

On some multi-phase problems in continuum mechanics

Stefano Bosia

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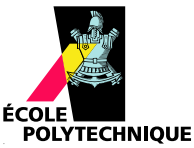
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UNIVERSITÀ ITALO FRANCESE



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On some multi-phase problems in continuum mechanics

Doctoral Dissertation of:
Stefano Bosia

Advisors:
Prof. Maurizio Grasselli
Prof. Andrei Constantinescu

Tutor:
Prof. Filippo Gazzola

Chair of the PhD Program:
Prof. Roberto Lucchetti

Committee:
Prof. Maurizio Grasselli
Prof. Andrei Constantinescu
Prof. Ferdinando Auricchio
Prof. Tomás Caraballo
Prof. Giuseppe Geymonat
Prof. Dietmar Hömberg

Referees:
Prof. Tomás Caraballo
Prof. Alexander Korsunsky

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Synopsis

In this thesis we study some problems arising within the context of continuum mechanics in the description of multi-phase physical situations. This analysis is carried out by means of tools from the theory of dynamical systems More precisely, we consider the following three problems: (I) the flow of binary mixtures, (II) p-n junctions in semiconductors under strain and (III) fatigue in polycrystalline metals.

On the flow of binary mixtures. The flow of binary mixtures can be described by two variables: the velocity of the medium $\mathbf{u}$ and an order parameter ψ. This last represents the difference in the relative concentrations of the two constituents of the mixture. The basic model we consider is the well known model H

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \varepsilon\nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \nabla\cdot(M\nabla\mu) \\ \mu = \varepsilon^{-1}f'(\psi) - \varepsilon\Delta\psi. \end{cases}$$

Here $f(\psi)$ is a double-well potential describing the natural separation tendency of the two components of the fluid. This system is an example of a diffuse interface model for binary flows, a class of models, which has been proven to be effective for numerical simulations and applications. In Chapter 1, we account for the models considered and we briefly review the theory of infinite-dimensional dynamical systems used in the rest of the first part. In particular, we prove the following

- For non-newtonian fluids (shear-thickening fluids of Ladyzhenskaya type) on a bounded do-

main of $\mathbb{R}^3$ and for a singular (i.e. logarithmic) double-well potential, we prove the existence of solutions and the existence of a trajectory attractor (Chapter 2).

- For the original model H on a bounded domain of $\mathbb{R}^2$ with a polynomial potential, we show the existence of a pullback exponential attractor. In particular, we explicitly account for arbitrarily fast growth of the potential at infinity. Although we are able to deduce results on the asymptotic behaviour of the system without limitations on the growth of the potential, the estimates we deduce are not strong enough to pass to the limit for regular potentials converging towards singular ones (Chapter 3).

- We then enquiry the effects of a reaction term on the behaviour of the binary fluid. This can be seen as a model describing chemically reacting fluids, whose average composition might vary over time. In particular, we prove the existence and the uniqueness of solutions on bounded domains of $\mathbb{R}^2$ for polynomial potentials. Moreover, we deduce the existence of a robust (with respect to the rate of the chemical reaction) family of exponential attractors (Chapter 4).

- Finally we consider a non-local version of the Cahn-Hilliard equation with a singular interaction kernel. This is a preliminary step in the study of a non-local model H with singular kernels. In the case of bounded domains in $\mathbb{R}^3$ with a singular potential, we prove the existence of variational solutions satisfying natural boundary conditions and study their regularity. Although the natural boundary conditions for the phase variable seems difficult to characterise in this setting, we are able to show that for regular solutions they reduce to the usual homogeneous Neumann (no flux) boundary conditions (Chapter 5).

Several interesting but challenging issues remain open, for instance:

- the study of the regularity properties and in particular the regularity up to the boundary for the non-local Cahn-Hilliard equation considered in Chapter 5;

- the investigation of the well-posedness properties and the asymptotic behaviour of the non-local model-H with singular kernel;

- a further study of the long-term properties of the Navier-Stokes-Cahn-Hilliard-Oono system already treated in Chapter 4. In particular, the problem of the convergence towards stationary states for this system seems particularly worth investigation.

On the effects of strain on semiconductor-based p-n junctions. Semiconductor devices essentially operate using the differences in the physical properties of two sharply separated regions,

one rich in electrons and one rich in holes (or, equivalently, lacking of electrons), which can ideally be considered as two phases of a continuum. However, with respect to the previous part, in this case the position of the interfaces is in general a priori given by the knowledge of the doping profile of the semiconductor.

Here we are interested in studying how deformations affect the properties of semiconductors. Our line of reasoning is based on the following approach:

- we start by reviewing fundamental semiconductor physics both for intrinsic and for doped silicon (Chapter 6).
- we then derive the drift-diffusion model and investigate which of its parameters depend on strain. Moreover, we give explicit models for the effects of strain on the band-gap width, on the mobilities and on the concentration of minority carriers in doped semiconductors (Chapter 7).
- we derive the Shockley relation in dependence of strain. In particular, we discuss the relevance of the reverse coupling of electronic properties on mechanical deformations through Maxwell stresses and conclude that it can be neglected at first approximation (Chapter 8).

The analysis has shown that several questions have still to be answered as, for example:

- the construction of a complete thermodynamically consistent continuum model for the coupled electro-mechanical effects in semiconductors;
- a rigourous treatment through perturbation analysis of the strain at the p-n junction;
- applications to other device architectures such as transistors and sensors.

On the lifetime estimate in high cycle fatigue regime for alloys. In the last part, we apply the theory of finite-dimensional dynamical systems to the field of lifetime predictions of polycrystalline metals in the high cycle fatigue regime. The model we consider is based on a homogenisation procedure which will relate local strains and stresses in the elastic and plastified grains at the microscopic level with the global strain and stress at the scale of the structure. The fatigue predictions are carried out using techniques from dynamical systems to track the progress of the accumulated plastic deformation in the grains. The proposed model for fatigue lifetime predictions offers greater flexibility in accommodating experimental data than those already presented in the literature. At the same time, it remains amenable to explicit analytical treatment.

Some possible developments of these results are:

- the investigation of the effects of stochastic terms and, in particular, the treatment of the resulting models within the framework of stochastic dynamical systems;
- the study of other loading regimes, such as quasiperiodic loadings or nondeterministic loadings;
- the extension to shape memory alloys accounting for the phase change occurring in these materials.

Publications

Most of the results of this thesis are contained int he following research articles:

- S. Bosia, *Analysis of a Cahn-Hilliard-Ladyzhenskaya system with singular potential*, J. Math. Anal. Appl. 397 (2013) 307–321, Chapter 2;
- S. Bosia, M. Grasselli, A. Miranville, *On the longtime behavior of a 2D hydrodynamic model for chemically reacting binary fluid mixtures*, Math. Methods Appl. Sci. (2013), Chapter 4;
- S. Bosia, A. Constantinescu, *Fast time-scale average for a mesoscopic high cycle fatigue criterion*, Int. J. Fatigue 45 (2012), 39–47, Chapter 9;
- S. Bosia, S. Gatti, *Pullback exponential attractors for a Cahn-Hilliard-Navier-Stokes system in 2D*, arXiv:1304.0933 (2013), submitted, Chapter 3
- H. Abels, S. Bosia, M. Grasselli, *Cahn-Hilliard Equation with Nonlocal Singular Free Energies*, arXiv:1311.3642 (2013), Chapter 5.
- S. Bosia, A. Constantinescu, M. Jabbour, N. Triantafyllidis, *On the modelling of strained semiconductors*, in preparation, Chapters 7–8.

Sinthèse

Cette thèse est dédiée à l'étude de certains problèmes de la mécanique des milieux continu qui apparaissent lors de la modélisation de systèmes multi-phase. Cette analyse est conduite grâce aux instruments de la théorie des systèmes dynamiques. Plus précisément, les trois problèmes suivant sont considérés : (I) l'écoulement de fluides binaires (II) les jonctions p-n à semi-conducteur soumises à déformations et (III) la fatigue dans les métaux polycristallins.

Sur l'écoulement de fluides binaires. L'écoulement d'un fluide binaire peut être décrit par deux variables : la vitesse du milieux $\mathbf{u}$ et un paramètre d'ordre ψ. Ce dernier représente la différence entre les concentrations relatives des deux composants du mélange. Le système fondamental que nous considérons est connu sous le nom de modèle H et peut être ecrit comme il suit :

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \varepsilon\nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \nabla\cdot(M\nabla\mu) \\ \mu = \varepsilon^{-1}f'(\psi) - \varepsilon\Delta\psi. \end{cases}$$

Ici $f(\psi)$ est un potentiel à double puits qui décrit la tendance naturelle à la séparation des deux composants du fluide. Ce système est un exemple d'un modèle à interface diffuse pour fluides binaires, une famille de modèles qui s'est démontrée efficace pour les simulations numériques et pour les applications. Le premier chapitre de cette thèse présente les modèles considérés tout en fournissant une vue générale sur la théorie des systèmes dynamiques infini-dimensionnels utilisée au cours du reste de la première partie. Plus précisément, on prouve les résultats suivants :

- pour des fluides non-newtoniens (fluides rhéoépaississant du type de Ladyzhenskaya) dans un domaine borné de $\mathbb{R}^3$ et dans le cas d'un potentiel singulier (c'est-à-dire logarithmique), on prouve l'existence de solutions et l'existence d'un attracteur de trajectoires (Chapitre 2) ;

- dans le cas du modèle H originaire donné sur un domaine borné de $\mathbb{R}^2$ avec un potentiel polynomial, on prouve l'existence d'un attracteur pullback exponentiel. Plus précisément, on tien compte d'une croissance arbitrairement rapide du potentiel à l'infini. Tout en pouvant déduire ces résultats de dynamique asymptotique sans limitations sur la croissance du potentiel, les estimations que nous dérivons ne sont pas suffisamment fortes pour passer à la limite pour suites de potentiels singuliers convergents à un potentiel singulier (Chapitre 3) ;

- successivement, on étudie les effets d'un terme de réaction sur le comportement du fluide binaire. Ceci représente un modèle qui décrit des fluides réagissant chimiquement, dont la composition moyenne peut changer dans le temps. Plus précisément, en des domaines bornés de $\mathbb{R}^2$ et pour des potentiels polynomiaux, on prouve l'existence et l'unicité de solutions. On déduit aussi l'existence d'une famille robuste (par rapport à la vitesse de la réaction chimique) de attracteurs exponentiels (Chapitre 4) ;

- enfin, on considère une version non-locale de l'équation de Cahn-Hilliard qui présente un noyau d'interaction singulier. Ces résultats représentent un passage préalable pour l'étude d'un model H non-local avec noyaux singuliers. Dans le cas d'un domaine borné en $\mathbb{R}^3$ avec un potentiel singulier, on prouve l'existence de solutions variationelles satisfaisant les conditions aux limites naturelles et on étudie leurs régularité. Même si ces conditions aux limites naturelles pour le paramètre d'ordre semblent difficiles à caractériser, on démontre que, pour des solutions régulières, elles se réduisent aux usuelles conditions de Neumann homogènes (Chapitre 5).

Plusieurs problèmes intéressants et difficiles restent sans solution. Parmi ceci on rappelle :

- l'étude des propriétés de régularité et en particulier la régularité jusqu'au bord pour l'équation de Cahn-Hilliard non-locale considérée au Chapitre 5 ;

- la réponse à la question si le modèle H non-locale est bien posé ou pas et l'examen de son comportement asymptotique ;

- une investigation ultérieure des propriétés asymptotiques du système de Navier-StokesCahn-Hilliard-Oono déjà étudié aux Chapitre 4. Plus précisément, le problème de la convergence des solutions aux états stationnaires parait particulièrement intéressant.

Sur les effets des déformations sur les jonctions p-n à semi-conducteur. Les dispositifs électroniques travaillent on exploitant les différences entre les propriétés physiques de deux régions nettement séparées, l'une riche en électrons et l'autre riche en trous (ou bien, pauvre en électrons), qui idéalement peuvent être considérées comme deux phase d'un même milieu continu Tout-de-même, par rapport à la partie précédente de cette thèse, dans ce cas la position des interfaces est généralement donnée grâce à la connaissance du profil de dopage du semi-conducteur.

L'objet principal de notre étude est la compréhension de comment les déformations affectent les propriétés des semi-conducteurs. Notre approche se base sur les phases qui suivent :

- on commence par présenter les éléments de physique des semi-conducteurs soit pour le silicium intrinsèque, soit dopé (Chapitre 6) ;
- par la suite, on dérive le modèle de diffusion-dérive et on étudie quels de ses paramètres dépendent des déformations. On donne aussi des lois explicites pour les effets des déformations sur l'intervalle de bande, sur les mobilités des porteurs de charge et sur les concentrations des porteurs de minorité dans les semi-conducteurs dopés (Chapitre 7) ;
- on obtient la loi de Shockley en dépendance des déformations. En particulier, on discute l'importance des effets du couplage inverse entre les propriétés électroniques et les déformations mécaniques (contraintes de Maxwell) et on déduit que ceux-ci peuvent être négligés en première approximation (Chapitre 8).

Nos analyses laissent ouverte des nombreuses questions comme, par exemple :

- la construction d'un modèle continu complet, thermodynamiquement consistent pour les effets électromécaniques couplés dans les semi-conducteurs ;
- un traitement rigoureux des déformations à la jonction p-n par la théorie des perturbations ;
- les applications à autres dispositifs comme transistors et senseurs.

Sur l'estimation de la durée de vie des alliages en fatigue à grand nombre de cycles. Dans la dernière partie, on utilise la théorie des systèmes dynamiques fini-dimensionnels dans le contexte des prédictions de la durée de vie des métaux polycristallins suomis à un grand nombre de cycles de chargement. Le model que l'on considère se base sur une procédure de homogénéisation qui lie les contraintes et les déformations locales dans les grains élastiques et plastiques au niveau microscopique avec les déformations et les contraintes à l'échelle de la structure. Les prédictions de fatigue sont menées en utilisant des techniques de la théorie des systèmes dynamique qui permettent de tracer l'évolution des déformations plastiques cumulées dans les grains. Le modèle

de fatigue proposé offre, en comparaison avec les résultats déjà connus, une plus grande flexibilité pour accommoder les données expérimentales. Au même temps, il reste accessible à une analyse explicite.

Des possibles développements de ces résultats sont :

- l'étude des effets de termes stochastiques et, en particulier, le traitement des modèles résultant dans le contexte de la théorie des systèmes dynamiques stochastiques ;
- l'examen d'autre genre d'histoires chargement, comme les chargements quasipériodiques ou les chargements non-déterministe ;
- l'extension de ces techniques aux alliages à mémoire de forme tenant compte des transition de phase qui se vérifient dans ces matériaux.

Publications

La plus grande partie des résultats de cette thèse sont contenus dans les articles suivants :

- S. Bosia, *Analysis of a Cahn-Hilliard-Ladyzhenskaya system with singular potential*, J. Math. Anal. Appl. 397 (2013) 307–321, Chapitre 2 ;
- S. Bosia, M. Grasselli, A. Miranville, *On the longtime behavior of a 2D hydrodynamic model for chemically reacting binary fluid mixtures*, Math. Methods Appl. Sci. (2013), Chapitre 4 ;
- S. Bosia, A. Constantinescu, *Fast time-scale average for a mesoscopic high cycle fatigue criterion*, Int. J. Fatigue 45 (2012), 39–47, Chapitre 9 ;
- S. Bosia, S. Gatti, *Pullback exponential attractors for a Cahn-Hilliard-Navier-Stokes system in 2D*, arXiv :1304.0933 (2013), soumis à comité de lecture, Chapitre 3
- H. Abels, S. Bosia, M. Grasselli, *Cahn-Hilliard Equation with Nonlocal Singular Free Energies*, arXiv :1311.3642 (2013), soumis à comité de lecture, Chapitre 5.
- S. Bosia, A. Constantinescu, M. Jabbour, N. Triantafyllidis, *On the modelling of strained semiconductors*, en préparation, Chapitres 7–8.

Sintesi

Lo scopo di questa tesi è lo studio di alcuni problemi che traggono origine dalla descrizione di processi fisici multifase nel contesto della dinamica dei continui e che possono essere affrontati con strumenti della teoria dei sistemi dinamici. In particolare verranno considerate le seguenti tre situazioni: (i) la dinamica di fluidi binari (ii) le proprietà dei semiconduttori inorganici sottoposti a deformazioni e (iii) la fatica in metalli policristallini.

Della dinamica dei fluidi binari. Lo scorrimento di un fluido binario può essere descritto tramite due variabili: la velocità del mezzo, di seguito indicata con il simbolo $\mathbf{u}$, e un parametro d'ordine per cui verrà utilizzato il simbolo ψ e che rappresenta la differenza tra le concentrazioni relative dei due componenti della miscela. Il modello fondamentale considerato in questo lavoro è il modello H che può essere scritto come segue

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \varepsilon\nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \nabla\cdot(M\nabla\mu) \\ \mu = \varepsilon^{-1}f'(\psi) - \varepsilon\Delta\psi. \end{cases}$$

Qui $f(\psi)$ è un potenziale a doppio pozzo che descrive la naturale tendenza delle due componenti del fluido a scindersi. Osserviamo che questo sistema è un esempio di modello a interfaccia diffusa per la descrizione del flusso di fluidi binari. In particolare, i modelli a interfaccia diffusa si sono rivelati particolarmente efficienti sia dal punto di vista numerico sia per le loro applicazioni. Nel Capitolo 1 esamineremo in dettaglio questo modello per poi passare in rassegna la teoria dei

sistemi dinamici infinito dimensionali usata in tutta la prima parte di questo lavoro. In particolare dimostreremo i seguenti risultati:

- nel caso di fluidi non-newtoniani (fluidi dilatanti o fluidi ispessenti al taglio del tipo di Ladyzhenskaya) su domini limitati di $\mathbb{R}^3$ e per un potenziale a doppio pozzo singolare (in particolare di tipo logaritmico) dimostreremo che esistono soluzioni deboli e che il sistema dinamico associato al modello considerato ammette un attrattore di traiettorie (Capitolo 2);

- considereremo poi il modello H originario su un dominio limitato di $\mathbb{R}^2$ con un potenziale a doppio pozzo polinomiale. In questo caso dimostreremo l'esistenza di un attrattore pullback esponenziale tenendo conto in modo esplicito della crescita polinomiale all'infinito del potenziale che potrà essere arbitrariamente rapida. Benché i risultati relativi alla caratterizzazione del comportamento asintotico siano qualitativamente indipendenti dalla crescita del potenziale, le stime dedotte non sono sufficientemente forti da permettere il passaggio al limite per potenziali regolari che approssimino un potenziale singolare (Capitolo 3);

- indagheremo poi gli effetti di un termine di reazione sul comportamento del fluido binario. Questo termine può, ad esempio, modellare fluidi che reagiscono chimicamente in cui una delle componenti può trasformarsi nell'altra e viceversa e la cui composizione media, quindi, può variare nel tempo. In particolare, dimostreremo l'esistenza e l'unicità delle soluzioni nel caso di domini limitati di $\mathbb{R}^2$ e per potenziali polinomiali. Inoltre, proveremo l'esistenza di una famiglia di attrattori esponenziali robusta rispetto alla costante cinetica della reazione chimica (Capitolo 4);

- infine, studieremo anche una versione non-locale della equazione di Cahn-Hilliard con un nucleo di interazione singolare. Questa indagine rappresenta un passaggio preliminare per lo studio di un modello H non-locale con nuclei singolari. Più precisamente, nel caso di domini limitati di $\mathbb{R}^3$ con un potenziale a doppio pozzo singolare (i.e. logaritmico), dimostreremo l'esistenza di una soluzione variazionale che soddisfa condizioni al contorno di tipo naturale e ne studieremo la regolarità. Benché in questo contesto le condizioni al contorno naturali per il parametro di fase sembrino difficili da caratterizzare, mostreremo che, nel caso di soluzioni regolari, queste si riducono all'usuale condizione di Neumann omogenea (Capitolo 5).

I risultati di questa parte lasciano aperti diversi ulteriori problemi interessanti e al contempo difficili. Tra questi ricordiamo:

- lo studio delle proprietà di regolarità (e in particolare della regolarità fino al contorno) per l'equazione di Cahn-Hilliard non-locale analizzata nel Capitolo 5;

- l'indagine della buona-positura e del comportamento asintotico del modello H non-locale con potenziali singolari;

- una analisi ulteriore delle proprietà asintotiche del sistema di Navier-Stokes-Cahn-Hilliard-Oono già affrontato nel Capitolo 4, con particolare riferimento all'interessante problema della convergenza delle soluzioni a singoli stati stazionari.

Dell'effetto delle deformazioni sulle giunzioni p-n. I dispositivi elettronici basati su materiali semiconduttori operano sfruttando le differenze nelle proprietà fisiche di due domini nettamente separati: i primi sono ricchi in elettroni; i secondi abbondano in lacune (o, equivalentemente, mancano di elettroni). Benché queste diverse zone possano essere considerate idealmente come due diverse fasi di uno stesso mezzo continuo, a differenza di quanto visto nella prima parte della presente tesi, in questo caso la posizione delle interfacce è generalmente nota a priori grazie alla conoscenza del profilo di drogaggio del semiconduttore.

La motivazione principale del nostro lavoro è lo studio degli effetti delle deformazioni sulle proprietà fisiche dei semiconduttori. In particolare, l'approccio da noi proposto all'analisi del problema è il seguente:

- inizieremo con una breve revisione dei fondamenti della fisica dei semiconduttori dedicando particolare attenzione al caso del silicio intrinseco e del silicio drogato (Capitolo 6);

- ripercorreremo poi la deduzione del modello di diffusione e trasporto evidenziando in particolare quali dei suoi parametri dipendano dalle deformazioni. Introdurremo, inoltre, modelli quantitativi per descrivere gli effetti delle deformazioni sulla banda proibita (band gap), sulle mobilità e sulla concentrazione dei portatori di carica minoritari nei semiconduttori drogati (Capitolo 7);

- infine, deriveremo la relazione di Shockley per giunzioni p-n evidenziandone la dipendenza dalle deformazioni. In particolare, discuteremo l'importanza dell'accoppiamento inverso relativo agli effetti delle proprietà elettroniche su quelle meccaniche tramite la valutazione degli sforzi di Maxwell. I nostri risultati permetteranno di concludere che, almeno in prima approssimazione, questo accoppiamento inverso può essere trascurato (Capitolo 8).

Le nostre analisi lasciano senza risposta numerosi quesiti interessanti, tra cui riportiamo, a titolo di esempio, i seguenti:

- la costruzione di un modello continuo termodinamicamente consistente per i fenomeni elettro-meccanici nei semiconduttori;

- una trattazione rigorosa tramite la teoria degli sviluppi perturbativi dei campi di deformazione in prossimità delle giunzioni p-n;
- l'applicazione dei risultati fin qui ottenuti ad altre architetture circuitali come transistor e sensori più complessi.

Della stima della durata di vita per leghe sottoposte ad un alto numero di cicli di carico. Nell'ultima parte del presente lavoro, applicheremo la teoria dei sistemi dinamici finito-dimensionali al campo della predizione di vita dei metalli policristallini sottoposti al regime di fatica materiale ad alto numero di cicli. Il modello da noi considerato è basato su una procedura di omogeneizzazione che lega tra loro gli sforzi e le deformazioni locali nei grani elastici o deformati plasticamente a livello microscopico con le analoghe quantità globali definite macroscopicamente alla scala della struttura studiata. Le stime della durata di vita del materiale possono essere ottenute tramite tecniche tratte dalla teoria dei sistemi dinamici che permettono di tenere conto dell'avanzamento della deformazione plastica cumulata nei grani. Il modello proposto per la predizione della durata di vita per materiali sottoposti ad un grande numero di cicli di carico offre una maggiore adattabilità nei confronti dei dati sperimentali rispetto a quelli presenti in letteratura rimanendo tuttavia trattabile in modo esplicito dal punto di vista analitico.

Alcuni possibili sviluppi dei risultati ottenuti in questa parte della tesi sono i seguenti:

- lo studio degli effetti di termini stocastici e in particolare il trattamento dei modelli risultanti nel contesto della teoria dei sistemi dinamici stocastici;
- l'analisi di altri regimi di carico, come carichi quasiperiodici e/o nondeterministici;
- l'estensione dei risultati al caso delle leghe a memoria di forma, tenendo conto in particolare delle transizioni di fase che hanno luogo in questi materiali.

Pubblicazioni

La maggior parte dei risultati riportati nella presente tesi sono contenuti nei seguenti articoli di ricerca:

- S. Bosia, *Analysis of a Cahn-Hilliard-Ladyzhenskaya system with singular potential*, J. Math. Anal. Appl. 397 (2013) 307–321, Capitolo 2;
- S. Bosia, M. Grasselli, A. Miranville, *On the longtime behavior of a 2D hydrodynamic model for chemically reacting binary fluid mixtures*, Math. Methods Appl. Sci. (2013), Capitolo 4;

- S. Bosia, A. Constantinescu, *Fast time-scale average for a mesoscopic high cycle fatigue criterion*, Int. J. Fatigue 45 (2012), 39–47, Capitolo 9;
- S. Bosia, S. Gatti, *Pullback exponential attractors for a Cahn-Hilliard-Navier-Stokes system in 2D*, arXiv:1304.0933 (2013), sottoposto per pubblicazione, Capitolo 3
- H. Abels, S. Bosia, M. Grasselli, *Cahn-Hilliard Equation with Nonlocal Singular Free Energies*, arXiv:1311.3642 (2013), sottoposto per pubblicazione, Capitolo 5.
- S. Bosia, A. Constantinescu, M. Jabbour, N. Triantafyllidis, *On the modelling of strained semiconductors*, in preparazione, Capitoli 7–8.

Contents

I Long term analysis of two fluid flows **1**

1 Two phase fluid flows **5**

1.1 Motivation—The model H . . . 6

1.1.1 On the Cahn-Hilliard equation . . . 6

1.1.2 On the Navier-Stokes equations . . . 9

1.1.3 Coupling Cahn-Hilliard and Navier-Stokes models . . . 10

1.2 Some generalisations of the model H . . . 12

1.2.1 Non-newtonian fluids . . . 12

1.2.2 Oono reaction term . . . 14

1.2.3 Non-local models . . . 16

1.3 Large-time behaviour for solutions of parabolic systems . . . 17

1.3.1 Short overview of the classical theory of attractors . . . 17

1.3.2 Trajectory attractors . . . 19

1.3.3 Exponential attractors . . . 20

1.3.4 Pullback attractors . . . 22

1.3.5 Convergence to stationary states . . . 24

1.4 Notation . . . 25

1.4.1 General notation . . . 25

1.4.2 Functional spaces . . . 27

2 A LCH system **37**

2.1 Functional setting . . . 39

2.2 Main assumptions and weak formulation . . . 40
2.3 The convective Cahn-Hilliard equation . . . 42
2.4 Some results on the Ladyzhenskaya model . . . 43
2.5 Weak solutions and energy estimates . . . 44
2.6 A weak trajectory attractor . . . 49
2.7 A strong trajectory attractor . . . 55

3 A 2*D* CHNS system 61
3.1 Functional setting and main results . . . 64
3.2 Exponential pullback attractors . . . 67
3.3 Existence results and basic energy estimate . . . 71
3.4 Higher regularity estimates . . . 75
3.5 Continuous dependence . . . 85
3.6 Time regularity . . . 93
3.7 Proof of the main results . . . 95

4 2*D* NSCHO 103
4.1 Functional setting and main results . . . 106
4.2 Existence and dissipation . . . 111
4.3 Continuous dependence . . . 114
4.4 Higher-order dissipative estimate . . . 118
4.5 A robust family of exponential attractors . . . 121

5 Nonlocal CH 131
5.1 Basic tools and well-posedness . . . 133
5.1.1 Function spaces . . . 133
5.1.2 Weak formulation and main result . . . 135
5.1.3 Evolution equations with monotone operators . . . 136
5.1.4 Results on the nonlocal operator $\mathcal{L}$ . . . 137
5.2 Subgradients . . . 141
5.3 Existence of unique solutions . . . 150
5.4 Long-time behaviour . . . 156
5.5 Boundary conditions for variational solutions . . . 159
5.5.1 Proof of Theorem 5.5.1: case $n = 1$ . . . 161
5.5.2 Proof of Theorem 5.5.1: case $n \geqslant 2$ . . . 163

II Strain deformation in p-n junctions **169**

Notation used in Part II **173**

6 Statement of the problem **175**

6.1 On the physics of semiconductors . . . 177

6.1.1 Energy bands . . . 179

6.1.2 Doping . . . 183

7 The Drift-Diffusion model and strain **187**

7.1 Derivation of the DD model . . . 188

7.2 A brief history of strain effects on SCs' properties . . . 194

7.3 Strain effects in silicon . . . 195

7.3.1 Shift of the energy bands . . . 195

7.3.2 Changes in effective masses . . . 199

7.3.3 Shift of the Fermi level . . . 201

7.3.4 Changes for n_i . . . 203

7.3.5 Changes in mobilities . . . 203

8 P-N junctions under strain **209**

8.1 P-N junctions in operation . . . 210

8.2 The Shockley relation with strain effects . . . 214

8.3 Maxwell stresses and reverse coupling . . . 218

III High cycle fatigue in alloys **223**

Notation used in Part III **227**

9 A HCF criterion **229**

9.1 The models at the mesoscopic scale . . . 231

9.2 Separation of time scales . . . 236

9.3 Lifetime estimates in HCF . . . 239

9.4 A priori estimates . . . 240

9.5 Identification of parameters from fatigue experiments . . . 243

9.6 Results and discussion . . . 245

9.7 Conclusions . . . 248

Acknowledgements **251**

Bibliography **255**

"When people thought the earth was flat, they were wrong. When people thought the earth was spherical, they were wrong. But if you think that thinking the earth is spherical is just as wrong as thinking the earth is flat, then your view is wronger than both of them put together."

(Isaac Asimov — The Relativity of Wrong)

Part I

Long term analysis of two fluid flows

Summary

The fist part of this thesis is devoted to the study of several model describing the evolution of a binary fluid flow. The evolution partial differential equations considered belong to the class of diffuse interface models and can be seen as generalisations of the well-known model H. Formally, these equations can be seen as the result of the coupling between the Cahn-Hilliard equation for phase separation and the Navier-Stokes equation describing the flow of the fluid. The generalisations considered concern non-newtonian Ladyzhenskaya-type fluids and chemically reacting mixtures. Non-local interactions between the constituents of the mixture are also partially considered.

The main results obtained concern the well-posedness of the systems studied as well as some characterisation of the large-time behaviour of the solutions. In particular many of the known techniques in the theory of infinite-dimensional dynamical systems find here an application. Among these we recall, trajectory attractors, exponential attractors and pullback attractors.

CHAPTER 1

Introduction to two-phase fluid flows models

Outline

In this chapter the mathematical literature concerning diffuse interface models for binary fluids is reviewed. This is the source of the main motivation of the first part of the present manuscript. In particular, the so-called model H and some of its generalisations are introduced. A brief review of the main instruments used in describing the large-time dynamics of evolution equation is given. Finally, the common notation, which will be used throughout this part of the present work, is introduced and discussed.

The mathematical modeling of multi-phase flows is particularly challenging and crucial for applications (see, e.g., Gurtin et al. (1996); Hohenberg and Halperin (1977); Heida et al. (2012); Lamorgese et al. (2011); Morro (2010) and references therein). One of the most interesting (and essentially still open) issue concerns efficient approaches to track the evolution of the interfaces between the different phases of the flow. This problem has been traditionally tackled from two different and complementary perspectives:

Sharp-interface models In this family of models, perfect immiscibility of the constituents of the mixture is assumed. From the mathematical viewpoint, this corresponds to solving for each constituent a suitable evolution equation in an unknown evolving domain, whose boundary corresponds with the sharp interface itself. Concerning theoretical results, only little regularity of the evolving boundaries can be expected in general (see e.g., Denisova and Solonnikov (1991); Abels and Wilke (2013) and references therein). Moreover, sharp-

interface modelling leads to severe numerical difficulties, in particular related to topological reconnections of the interfaces themselves, occurring, for example, during coalescence phenomena.

Diffuse-interface models This case accounts for a partial miscibility between the different constituents of the fluid mixture. This leads to models in which a unique continuum is described through a finite family of order-parameter fields (one order parameter in the case of binary fluids) giving the local composition of the mixture. An archetype of this class of models is given by the model H, which will be described in detail in Section 1.1 below. These models seem to be much more flexible from the numerical point of view and therefore relevant for applications (see Elliott et al. (2011) and references therein).

In the first part of this thesis, we will focus on the second class of models, discussing in particular the large-time behaviour of several "variations" of the classical model H. We start this introductory chapter by briefly reviewing both the model H and some of its modifications as well as the theory of attractors for evolution equations.

1.1 Motivation—The model H

The so called model H was first proposed in Hohenberg and Halperin (1977) and Siggia (1979) and then rigorously derived in Gurtin et al. (1996). The corresponding differential system appears to be the coupling between the Navier-Stokes equation for fluid mechanics and the Cahn-Hilliard equation describing, in the simplest case, the evolution of a mixture of two constituents, such as an alloy. Before introducing the full model we briefly review both these equations and the main mathematical questions related to them.

1.1.1 On the Cahn-Hilliard equation

The Cahn-Hilliard equations were first derived at the end of the 50s to model spinodal decomposition and coarsening of metallic alloys during quenching (see Cahn and Hilliard (1958); Cahn (1961)). During cooling of a metallic alloy, the originally stable uniform composition becomes unstable. This leads to phase separation and to the appearance of complex patterns in which domains having different chemical composition can be recognised (see Figure 1.1).

The spinodal decomposition differs significantly from phase transitions involving nucleation and growth of one phase in another one (e.g., during the cooling and solidification of water into ice). In the latter case, a thermodynamical barrier between the two phases of the continuum involved in the transition has to be overcome. This leads to phase transitions starting in a

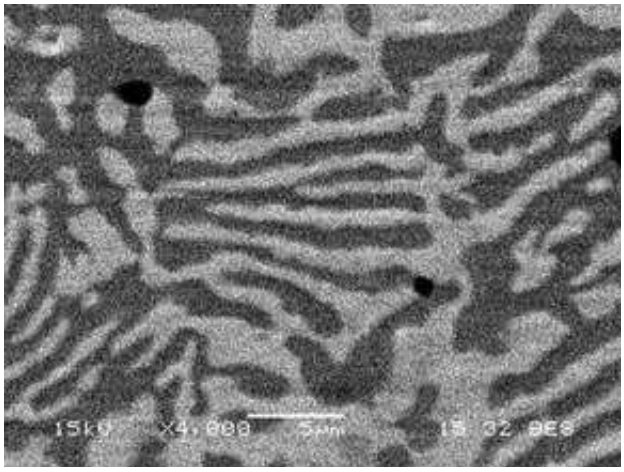


Figure 1.1: The microstructure of a steel alloy after quenching.

very localised portion of the material (selected by stochastic fluctuations) and then invading all the domain. Pertinent models for these phenomena can be found in the literature devoted to free-boundary problems (see Meirmanov (1992); Visintin (1996)).

On the other hand, spinodal decomposition is not associated with nucleation phenomena, but to a transition happening throughout the domain as soon as the homogeneous composition state becomes thermodynamically unstable. This instability is seen to occour as soon as the temperature of the mixture θ falls below a critical temperature θ_c. The microscopic explanation of the phase separation phenomena observed during spinodal decomposition is to be found in diffusion mechanisms of the different constituents of the mixture, which fails to lead to a stable uniform composition for temperatures below the critical one.

In the mathematical model proposed by Cahn and Hilliard, spinodal decomposition of a binary allow is modeled through a single order parameter field ψ representing the difference of the relative concentrations of the two chemical species involved in the phase separation. Physically relevant values for ψ thus belong to the interval $[-1, 1]$. A temperature dependent potential energy $F(\psi)$ can then be introduced. In order to consistently describe the physical situation just introduced, F is assumed to be a temperature-dependent quadratic perturbation of a super-quadratic convex function F_0 so that for $\theta < \theta_c$ global convexity is lost:

$$F(\psi) = F_0(\psi) + \frac{\theta - \theta_c}{2}\psi^2$$

Moreover, an energy functional is associated to the configuration of the order parameter field accounting for both the phase separation and the "energetic cost" of the mixing regions. This

leads to the following assumption

$$E_P(\psi) = \frac{\varepsilon}{2}\int_\Omega |\nabla\psi(\mathbf{x})|^2\,\mathrm{d}\mathbf{x} + \frac{1}{\varepsilon}\int_\Omega F(\psi(\mathbf{x}))\,\mathrm{d}\mathbf{x}. \tag{1.1.1}$$

Here, the first term penalises the size of the transition areas between the different domains of (almost) pure composition, while, for under-critical temperatures, the second favours the phase separation between the two constituents. The parameter ε appearing in this last expression is seen to be related with the thickness ($\propto\sqrt{\varepsilon}$) of the transition region between different phases.

Having introduced an energy for the order parameter field, the next step consists in the derivation of an associated evolution equation describing spinodal decomposition. This goal can be achieved by considering a gradient flow approach in a suitable Hilbert space. Choosing as ambient space $(H^1(\Omega))^*$ (see Section 1.4 below for the notation generally used in this part), the resulting system of partial differential equations is

$$\begin{cases} \partial_t\psi = -\nabla\cdot(M\nabla\mu) \\ \mu = -\varepsilon\Delta\psi + \frac{1}{\varepsilon}f'(\psi). \end{cases} \tag{1.1.2}$$

Here, the variable μ is usually called chemical potential, while the quantity M is known as mobility and will be kept positive and constant for all the extent of this work (see Cahn et al. (1996); Elliott and Garcke (1996) for an account of the physical relevance of degenerate mobilities). This system is usually supplemented with homogeneous Neumann boundary conditions both on the order parameter field ψ and on the chemical potential μ.

$$\partial_{\mathbf{n}}\psi = \partial_{\mathbf{n}}\mu = 0.$$

The boundary condition on ψ corresponds to the physically relevant case of no-flux boundary conditions leading to the conservation of the mean composition of the mixture

$$\int_\Omega \psi(t),\mathrm{d}\mathbf{x} = \int_\Omega \psi(t_0)\,\mathrm{d}\mathbf{x},$$

while the assumption on the chemical potential is consistent with the observation that isolines of equilibrium solutions are orthogonal to domain boundaries.

One of the major challenges associated with the Cahn-Hilliard equation is given by the analytical form of the potential F. The derivation of the model from thermodynamical principles leads to a singular expression for the potential $F(\psi)$, being bounded, but defined only on the interval $[-1,1]$ (see Cahn (1961)):

$$F(\psi) = \frac{\theta}{2}\left((1+\psi)\ln(1+\psi) + (1-\psi)\ln(1-\psi)\right) - \frac{\theta_c}{2}\psi^2. \tag{1.1.3}$$

However, the associated potential term $f(\psi)$ appearing in (1.1.2) is not bounded thus leading to some difficulties in the theory of the well-posedness and asymptotic behaviour of the Cahn-Hilliard

system. A popular alternative to (1.1.3) is given by regular potentials of the form

$$F(\psi) = \psi^p - \psi^2, \qquad \text{with } p > 2 \text{ (and often } p = 4).$$

These double-well smooth potentials are qualitatively similar to the theoretically relevant singular potential introduced above featuring two symmetric minima separated by an energy barrier. However, they lead to a much simpler well-posedness theory based exclusively on compactness methods (see, e.g., Lions (1969) for a general introduction to these techniques). Moreover, smooth potentials are much easier to implement in numerical simulations (see the seminal paper Elliott and French (1987) as well as the references in Cherfils et al. (2011)). However, being the Cahn-Hilliard equation a fourth order evolution equation, no comparison principle is available and hence, when using smooth potentials, no guarantee is given that the solution will remain in the physically significant interval $[-1, 1]$. Indeed, in simulations it is observed that this is not the case. This justifies the interest in precise information on the behaviour of solution for smooth potentials approximating the regular ones. This issue will be partially addressed in Chapter 3 (see also Frigeri and Grasselli (2012b,a)).

Finally, another important open problem associated with the singular potential F is the so called "separation from pure phases property". Indeed, for solutions of the Cahn-Hilliard equation on bounded domains in $\mathbb{R}^2$, it can be seen that after a sufficiently long time (which is however uniform with respect to the norm of the initial data) the order parameter field ψ is uniformly separated from the pure phases 1 and -1 (see Miranville and Zelik (2004)). This property is still unknown in the three-dimensional case and the techniques used in its proof do not seem to be carried over in a physically significant way to the full model H. We refer the interested reader to Cherfils et al. (2011) for a recent thorough review of the mathematical theory associate to the Cahn-Hilliard equation.

1.1.2 On the Navier-Stokes equations

In order to describe the flow of an incompressible fluid, one of the best known models is given by Navier-Stokes equations. These model linear viscous fluids where the stress tensor $\boldsymbol{\sigma}$ linearly depends on the (symmetric part of) velocity gradient $D\mathbf{u}$ through a relation of the form

$$\boldsymbol{\tau} = -\pi \mathbf{I} + 2\nu D\mathbf{u}. \tag{1.1.4}$$

Here and in the following, the velocity of the fluid will be denoted by $\mathbf{u}$, while π will be the isotropic component of the stress (pressure) and ν the viscosity coefficient. This gives rise to the

following system of partial differential equations

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} = \nabla\pi + \mathbf{g} \\ \nabla\cdot\mathbf{u} = 0. \end{cases} \tag{1.1.5}$$

Natural boundary conditions are given by the no-slip boundary conditions

$$\mathbf{u} = \mathbf{0}$$

Although the Navier-Stokes equations are among the most studied equations of mathematical physics (see Temam (1984) for an thorough introduction), very little has been discovered on their well-posedness after the seminal work of Leray in the 30's (see Leray (1934)). The situation, as known today for bounded domains, is as follows

2D case In this case, the Navier-Stokes equations are well posed in the Hadamard sense. By this we mean that for square integrable initial data and forcig term $\mathbf{g}$, there exists a unique weak solution, which depends continuously on these data. Moreover, for more regular initial conditions, also strong solutions can be constructed and these are unique as well.

3D case On bounded domains in $\mathbb{R}^3$, equation (1.1.5) admits a weak solution starting from square-integrable initial data. However, this solution is not known to be unique. Nonetheless, one can show the following "strong-weak" uniqueness property: if a strong solution exists (i.e., a solution belonging to $L^2(0,T;\mathbf{H}^2(\Omega)) \cap \mathbf{C}([0,T];\mathbf{H}^1(\Omega))$—see Section 1.4 for the notation), then it is unique in the class of weak solutions. The question whether strong solutions exist for any regular (i.e. $\mathbf{H}^1(\Omega)$) initial datum remains still unanswered.

For a thorough introduction to the mathematical theory of Navier Stokes equations, we refer the interested reader to the monographs Temam (1984, 1995).

1.1.3 Coupling Cahn-Hilliard and Navier-Stokes models

Having briefly reviewed the Cahn-Hilliard and the Navier-Stokes equations, we can now introduce the system of partial differential equations resulting from the physical description of a binary fluid. As stated before, we will discuss the so called model H, which can also be seen as arising from the coupling of the two models just discussed. This model has been rigourously derived in the works by Gurtin et al. Gurtin et al. (1996), by Hohenberg and Halperin Hohenberg and Halperin (1977) and, more recently, in the works by Morro Morro (2010) and Heida Heida et al. (2012). One of the fundamental assumptions in its derivation is that both constituents have the same density (see Abels (2009b) for the "unmatched densities" case).

The resulting system, which will be the object of investigation in the next four chapters is

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \varepsilon\nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \nabla\cdot(M\nabla\mu) \\ \mu = \varepsilon^{-1}f'(\psi) - \varepsilon\Delta\psi. \end{cases} \tag{1.1.6}$$

We use here a notation consistent to the one described for the Cahn-Hilliard and the Navier-Stokes equation earlier in this section. However, we emphasise the exact meaning, which has to be given to the velocity $\mathbf{u}$ in this setting. In principle, one can assume that a velocity can be assigned to each fluid constituting the mixture (and, indeed, this can be done in the derivation of the model from basic principles of continuum mechanics). In the case of "matched densities" fluids considered here, $\mathbf{u}$ is the averaged velocity of the two constituents of the mixture. We also observe that in system (1.1.6) the coupling between the Navier-Stokes equations and the Cahn-Hilliard equation occours in three places:

- in the additional convective term $(\mathbf{u}\cdot\nabla)\psi$ appearing in the evolution equation for the order parameter field (cf. equation (1.1.2));
- in the Korteweg force $\nabla\cdot(\nabla\psi\otimes\nabla\psi)$ giving rise to an additional bulk force in the Navier Stokes equations. We note that, up to a gradient term (which can however be easily reabsorbed in the pressure π), this term can also be conveniently written as $\mu\nabla\psi$ or as $-\psi\nabla\mu$;
- in the viscous term of the momentum equation in the form of an order-parameter-dependent viscosity $\boldsymbol{\tau} = \nu(\psi)\nabla\mathbf{u}$ (cf. equation (1.1.5)).

Finally, system (1.1.6) is usually supplemented by no-slip boundary conditions on the velocity field and by no-flux boundary conditions on the order-parameter field and chemical potential:

$$\mathbf{u} = \mathbf{0}, \quad \partial_{\mathbf{n}}\psi = 0, \quad \partial_{\mathbf{n}}\mu = 0, \qquad \text{on } \partial\Omega. \tag{1.1.7}$$

and by a given initial datum

$$\mathbf{u}(0) = \mathbf{u}_0, \quad \psi(0) = \psi_0, \qquad \text{in } \Omega.$$

In the case of Newtonian fluids (i.e. for $\boldsymbol{\tau}(D\mathbf{u}) \doteq 2\nu D\mathbf{u}$), the well-posedness of the model H (also referred to as Cahn-Hilliar-Navier-Stokes system—CHNS—in the following) has been widely investigated in the literature (see also Liu and Shen (2003) for contributions to a very similar model). As can be easily expected from our preliminary discussion of the Cahn-Hilliard and Navier-Stokes equations, when discussing existence results for the model H, the space dimension

and the hypothesis on the double-well potential play a crucial role. System (1.1.6)–(1.1.7) has been firstly studied in Starovoitov (1997) for $\Omega = \mathbb{R}^2$ and regular potential. Then, in the case of bounded domains in $\mathbb{R}^2$ and for non-constant viscosity $\nu = \nu(\psi)$, global existence results for both weak and strong solutions were obtained in Boyer (1999) (see also Boyer (2001) as well as Abels and Feireisl (2008) for the compressible case). More recently, the case of logarithmic potentials has been considered in Abels (2009b) (see also Abels (2009a)), where, in the absence of non-gradient external forces, the convergence of solutions to a single equilibrium has been established. This issue has also been investigated in Zhao et al. (2009) for smooth potentials. A further related contribution (see Abels (2009b)) proves the existence of a (weak) global attractor (which is strong in dimension two—see Section 1.3 for pertinent definitions). A rather complete picture of the longtime behavior in the case of bounded domain in $\mathbb{R}^2$ can be found in Gal and Grasselli (2010a). Finally, in the case of $3D$ bounded domains and assuming time-dependent external forces, existence of trajectory attractors has been demonstrated in Gal and Grasselli (2010b).

Essentially, in all the above contributions to this field, the well-posedness results obtained for the model H are equivalent to those known for the uncoupled Navier-Stokes equations. In particular well-posedness in the Hadamard sense is obtained in the case of bounded domains in $\mathbb{R}^2$, while only partial information as described in Section 1.1.2 above is available in the case of bounded domain in $\mathbb{R}^3$.

The effectiveness of model H for numerical simulations has also been widely assessed. We refer the interested reader to, among others, Badalassi et al. (2003); Kay et al. (2008); Kim et al. (2004); Shen and Yang (2010) and references therein.

1.2 Some generalisations of the model H

Having reviewed the standard model H, we now introduce some of its generalisations that will be discussed in the present work. These essentially involve two terms appearing in (1.1.6): modifications in the viscosity term $\nabla \cdot \boldsymbol{\tau}$ with respect to the linear assumption (1.1.4) lead to the so called non-Newtonian fluid models; changes in the description of the interaction between the constituents of the mixture, may lead to chemically reacting and/or non-local interactions. We will briefly discuss these phenomena in this section.

1.2.1 Non-newtonian fluids

The so-called Ladyzhenskaya model for non-Newtonian fluids was proposed in the 60's (see Ladyzhenskaya (1967)) both on physical and mathematical grounds. Through the introduction of

a suitable non-linearity in the stress-velocity gradient relation, both shear-thinning (as lava or blood) and shear-thickening fluids (like cornstarch–water mixtures or soaked sand) can be effectively modeled. These materials exhibit smaller and smaller (respectively greater and greater) resistance to motion as the gradient of the deformation rate becomes larger. In particular, for binary fluid flows, the following non-linear constitutive relation for the fluid may be assumed

$$\boldsymbol{\tau}(D\mathbf{u},\psi) \doteq \left(\nu_1(\psi)+\nu_2(\psi)|D\mathbf{u}|^{p-2}\right) D\mathbf{u} \tag{1.2.1}$$

where ν_1 and ν_2 are suitable positive and sufficiently smooth functions and where the exponent p is assumed to be larger than 1. The case $p<2$ corresponds to a concave relation between stress and velocity gradient and can model shear thinning fluids. On the contrary, for $p>2$, $\boldsymbol{\tau}$ is a convex function of $D\mathbf{u}$ and therefore, shear-thickening fluids are described. In the case $p=2$ the standard Navier-Stokes equations are recovered.

Concerning the mathematical theory of single component Ladyzhenskaya fluids, many interesting results have been obtained in recent years (see Feireisl and Pražák (2010) for a recent review on the subject). In particular, focusing on the case of bounded domains of $\mathbb{R}^3$ and for shear-thickening fluids, it has been shown that full well-posedness in the Hadamard sense can be recovered. This is in contrast to what happens for the standard Navier-Stokes equations. Indeed, in the regime $p>\frac{11}{5}$, existence and uniqueness of weak solutions can be proven for the system

$$\begin{cases} \partial_t\mathbf{u}+(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi+\nabla\cdot(\boldsymbol{\tau}(D\mathbf{u}))+\mathbf{g} \\ \nabla\cdot\mathbf{u}=0 \end{cases}$$

with homogeneous Dirichlet boundary conditions $\mathbf{u}=\mathbf{0}$ (see Ladyzhenskaya (1967); Lions (1969). The key point for obtaining these enhanced well-posedness results lies in a change of the functional setting where solutions are searched: instead of the usual weak regularity $L^2(\mathbf{H}^1_{0,\mathrm{div}}(\Omega))$, one can now look for weak solutions belonging to $L^p(\mathbf{W}^{1,p}_{0,\mathrm{div}}(\Omega))$ (see Section 1.4 for the notation used here). This allows testing the equation against a solution obtained through any suitable approximation method (or through monotonicity arguments, like in Lions (1969)) thus deducing energy identities for the solution as well as suitable continuous dependence estimates.

Concerning the system arising from (1.1.6) with (1.2.1) (which may be called Ladyzhenskaya-Cahn-Hilliard—or LCH—system), some results are already available in the literature. In particular, the case of a regular double well potential F has been studied in Kim et al. (2006) and well-posedness results obtained, that are analogous to those just discussed in the case of a single fluid. A complete overview of the regular case can be found in Grasselli and Pražák (2011), where also the large-time behaviour of the system is studied and the existence of global as well as exponential attractors proven (see Section 1.3 below).

One could expect the situation to be similar also in the case of singular potentials. However, as we shall see in Chapter 2, for the LCH system with singular (i.e., logarithmic) potential a complete well-posedness theory seems to be out-of-reach. This is due to the worsening in the time regularity of the velocity field when p becomes larger (see the Remark 2.5.1). In particular we will discuss existence results as well as a characterisation of the large-time behaviour of solutions through trajectory attractors (see Section 1.3 below).

1.2.2 Oono reaction term

The model H can also be suitably modified to account for possible transitions between the two components of the mixture. This is particularly relevant in the case of chemically reacting fluid flows (see Huo et al. (2003, 2004); Teramoto and Nishiura (2002); Villain-Guillot (2010)). Usually, the corresponding modified Cahn-Hilliard equation for describing the phase separation process in the presence of chemical reaction is known as the Cahn-Hilliard-Oono equation—CHO—see Oono and Puri (1987). Moreover, such an equation also arises in slightly different contexts (e.g., phase separation in diblock polymers) with other names (see, for instance, Aristotelous et al. (2012); Choksi et al. (2011) and references therein). In particular, the resulting CHO system is

$$\begin{cases} \partial_t \psi + \epsilon(\psi - c_0) = -\nabla \cdot (M \nabla \mu) \\ \mu = -\varepsilon \Delta \psi + \frac{1}{\varepsilon} f'(\psi). \end{cases} \tag{1.2.2}$$

where ϵ is proportional to the reaction rate and c_0 is the thermodynamical equilibrium composition of the mixture considered. As for the boundary conditions, the usual no-flux boundary conditions used in the Cahn-Hilliard equation can be retained also in this case.

Several features distinguish the solutions of the usual Cahn-Hilliard equation from those of the CHO system. First, the equilibria of the CHO equation display some clear periodic patter, such as dots or lamellæ according to the relative equilibrium concentration of the constituents (see Figure 1.2). Secondly, the mean composition of the mixture is not fixed by the initial condition (as happens, e.g., for an alloy), but changes with time converging to the prescribed thermodynamical equilibrium c_0 (see equation (1.2.4) for the analogous result for the full variation on the model H below).

Coupling the CHO system with the Navier-Stokes equations and proceeding exactly as in the derivation of the model H, one obtains the following system of Partial differential equations

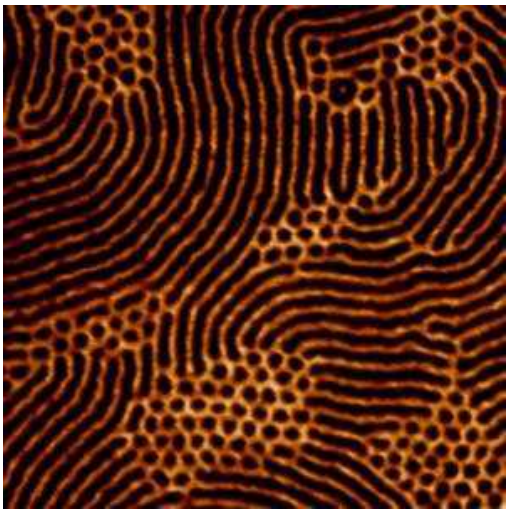


Figure 1.2: Pattern formation in a mixture of diblock copolimers. Observe the regular dotted regions and the lamellæ appearing as a consequence of small local fluctuations of the mean composition of the mixture. Compare with the pattern arising in alloys (see Figure 1.1).

usually called the Navier-Stokes-Cahn-Hilliard-Oono system (or NSCHO system, for short)

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla\cdot(\nu(\psi)D\mathbf{u}) = \nabla\pi + \mu\nabla\psi \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi + \epsilon(\psi - c_0) = \Delta\mu \\ \mu = -\Delta\psi + f(\psi). \end{cases} \tag{1.2.3}$$

This system can be supplemented by the same boundary conditions used for the model H itself (see (1.1.7)).

As anticipated above for the simpler CHO system, an important feature of the NSCHO model concerns the evolution of the mean composition of the mixture. Indeed, integrating the third equation in (1.2.3) over the domain Ω and taking (1.1.7) into account, we obtain the following evolution equation for the (spatial) average $\langle\psi\rangle$

$$\partial_t\langle\psi\rangle + \epsilon(\langle\psi\rangle - c_0) = 0,$$

from which we deduce

$$\langle\psi\rangle(t) = c_0 + e^{-\epsilon t}(\langle\psi_0\rangle - c_0). \tag{1.2.4}$$

Hence, if $\langle\psi_0\rangle = c_0$, then the total mass is conserved as in the classical Cahn-Hilliard equation. Otherwise, we are in the off-critical mixture case, i.e. the order parameter average at steady state differs from $\langle\psi_0\rangle$ (cf. Huo et al. (2003) where numerical simulations are performed in 2D by taking

periodic boundary conditions). This feature leads to interesting problems for the description of the long-term behaviour of solutions.

In Chapter 4, we will study the well-posedness as well as robustness of the asymptotic behaviour of solution with respect to the parameter ϵ.

1.2.3 Non-local models

The Cahn-Hilliard equation derived from the potential energy (1.1.1) implicitly assumes that the interactions between the components of the mixture are short-ranged (i.e., local). However, we may also assume that the interaction energy between two particle of the mixture at points $\mathbf{x}$ and $\mathbf{y}$ is given by a Kac potential of the form

$$\gamma^n K(\gamma|\mathbf{x}-\mathbf{y}|) \qquad \text{with } \gamma > 0.$$

In this case, a statistical mechanical derivation of the model leads to the following non-local total energy for the system (see Giacomin and Lebowitz (1997, 1998))

$$E_P(\psi) = \frac{\varepsilon}{2}\int_\Omega\int_\Omega K(|\mathbf{x}-\mathbf{y}|)|\psi(\mathbf{x})-\psi(\mathbf{y})|^2\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} + \varepsilon\int_\Omega\int_\Omega K(|\mathbf{x}-\mathbf{y}|)\psi(\mathbf{x})(1-\psi(\mathbf{x}))\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} + \frac{1}{\varepsilon}\int_\Omega F(\psi(\mathbf{x}))\,\mathrm{d}\mathbf{x}.$$

The resulting Cahn-Hilliard equation is then given by

$$\begin{cases} \partial_t\psi = -\nabla\cdot(M\nabla\mu) \\ \mu = \varepsilon a\psi - \varepsilon K \ast \psi + \frac{1}{\varepsilon}f'(\psi). \end{cases}$$

where $a(\mathbf{x})$ is defined by

$$a(\mathbf{x}) \doteq \int_\Omega K(|\mathbf{x}-\mathbf{y}|)\,\mathrm{d}\mathbf{y}$$

and where $\ast$ denotes the convolution operator. In the case of smooth interaction kernels K, this system has been studied in Gajewski and Zacharias (2003); Bates and Han (2005). We also note that the non-local model can be reduced to the classical local one by suitably rescaling the interaction kernel K so that its mass is concentrated around the origin.

An interesting problem related to this non-local formulation of the Cahn-Hilliard equations is given by its effects on the properties of the full model H when it is substituted to the local Cahn-Hilliard one. In the case of regular interaction kernels, this issue has recently been addressed in a series of research papers (see Colli et al. (2012); Frigeri and Grasselli (2012a,b)). In particular, in these papers, well-posedness results have been obtained and a description of the asymptotic behaviour of the system has been given.

However, not only regular kernels can be studied, but also singular ones are of great interest for applications. This choice leads to operators somehow similar to the so-called s-Laplacian, although defined on bounded domains (see Silvestre (2007) for an introduction to these operators on the whole space). We will give some preliminary results on the well-posedness of the Cahn-Hilliard equation with non-local interactions described by a singular kernel in Chapter 5. These have to be considered a preliminar work towards the study of the full nonlocal model H with singular kernels.

1.3 Large-time behaviour for solutions of parabolic systems

We now wish to review some of the theory of (infinite dimensional) dynamical system introducing the tools that will be used to describe the large-time behaviour of solutions to evolution equations. We refer the interested reader to the monographs Temam (1997); Robinson (2001) for a more comprehensive introduction to the subject (see also the review Miranville and Zelik (2008)). After briefly recalling the basic theory of global attractors we shortly discuss some of its generalisations, which are needed to study the behaviour exhibited by evolution equations arising in examples of practical interest. In order not to break the exposition into pieces, we refer to Section 1.4 for a detailed description of the notation used in this section and in the remaining of this part of the present manuscript.

1.3.1 Short overview of the classical theory of attractors

The theory of attractors for infinite-dimensional dynamical systems was originally developed by Ladyzhenskaya, Vishik and collaborators in the 70s (see Babin and Vishik (1992) for an early account on the subject). For the sake of clarity, we will briefly discuss here only the case of autonomous systems referring to Section 1.3.4 for the discussion of the pertinent setting for the non-autonomous case (see also Section 3.2 as well as Carvalho et al. (2013) and the references therein).

The starting point of the theory of (global) attractors is an abstract reinterpretation of the structure of the solutions of an evolution equations through the notion of (possibly non-linear) semigroup.

Definition 1.3.1. Let H be a metric. A family of operators $\{S(t)\}_{t\in\mathbb{R}^+}$ s.t. $S(t)\colon H \to H$ for all $t \geqslant 0$ is called *semigroup* if the following properties hold

- $S(0) = I$
- $S(t+s) = S(t) \circ S(s)$ for all non-negative s, t (semigroup property).

The variable t is usually called *time*.

Remark 1.3.1. For the purposes of this work we will always assume that H is an Hilbert or a Banach space.

One of the main goals of the contemporary theory of dynamical systems is to prove significant properties on the solutions of an evolution equation after large time. Among many others, natural question are whether the solutions eventually regularise (this may also happen after a finite time, e.g., in the case of parabolic systems as those which will be studied in the present work), how complex the asymptotic behaviour of the system can be and how fast this significant regime can be reached (at least from a practical point of view). The theory of (global) attractors for evolution PDEs tries to give an answer to these question by constructing "small" sets in the *phase space* H, which contain the eventual evolution of the system. Moreover, precious quantitative information may be deduced from the fractal dimension of these sets and from the rate at which they attract all other physically possible initial data.

From the abstract semigroup description just introduced, the answers to the above questions can be translated in simple properties of the semigroup in the phase space. In particular, regularising properties are epitomised in the requirement that there exists a compact subset of H which absorbs all solutions in the sense made precise by the following definition.

Definition 1.3.2. Let $\{S(t)\}_{t\in\mathbb{R}^+}$ be a semigroup on a metric space H. A subset B is *absorbing* for the semigroup $\{S(t)\}_{t\in\mathbb{R}^+}$ if for all bounded sets $U \subset H$, there exists a time $\overline{t} = \overline{t}(B)$ such that

$$S(t)U \subset B \qquad \forall t \geqslant \overline{t}.$$

In order to describe more precisely (and quantitatively) the behaviour of solutions we will also need to use the metric structure of the phase space H. In particular, we introduce the Hausdorff semi-distance between sets

Definition 1.3.3. Let H be a metric space with distance $d\colon H \times H \to \mathbb{R}$. Given two sets A and B the *Hausdorff semi-distance* between A and B is given by

$$\operatorname{dist}_H(A, B) \doteq \sup_{x\in A} \inf_{y\in B} d(x, y).$$

We can now introduce the main object of interest of this section.

Definition 1.3.4. Let $\{S(t)\}_{t\in\mathbb{R}^+}$ be a semigroup on a metric space H. The *global attractor* for $\{S(t)\}_{t\in\mathbb{R}^+}$ is a set $\mathcal{A} \subset H$ such that

- $\mathcal{A}$ is compact;

- $\mathcal{A}$ is invariant (i.e. $S(t)\mathcal{A} = \mathcal{A}$, for all $t \geqslant 0$);
- $\mathcal{A}$ attracts all bounded subsets $B \subset H$. By this we mean that

$$\lim_{t\to\infty} \mathrm{dist}_H(S(t)B, \mathcal{A}) = 0 \quad \text{for all } B \subset H \text{ with } B \text{ bounded.}$$

It is easy to see that, if the (global) attractor exists, then, by invariance, it has to be unique. Loosely speaking, the attractor contains all the "relevant" information for understanding the persistent dynamics of the evolution equation (or semigroup) of interest. To give examples related to the questions introduced before, the complexity of the asymptotic dynamics can be measured through the evaluation of the fractal dimension of the (global) attractor. Moreover, the rate at which solutions approach the asymptotic regime(s) corresponds to the rate at which $\mathrm{dist}_H(S(t)B, \mathcal{A})$ goes to 0.

We only recall the following fundamental existence result for (global) attractors (cf. (Temam, 1997, Theorem 1.1))

Theorem 1.3.1. *Let $\{S(t)\}_{t\in\mathbb{R}^+}$ be a (non-linear) semigroup acting on a metric space H. Assume that $S(t)$ is continuous for any $t \geqslant 0$ and that there exists a compact absorbing set $B \subset H$. Then, $\{S(t)\}_{t\in\mathbb{R}^+}$ has a (compact) global attractor $\mathcal{A}$. Moreover*

$$\mathcal{A} = \bigcap_{s\geqslant 0} \overline{\bigcup_{t\geqslant s} S(t)B}^{H}$$

holds.

1.3.2 Trajectory attractors

The simple picture of global attractors just introduced, although appealing, cannot in general be used as it is to deal with the solution semigroups arising from applications. Without any attempt of completeness, we would now like to bring to the attention of the reader some of its possible extensions and the subjacent reasons for their development. In particular, we will focus on possible cures to the lack of uniqueness (also related to possible issues with the continuity of the semigroup), on the problems related with the rate of decay of solutions towards the attractor itself and on a possible extension of the theory of global attractors to the non-autonomous case. We start here by addressing the issue related to non-uniqueness.

In the case when uniqueness of solutions is not known, a possible approach to the description of the asymptotic behaviour is given by the theory of trajectory attractors developed by Chepyzhov and Vishik (see Chepyzhov and Vishik (2002, 1997)). This theory was introduced to address, among others, the issues related to the lack of information concerning uniqueness of solutions for the Navier-Stokes equations on $3D$ domains. The key ingredient of this approach is a different

interpretation of the phase space. Solutions are no longer considered as points evolving in the phase space H, but represented as trajectories (i.e. whole functions from $\mathbb{R}^+$ taking values in H), which are translated (with respect to time) by the actions of the semigroup. More rigourously, one can define the phase space to be

$$\Theta^+_{w,\mathrm{loc}} \doteq L^p_{\mathrm{loc}}(\mathbb{R}_+; H),$$

for some $p \geqslant 1$, endowed with a suitable (weak) topology (see Section 2.6 for more details on this technique). The corresponding translation semigroup acting on $\Theta^+_{w,\mathrm{loc}}$ is then simply defined by

$$T(h)\colon u(\,\cdot\,) \mapsto u(\,\cdot\, + h) \qquad \forall u \in \Theta^+_{w,\mathrm{loc}}.$$

It is easy to see that, if the evolution equation studied is well-posed and a continuous semigroup can be defined on the original phase space, the classical and the trajectory semigroup approach are equivalent. The trajectory attractor is then defined as the usual (global) attractor in this novel functional setting.

We briefly comment on some technical issues related to the technique of trajectories attractors. First, one could wonder how the compactness required in Theorem 1.3.1 is recovered in this new setting. However, the required compactness can usually be easily deduced by Aubin-Lions' type lemmata (for the details in a practical functional setting see, e.g., Lemma 2.6.2 below). Moreover, in the case both are well defined, the relation between this attractor in the space of trajectories and the (global) attractor of the previous section seems unclear. However, one can easily prove (see Chepyzhov and Vishik (2002)) that in this case the attractor in the trajectory space can be defined for all real times $t \in \mathbb{R}$ (and not only for positive ones) and that it is invariant with respect to time-shifts. Moreover, the global attractor defined before coincides with sections at fixed time of the trajectory attractor just introduced.

Finally, we note that the theory of trajectory attractors can also be extended to the case of non-autonomous dynamical systems. This leads to some regularity assumptions on the time-dependent terms, which are mainly related to compactness requirements in the theory. We refer again the interested reader to the results contained in Chepyzhov and Vishik (2002) as well to Chapter 2 below.

In Chapter 2, we will use the theory of trajectory attractors to describe the asymptotic behaviour of solutions of the LCH model briefly discussed in Section 1.2.1

1.3.3 Exponential attractors

In general, no information can be obtained on the rate of convergence of solutions towards the attractor when working in the framework of global attractors. Indeed, counterexamples are well-

known also in the simpler case of finite-dimensional dynamical system. For example, consider the ordinary differential equation

$$y'(x) = -\frac{1}{2}y^3(x), \qquad y(0) = y_0$$

which admits the global attractor $\mathcal{A} = \{0\}$, but whose solutions

$$y = \frac{1}{\sqrt{x + C}}, \qquad C \geqslant 0$$

are easily seen to decay polynomially fast to 0.

Since the global attractor as defined before is unique, if one wishes to ensure an exponential attraction property, some other requirements on the attractor itself have to be loosened. Moreover, in order to lead to significant results, the sought exponentially attracting object should also be finite-dimensional. One is thus led to the following definition of exponential attractor (see Eden et al. (1994); Efendiev et al. (2000, 2005)

Definition 1.3.5. Let $\{S(t)\}_{t\in\mathbb{R}^+}$ be a semigroup on a metric space H. An *exponential attractor* for $\{S(t)\}_{t\in\mathbb{R}^+}$ is a set $\mathcal{B} \subset H$ such that

- $\mathcal{B}$ is positively invariant (i.e. $S(t)\mathcal{B} \subset \mathcal{B}$, for all $t \geqslant 0$);
- $\mathcal{B}$ is compact and has finite fractal dimension;
- $\mathcal{B}$ attracts all bounded subsets $B \subset H$ exponentially fast. By this we mean that there exist two positive constants $C = C(B)$ and α such that

  $$\operatorname{dist}_H(S(t)B, \mathcal{B}) \leqslant Ce^{-\alpha t}$$

  holds.

In the Banach-space theory proposed by Efendiev, Miranville and Zelik, exponential attractors can be shown to exist for a semigroup $\{S(t)\}_{t\geqslant 0}$ as soon as the following two conditions are met:

i) the semigroup satisfies the so-called *smoothing property*. If H_1 is a compact subspace of H, this is equivalent to asking that there exists an absorbing set B and a time t such that

   $$S(t)\mathcal{O}_\delta(B) \subset B$$

   and

   $$\|S(t)u - S(t)v\|_{H_1} \leqslant C\|u - v\|_H \qquad \text{for all } u, v \in \mathcal{O}_\delta(B)$$

   hold, where $\mathcal{O}_\delta(B) \doteq \{v \in V \mid \inf_{w\in B} \|v - w\|_{H_1} < \delta\}$ is a δ-neighbourhood of the set B in H_1;

ii) the semigroup is Hölder continuous in time, i.e., there exist positive C and $\gamma \in [0,1]$ such that

$$\|S(t)u - u\|_{H_1} \leqslant C|t|^{\gamma} \qquad \text{for all } u \in \mathcal{O}_\delta(B)$$

holds.

Concerning the results known for the model H, we refer the interested reader to Gal and Grasselli (2010a), where the authors prove the existence of exponential attractors for system (1.1.6)–(1.1.7) on bounded domain in $\mathbb{R}^2$ and for smooth double-well potentials. We also refer to (see also Abels (2009b); Gal and Grasselli (2010b, 2011); Zhao et al. (2009) for related contributions).

We will discuss the existence of exponential attractors for some variations on the model H in Chapters 3 and 4.

1.3.4 Pullback attractors

We now wish to enquire the third and last question introduced before, concerning possible extensions of the theory of global attractors to the case of non-autonomous forcing terms. In particular, among the many possibilities, we will give here a brief account of the theory of pullback attractors (see Section 3.2 for further details and Carvalho et al. (2013) for a comprehensive introduction to this subject). We recall that this theory was first introduced in the context of stochastic differential equations in Schmalfuss (1992) and then brought to deterministic dynamical systems in the works by Kloeden, who also introduced the terminology pullback attractor, see Kloeden (2000). Pullback attractors theory gives a somehow different physical interpretation of the meaning of the attracting set. However, before delving into some of the details, we would like to recall that some other simple extensions of the standard theory of global attractors are also available.

The first issue one has to deal with in the non-autonomous setting is that the solution operator no longer naturally generates a semigroup. Indeed, in order to predict the evolution of a non-autonomous system, one not only needs to know the time that passed by, but also the time at which the system was "started". This leads to a generalisation of the notion of semigroup which goes under the name of process.

Definition 1.3.6. Let H be a metric. A family of operators $\{U(s,t)\}_{s \geqslant t \in \mathbb{R}_+}$ s.t. $U(s,t)\colon H \to H$ for all $s \geqslant t \geqslant 0$ is called *process* if the following properties hold

- $U(s,s) = I$ for all $s \geqslant 0$;
- $U(s,t) = U(s,\tau) \circ U(\tau,t)$ for all non-negative s, τ and t such that $s \geqslant \tau \geqslant t$ (composition property).

However, processes can often be reduced to semigroups by suitably extending the phase space on which they are defined. Assume that the time-dependence is summarised in only one (e.g.

forcing) term defined on the whole real axis (X is here a suitable Hilbert or Banach space)

$$f\colon \mathbb{R} \to X \qquad f(\,\cdot\,)\colon t \mapsto f(t).$$

If the natural phase space for the evolution problem is H, then we can define an extended phase space $\widetilde{H}$ as follows

$$\widetilde{H} \doteq H \times \mathbb{R}_+$$

Moreover, the process $\{U(s,t)\}_{s\geqslant t\in\mathbb{R}_+}$ naturally gives rise to a semigroup $\{\widetilde{S}(t)\}_{t\in\mathbb{R}_+}$ on $\widetilde{H}$:

$$\widetilde{S}(t)\colon H \times \mathbb{R}_+ \to H \times \mathbb{R}_+ \qquad \widetilde{S}(t)(u,s) \doteq (U(t+s,s)u, t+s)$$

A second difficulty now appears evident. This is related to the compactness usually required in order to deduce the existence of a global attractor (see Theorem 1.3.1 above). Unless quite strong assumptions are set on the forcing term f, the existence of a global attractor cannot be deduced in general. One possibility is to assume f to be translation compact in X i.e.

$$\bigcup_{t\in\mathbb{R}} \{f(t)\} \subset\subset X$$

(Here $\subset\subset$ denotes compact inclusion—see Section 1.4). For further details, we refer the interested reader to Chepyzhov and Vishik (2002). See also Bosia (2012) for an example of application of this technique in the case of quasi-periodic non autonomous terms.

On the other hand, the theory of pullback attractors gives a different interpretation to the physical meaning of the attractor itself. Instead of considering it as a representation of the final evolution of the system studied, the attractor is seen as describing the present state of the system arising from the past after an arbitrary long evolution. This change of viewpoint is summarized both in a slight change in the definition of the process (now $\{U(s,t)\}_{s\geqslant t}$ has to be defined for $s,t \leqslant T$ where $T \in \mathbb{R}$ is the present time) and in the reformulation of the attraction property as follows.

Definition 1.3.7. Let $\{U(s,t)_{t\leqslant s\leqslant T}\}$ be a process on a metric space H. The *pullback attractor* for $\{U(s,t)_{t\leqslant s\leqslant T}\}$ is a family of sets $\{\mathcal{A}(t)\}_{t\leqslant T} \subset 2^H$ such that

- $\mathcal{A}(t)$ is compact for all $t \leqslant T$;
- $\mathcal{A}(\,\cdot\,)$ is invariant with respect to $U(\,\cdot\,,\,\cdot\,)$, i.e.

$$U(s,t)\mathcal{A}(t) = \mathcal{A}(s) \qquad \text{holds for all } t \leqslant s \leqslant T;$$

- $\mathcal{A}(\,\cdot\,)$ pullback attracts all bounded subsets, i.e., for all $B \subset H$ there holds

$$\lim_{s\to-\infty} \operatorname{dist}_H(U(t,s)B, \mathcal{A}(t)) = 0 \qquad \text{for all } t \leqslant T;$$

- $\mathcal{A}(\,\cdot\,)$ is minimal, i.e., if $\{\mathcal{C}(t)\}_{t\leqslant T}$ is another family of sets satisfying the above properties, then

$$\mathcal{A}(t) \subset \mathcal{C}(t) \qquad \text{for all } t \leqslant T.$$

A few remarks are necessary. First, due to time-invariance, the definition of pullback and global attractor are equivalent for autonomous evolution equations. However, in the general case the two notions may differ significantly (see, e.g., the account of the Haraux example in Miranville and Zelik (2008)). Finally, in contrast again with the autonomous case, the fourth requirement in the definition of the pullback attractor is not redundant with invariance, but necessary in order to guarantee uniqueness.

Among the many existence results known for pullback attractors, we only recall this simple analogue of Theorem 1.3.1 (see (Carvalho et al., 2013, Theorem 2.12))

Theorem 1.3.2. *Let $\{U(s,t)\}_{t\leqslant s\leqslant T}$ be a (non-linear) process acting on a metric space H. Assume that $U(s,t)$ is continuous for any $s \geqslant t$ and that for any t there exists a compact set $B(t) \subset H$ pullback-attracting bounded subsets of H. Then, $\{U(s,t)\}_{t\leqslant s\leqslant T}$ has a pullback attractor $\{\mathcal{A}_t\}_{t\leqslant T}$. Moreover*

$$\mathcal{A}(t) = \overline{\bigcup_{\substack{B\subset H\\ B \text{ bounded}}} \bigcap_{\tau\leqslant s} \overline{\bigcup_{t\leqslant\tau} U(s,t)B}}^{H}$$

holds.

The theory of pullback attractors for non-autonomous evolution equations is still undergoing vigourous development. In particular, recent results suggest that, in comparison with other proposals, it is effective in giving insight on the structure and properties of the attracting set with detail similar to that achieved by the theory of global attractors in the autonomous setting (see Carvalho et al. (2013) and references therein for an account of the state-of-the-art of the theory).

We will give some results on the existence of (exponential) pullback attractors for the model H in Chapter 3.

1.3.5 Convergence to stationary states

Finally, we also recall that a complementary approach to attractors is available in the study of the asymptotic behaviour of the solutions of infinite dimensional dynamical systems. Studying the convergence to stationary states of a dynamical system means looking for an answer to the questions: "What happens to the system if all external energy source is switched off?", "Does it settle down to some equilibrium state?" and "Can we get rid of a priori possible, non-converging evolutions also in the case of dissipative systems?"

Although these queries may seem trivial when looking from the point of view of finite-dimensional dynamical systems, subtleties may (and do often) arise in the infinite-dimensional setting. For example, the Cahn-Hilliard equations admit a continuum of non-isolated equilibria making the answer to the above questions delicate. Usually, one has to invoke some Łojasiewicz-Simon type inequality (see Jendoubi (1998); Chill (2003)) to deduce convergence of a solution to a single stationary state.

In the case of the model H, convergence of solutions to stationary states under various assumptions has been deduced, e.g., in Abels (2009b); Gal and Grasselli (2010a); Zhao et al. (2009).

1.4 Notation

In this section we review the general notation used throughout the first part of the present manuscript. Additional specific notation might be introduced when needed in subsequent chapters.

1.4.1 General notation

We will use the symbol $\doteq$ in an expression as $A \doteq \mathcal{P}$ where A is a symbol and $\mathcal{P}$ is any well formed expression, to indicate how the quantity appearing on the left hand side is defined.

We will assume that the notion of *set* (equivalently, *family* or *collection*) and of *element* of a set are known to the reader. Given a set A and an element x we will write

$$x \in A \qquad \text{respectively} \qquad x \notin A$$

if x belongs to A (respectively if x does not belong to A). If all the elements of a set A belong also to a set B we will say that A is *included* in B and we will wite

$$A \subset B.$$

If A is any set, the notation 2^A will stand for the set consisting of all the possible subsets of A.

Given a topological space X and a set $A \subset X$, we will denote by $\overline{A}^X$ its *closure* with respect to the topology of X. When clear from the context the superscript X might be dropped to simplify notation. Moreover, ∂A will be the set of *boundary points* of A. If a subset A of X is *compact* with respect to the topology of X we will write

$$A \subset\subset X$$

With the symbol $\mathbb{R}^n$ we will denote the *n-dimensional Euclidean vector space* endowed with the topology generated by the Euclidean metric. We also introduce the notation $\mathbb{R}_+$ for the set

of non-negative real numbers. Moreover, by $\mathbb{R}^n_+$ we will denote the *n-dimensional half space*

$$\mathbb{R}^n_+ \doteq \{\mathbf{x} \in \mathbb{R}^n \mid x_n \geqslant 0\}.$$

In general, $\Omega \subset \mathbb{R}^n$, $n = 2, 3$ will be a smooth bounded *domain* on which the differential problem is given. The regularity of Ω will be specified from time to time, but, as a general rule, it will always be large enough to justify all computations performed. We will also write

$$Q_t \doteq \Omega \times [0, t) \qquad Q_{t,s} \doteq \Omega \times [t, s)$$

to denote the *parabolic domain* on which the considered evolution PDEs is given.

In general, *scalars* will be denoted by normal fonts (like in f or σ), while we will use bold for *vectors* and second rank *tensors* (e.g., $\mathbf{f}$ or $\boldsymbol{\sigma}$) leaving to the context the distinction between these quantities. The components of a vector $\mathbf{u} \in \mathbb{R}^n$ will be denoted by u_i, while the components of a rank two tensor $\boldsymbol{\sigma}$ will be identified by the symbol σ_{ij}. The trace of a rank two tensor on $\mathbb{R}^n$ will be denoted by

$$\operatorname{tr} \mathbf{A} \doteq \sum_{i=1}^{n} A_{ii}$$

The usual *scalar product* in $\mathbb{R}^n$ will be written as

$$\mathbf{u} \cdot \mathbf{v} \doteq \sum_{i=1}^{n} u_i v_i.$$

For the *composition* of rank two tensors on $\mathbb{R}^n$ we will write

$$\mathbf{A} \cdot \mathbf{B} \quad \text{or} \quad \mathbf{AB} \qquad \text{where} \quad (\mathbf{AB})_{ij} \doteq \sum_{k=1}^{n} A_{ik} B_{kj}.$$

We also introduce a scalar product on the space of rank two tensors (also called *saturation*) by the following rule

$$\mathbf{A} : \mathbf{B} \doteq \operatorname{tr}(\mathbf{AB}) = \sum_{i,j=1}^{n} A_{ij} B_{ij}.$$

We will denote by a prime p' the conjugate exponent to any given real number $p \in [1, \infty]$. In particular p' is defined by

$$\frac{1}{p} + \frac{1}{p'} = 1 \quad \text{for } p \in (0, \infty)$$

and is set equal to 1 (respectively ∞) for $p = \infty$ (respectively 1).

Derivatives with respect to time will be denoted by $\partial_t f$. Concerning spatial derivatives, we will use standard notation for the *gradient* of a scalar or vector valued function (e.g., ∇f), the *divergence* of a vector or tensor field (e.g., $\nabla \cdot \mathbf{f}$) and for the Hessian matrix of any function (e.g., $\nabla\nabla f$). Moreover, we will denote by $\Delta f \doteq \nabla \cdot (\nabla f) = \operatorname{tr}(\nabla\nabla f)$ the Laplace operator.

Given a regular domain Ω, we will denote by $\mathbf{n}$ its outward pointing normal. Moreover, given a regular function f defined on Ω, we will denote by $\partial_{\mathbf{n}} f$ the normal derivative of the function on the boundary.

We also introduce a special notation for the convolution operator. Indeed, given a set $\Omega \subset \mathbb{R}^n$ a function f defined on it and a kernel defined on the whole Euclidean space $\mathbb{R}^n$ we set

$$(K * f)(\mathbf{x}) \doteq \int_\Omega K(\mathbf{x}-\mathbf{y}) f(\mathbf{y})\, \mathrm{d}\mathbf{y}.$$

In all the computations the symbol C will denote a *generic constant*, which may change from line to line or from passage to passage. The constant C will depend only on the domain Ω, and on the physical parameters of the model considered. In particular, unless otherwise stated, C will always be assumed independent of time. However, for the sake of clarity, all possible dependencies of C on other quantities will be explicitly accounted in each of the subsequent chapters.

1.4.2 Functional spaces

Given a Banach or a Hilbert space X we will denote the norm of one of its element $f \in X$ by the symbol $\|f\|_X$. The *dual* space of X will be denoted by X^*. If a sequence $\{x_n\}_{n\in\mathbb{N}} \subset X$ converges strongly to x in X we will write

$$x_n \to x \quad \text{in } X.$$

Weak and weak-star convergences will be denoted by

$$x_n \rightharpoonup x \quad \text{or} \quad x_n \overset{*}{\rightharpoonup} x \quad \text{in } X.$$

The spaces $L^p(\Omega)$ will be the usual Banach spaces of p-integrable, Lebesgue-measurable functions defined on the set Ω, where p belongs to $[1,\infty]$. We shall use the bold symbols $\mathbf{L}^p(\Omega)$ for the corresponding spaces of vector valued functions. We will use the special shorthand notation $|\cdot|_p$ for the norm in $L^p(\Omega)$ spaces, $1 \leqslant p \leqslant \infty$.

The Sobolev-Hilbert space, which consists of k-times differentiable functions in the sense of distributions with square integrable derivatives, will be denoted by $H^k(\Omega)$. Again, the bold symbols $\mathbf{H}^k(\Omega)$ will be reserved to the corresponding spaces of vector valued functions. Moreover, we will denote by $W^{k,p}(\Omega)$ the non-hilbertian Sobolev space, which consists of k-differentiable functions in the sense of distributions with L^p integrable derivatives. As above, a bold symbol $\mathbf{W}^{k,p}(\Omega)$ will be used for spaces of vector-valued functions. We also introduce consistent notation for the *fractional Sobolev spaces*, by letting the index k take any positive real value: in this case we will usually write $H^s(\Omega)$ and $W^{s,p}(\Omega)$ (and we will introduce analogous notation for the vector-valued case) to emphasize that s can also be non-integer. Concerning the norms used for vector valued spaces we will adopt the following convention

$$|\nabla f|_2^2 \doteq \sum_{i=1}^n \int_\Omega \left|\frac{\partial f}{\partial x_i}\right|^2 \mathrm{d}\mathbf{x} \qquad |\nabla \mathbf{f}|_2^2 \doteq \sum_{i,j=1}^n \int_\Omega \left|\frac{\partial f_i}{\partial x_j}\right|^2 \mathrm{d}\mathbf{x}.$$

We will denote with an additional subscript 0 to the above notations (e.g., $H^k_0(\Omega)$) the spaces of functions belonging to the "base" functional space (e.g., $H^k(\Omega)$) and vanishing at the boundary of Ω in the sense of distributions. In the case the domain Ω has infinite measure, the subscript loc as in $L^p_{\mathrm{loc}}(\Omega)$ will denote the local spaces for whose elements

$$\|f\|_{L^p(B)} \leqslant C_B \qquad \forall B \subset\subset \Omega$$

holds. Analogous notations will be used for Sobolev spaces (as $H^1_{\mathrm{loc}}(\Omega)$ or $\mathbf{W}^{s,p}_{\mathrm{loc}}(\Omega)$).

Moreover, the *mean value* f a function over the domain Ω will be denoted by

$$\langle f \rangle \doteq \frac{1}{|\Omega|} \int_\Omega f \, \mathrm{d}\mathbf{x}.$$

Additionally, the mean free part of f will be denoted by

$$\overline{f} \doteq f - \langle f \rangle.$$

We will also use the additional subscript (m) for the (affine) subspaces of a given functional space consisting of prescribed mean functions:

$$X_{(m)} \subset X \qquad X_{(m)} \doteq \{f \in X \mid \langle f \rangle = m\}.$$

In order to study the velocity field, we introduce the usual spaces of divergence-free (solenoidal) functions. These will be denoted by a div subscript. In particular, let

$$\mathcal{V} \doteq \{\phi \in \mathbf{C}^\infty(\Omega; \mathbb{R}^n) \mid \nabla \cdot \phi = 0\}$$

be the usual space of divergence-free test functions. The divergence-free spaces are defined by

$$\begin{aligned} \mathbf{H}^s_{\mathrm{div}}(\Omega) &\doteq \overline{\mathcal{V}}^{\mathbf{H}^s(\Omega)}, \\ \mathbf{L}^2_{\mathrm{div}}(\Omega) &\doteq \overline{\mathcal{V}}^{\mathbf{L}^2(\Omega)} \equiv \mathbf{H}^0_{\mathrm{div}}(\Omega), \\ \mathbf{W}^{s,p}_{\mathrm{div}}(\Omega) &\doteq \overline{\mathcal{V}}^{\mathbf{W}^{s,p}(\Omega)}. \end{aligned}$$

for $s > 0$, $p \geqslant 1$. Analogously, also the corresponding spaces with homogeneous Dirichlet boundary conditions (as $\mathbf{H}^s_{0,\mathrm{div}}(\Omega)$) will be used. In view of the study of the equation for the velocity field, we also introduce the Leray projector $\mathbb{P}\colon \mathbf{L}^2(\Omega) \to \mathbf{L}^2_{\mathrm{div}}(\Omega)$ mapping every element of $\mathbf{L}^2(\Omega)$ to its divergence-free part.

The dual spaces of hilbertian and non-hilbertian Sobolev spaces will be denoted by

$$H^{-s}(\Omega) \doteq (H^s_0(\Omega)) \quad \text{and} \quad W^{-s,p'}(\Omega) \doteq (W^{s,p}_0(\Omega))^*$$

whenever these notations make sense. Analogous notations will be used for the space of divergence free functions.

Moreover, we will denote by $\langle f, g\rangle$ both the scalar product in $L^2(\Omega)$ (or $\mathbf{L}^2(\Omega)$) and the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$ (or their vector valued analogues), the exact meaning being clear from the context. When needed we will also use the notation

$$_{X*}\langle f, g\rangle_X$$

to denote the duality pairing between $g \in X$ and $f \in X^*$ and the notation

$$\langle f, g\rangle_Q$$

when referring to the scalar product in $L^2(Q)$ or to the duality pairing between $H^{-1}(Q)$ and $H_0^1(Q)$.

We also introduce notation for the classical spaces of k-times continuously differentiable functions defined on a set Ω and taking values in X: $\mathbf{C}^k(\Omega, X)$. This space will be endowed with the usual maximum norm. We will usually drop the exponent k when referring to continuous functions (i.e., when $k = 0$). Moreover, when $X = \mathbb{R}$ or when it will be clear from the context we will also use the shorten notation $\mathbf{C}^k(\Omega)$. As before a subscript 0 (as in $\mathbf{C}_0^k(\Omega)$) will denote the subset of those functions vanishing at the boundary, while a subscript c (e.g., $\mathbf{C}_c^k(\Omega)$) will refer to those functions having support compactly contained in Ω.

Finally we also introduce suitable notation for the Bochner spaces, i.e., for Banach valued L^p spaces. In particular, if X is a Banach space and s, t are real numbers such that $s > t$, we will denote by

$$L^p(t, s; X)$$

the set of all p-integrable Lebesgue-measurable functions defined on the interval $[t, s]$ and taking values in X. The norm in this space will be given by

$$\|f\|_{L^p(t,s;X)} \doteq \left(\int_t^s \|f(r)\|_X^p \,\mathrm{d}r\right)^{1/p}$$

When no misunderstanding is possible, we will also use the shorthand notation $L^p(X)$ for $L^p(t, s; X)$. We will also use the notation

$$L_{\mathrm{b}}^p(t, s; X)$$

to refer to translation bounded spaces. In this case the norm will be defined by

$$\|\chi\|_{L_{\mathrm{b}}^p(t,s;X))} \doteq \sup_{\tau\in[t,s-1]} \left(\int_\tau^{\tau+1} \|\chi(s)\|_X^p \,\mathrm{d}s\right)^{1/p}.$$

Bibliography

Abels, H. (2009a). Existence of weak solutions for a diffuse interface model for viscous, incompressible fluids with general densities. *Comm. Math. Phys.*, 289(1):45–73.

Abels, H. (2009b). Longtime behavior of solutions of a Navier-Stokes/Cahn-Hilliard system. In: *Nonlocal and abstract parabolic equations and their applications*, volume 86 of *Banach Center Publ.*, pages 9–19. Polish Acad. Sci. Inst. Math., Warsaw.

Abels, H. & Feireisl, E. (2008). On a diffuse interface model for a two-phase flow of compressible viscous fluids. *Indiana Univ. Math. J.*, 57(2):659–698.

Abels, H. & Wilke, M. (2013). Well-posedness and qualitative behaviour of solutions for a two-phase Navier-Stokes-Mullins-Sekerka system. *Interfaces Free Bound.*, 15(1):39–75.

Aristotelous, A. C., Karakashiany, O. A., & Wise, S. M. (2012). A mixed discontinuous Galerkin, convex splitting scheme for a modified Cahn–Hilliard equation. Preprint.

Babin, A. V. & Vishik, M. I. (1992). *Attractors of evolution equations*, volume 25 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co. Translated and revised from the 1989 Russian original by Babin.

Badalassi, V. E., Ceniceros, H. D., & Banerjee, S. (2003). Computation of multiphase systems with phase field models. *J. Comput. Phys.*, 190(2):371–397.

Bates, P. W. & Han, J. (2005). The Neumann boundary problem for a nonlocal Cahn-Hilliard equation. *J. Differential Equations*, 212(2):235–277.

Bosia, S. (2012). Well-posedness and long term behavior of a simplified Ericksen-Leslie non-autonomous system for nematic liquid crystal flows. *Commun. Pure Appl. Anal.*, 11(2):407–441.

Boyer, F. (1999). Mathematical study of multi-phase flow under shear through order parameter formulation. *Asymptot. Anal.*, 20(2):175–212.

Boyer, F. (2001). Nonhomogeneous Cahn-Hilliard fluids. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 18(2):225–259.

Cahn, J. W. (1961). On spinodal decomposition. *Acta Metallurgica*, 9(9):795 – 801.

Cahn, J. W., Elliott, C. M., & Novick-Cohen, A. (1996). The Cahn-Hilliard equation with a concentration dependent mobility: motion by minus the Laplacian of the mean curvature. *European J. Appl. Math.*, 7(3):287–301.

Cahn, J. W. & Hilliard, J. E. (1958). Free energy of a nonuniform system. i. interfacial free energy. *The Journal of Chemical Physics*, 28(2):258–267.

Carvalho, A. N., Langa, J. A., & Robinson, J. C. (2013). *Attractors for infinite-dimensional non-autonomous dynamical systems*, volume 182 of *Applied Mathematical Sciences*. Springer.

Chepyzhov, V. V. & Vishik, M. I. (1997). Evolution equations and their trajectory attractors. *J. Math. Pures Appl. (9)*, 76(10):913–964.

Chepyzhov, V. V. & Vishik, M. I. (2002). *Attractors for equations of mathematical physics*, volume 49 of *American Mathematical Society Colloquium Publications*. American Mathematical Society.

Cherfils, L., Miranville, A., & Zelik, S. (2011). The Cahn-Hilliard equation with logarithmic potentials. *Milan J. Math.*, 79(2):561–596.

Chill, R. (2003). On the łojasiewicz-Simon gradient inequality. *J. Funct. Anal.*, 201(2):572–601.

Choksi, R., Maras, M., & Williams, J. F. (2011). 2D phase diagram for minimizers of a Cahn-Hilliard functional with long-range interactions. *SIAM J. Appl. Dyn. Syst.*, 10(4):1344–1362.

Colli, P., Frigeri, S., & Grasselli, M. (2012). Global existence of weak solutions to a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Math. Anal. Appl.*, 386(1):428–444.

Denisova, I. V. & Solonnikov, V. A. (1991). Solvability in Hölder spaces of a model initial-boundary value problem generated by a problem on the motion of two fluids. *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)*, 188(Kraev. Zadachi Mat. Fiz. i Smezh. Voprosy Teor. Funktsii. 22):5–44, 186.

Eden, A., Foias, C., Nicolaenko, B., & Temam, R. (1994). *Exponential attractors for dissipative evolution equations*, volume 37 of *RAM: Research in Applied Mathematics*. Masson.

Efendiev, M., Miranville, A., & Zelik, S. (2000). Exponential attractors for a nonlinear reaction-diffusion system in $\mathbf{R}^3$. *C. R. Acad. Sci. Paris Sér. I Math.*, 330(8):713–718.

Efendiev, M., Zelik, S., & Miranville, A. (2005). Exponential attractors and finite-dimensional reduction for non-autonomous dynamical systems. *Proc. Roy. Soc. Edinburgh Sect. A*, 135(4):703–730.

Elliott, C. M. & French, D. A. (1987). Numerical studies of the Cahn-Hilliard equation for phase separation. *IMA J. Appl. Math.*, 38(2):97–128.

Elliott, C. M. & Garcke, H. (1996). On the Cahn-Hilliard equation with degenerate mobility. *SIAM J. Math. Anal.*, 27(2):404–423.

Elliott, C. M., Stinner, B., Styles, V., & Welford, R. (2011). Numerical computation of advection and diffusion on evolving diffuse interfaces. *IMA J. Numer. Anal.*, 31(3):786–812.

Feireisl, E. & Pražák, D. (2010). *Asymptotic behavior of dynamical systems in fluid mechanics*, volume 4 of *AIMS Series on Applied Mathematics*. American Institute of Mathematical Sciences (AIMS), Springfield, MO.

Frigeri, S. & Grasselli, M. (2012a). Global and trajectory attractors for a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Dynam. Differential Equations*, 24(4):827–856.

Frigeri, S. & Grasselli, M. (2012b). Nonlocal Cahn-Hilliard-Navier-Stokes systems with singular potentials. *Dyn. Partial Differ. Equ.*, 9(4):273–304.

Gajewski, H. & Zacharias, K. (2003). On a nonlocal phase separation model. *J. Math. Anal. Appl.*, 286(1):11–31.

Gal, C. G. & Grasselli, M. (2010a). Asymptotic behavior of a Cahn-Hilliard-Navier-Stokes system in 2D. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(1):401–436.

Gal, C. G. & Grasselli, M. (2010b). Trajectory attractors for binary fluid mixtures in 3D. *Chin. Ann. Math. Ser. B*, 31(5):655–678.

Gal, C. G. & Grasselli, M. (2011). Instability of two-phase flows: a lower bound on the dimension of the global attractor of the Cahn-Hilliard–Navier-Stokes system. *Phys. D*, 240(7):629–635.

Giacomin, G. & Lebowitz, J. L. (1997). Phase segregation dynamics in particle systems with long range interactions. I. Macroscopic limits. *J. Statist. Phys.*, 87(1-2):37–61.

Giacomin, G. & Lebowitz, J. L. (1998). Phase segregation dynamics in particle systems with long range interactions. II. Interface motion. *SIAM J. Appl. Math.*, 58(6):1707–1729.

Grasselli, M. & Pražák, D. (2011). Longtime behavior of a diffuse interface model for binary fluid mixtures with shear dependent viscosity. *Interfaces Free Bound.*, 13:507–530.

Gurtin, M. E., Polignone, D., & Viñals, J. (1996). Two-phase binary fluids and immiscible fluids described by an order parameter. *Math. Models Methods Appl. Sci.*, 6(6):815–831.

Heida, M., Málek, J., & Rajagopal, K. (2012). On the development and generalizations of Cahn–Hilliard equations within a thermodynamic framework. *Zeitschrift für Angewandte Mathematik und Physik (ZAMP)*, 63:145–169.

Hohenberg, P. C. & Halperin, B. I. (1977). Theory of dynamic critical phenomena. *Rev. Mod. Phys.*, 49:435–479.

Huo, Y., Jiang, X., Zhang, H., & Yang, Y. (2003). Hydrodynamic effects on phase separation of binary mixtures with reversible chemical reaction. *J. Chem. Phys.*, 118:9830–9837.

Huo, Y., Zhang, H., & Yang, Y. (2004). Effects of reversible chemical reaction on morphology and domain growth of phase separating binary mixtures with viscosity difference. *Macromol. Theory Simul.*, 13(3):280–289.

Jendoubi, M. A. (1998). A simple unified approach to some convergence theorems of L. Simon. *J. Funct. Anal.*, 153(1):187–202.

Kay, D., Styles, V., & Welford, R. (2008). Finite element approximation of a Cahn-Hilliard-Navier-Stokes system. *Interfaces Free Bound.*, 10(1):15–43.

Kim, J., Kang, K., & Lowengrub, J. (2004). Conservative multigrid methods for Cahn-Hilliard fluids. *J. Comput. Phys.*, 193(2):511–543.

Kim, N., Consiglieri, L., & Rodrigues, J. F. (2006). On non-Newtonian incompressible fluids with phase transitions. *Math. Methods Appl. Sci.*, 29(13):1523–1541.

Kloeden, P. E. (2000). Pullback attractors in nonautonomous difference equations. *J. Differ. Equations Appl.*, 6(1):33–52.

Ladyzhenskaya, O. (1967). New equations for the description of the motions of viscous incompressible fluids, and global solvability for their boundary value problems. *Trudy Matematicheskogo Instituta im. VA Steklova*, 102:85–104.

Lamorgese, A., Molin, D., & Mauri, R. (2011). Phase field approach to multiphase flow modeling. *Milan J. Math.*, 79:597–642.

Leray, J. (1934). Sur le mouvement d'un liquide visqueux emplissant l'espace. *Acta Math.*, 63(1):193–248.

Lions, J.-L. (1969). *Quelques méthodes de résolution des problèmes aux limites non linéaires*. Dunod.

Liu, C. & Shen, J. (2003). A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. *Phys. D*, 179(3-4):211–228.

Meirmanov, A. M. (1992). *The Stefan problem*, volume 3 of *de Gruyter Expositions in Mathematics*. Walter de Gruyter & Co. Translated from the Russian by Marek Niezgódka and Anna Crowley, With an appendix by the author and I. G. Götz.

Miranville, A. & Zelik, S. (2004). Robust exponential attractors for Cahn–Hilliard type equations with singular potentials. *Math. Methods Appl. Sci.*, 27(5):545–582.

Miranville, A. & Zelik, S. (2008). Attractors for dissipative partial differential equations in bounded and unbounded domains. In: *Handbook of differential equations: evolutionary equations. Vol. IV*, Handb. Differ. Equ., pages 103–200. Elsevier/North-Holland, Amsterdam.

Morro, A. (2010). Phase-field models of Cahn–Hilliard fluids and extra fluxes. *Adv. Theor. Appl. Mech*, 3:409–424.

Oono, Y. & Puri, S. (1987). Computationally efficient modeling of ordering of quenched phases. *Physical review letters*, 58(8):836–839.

Robinson, J. C. (2001). *Infinite-dimensional dynamical systems*. Cambridge Texts in Applied Mathematics. Cambridge University Press. An introduction to dissipative parabolic PDEs and the theory of global attractors.

Schmalfuss, B. (1992). Backward cocycles and attractors of stochastic differential equations. In: *International Seminar on Applied Mathematics-Nonlinear Dynamics: Attractor Approximation and Global Behaviour*, pages 185–192.

Shen, J. & Yang, X. (2010). Energy stable schemes for Cahn-Hilliard phase-field model of two-phase incompressible flows. *Chin. Ann. Math. Ser. B*, 31(5):743–758.

Siggia, E. D. (1979). Late stages of spinodal decomposition in binary mixtures. *Phys. Rev. A*, 20:595–605.

Silvestre, L. (2007). Regularity of the obstacle problem for a fractional power of the Laplace operator. *Comm. Pure Appl. Math.*, 60(1):67–112.

Starovoitov, V. (1997). The dynamics of a two-component fluid in the presence of capillary forces. *Mathematical Notes*, 62(2):244–254.

Temam, R. (1984). *Navier-Stokes equations*, (third ed.), volume 2 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co. Theory and numerical analysis, With an appendix by F. Thomasset.

Temam, R. (1995). *Navier-Stokes equations and nonlinear functional analysis*, (second ed.), volume 66 of *CBMS-NSF Regional Conference Series in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM).

Temam, R. (1997). *Infinite-dimensional dynamical systems in mechanics and physics*, (second ed.), volume 68 of *Applied Mathematical Sciences*. Springer-Verlag.

Teramoto, T. & Nishiura, Y. (2002). Double gyroid morphology in a gradient system with nonlocal effects. *J. Phys. Soc. Jpn.*, 71(7):1611–1614.

Villain-Guillot, S. (2010). 1D Cahn–Hilliard equation for modulated phase systems. *Journal of Physics A: Mathematical and Theoretical*, 43:205102.

Visintin, A. (1996). *Models of phase transitions*. Progress in Nonlinear Differential Equations and their Applications, 28. Birkhäuser Boston Inc.

Zhao, L., Wu, H., & Huang, H. (2009). Convergence to equilibrium for a phase-field model for the mixture of two viscous incompressible fluids. *Commun. Math. Sci.*, 7(4):939–962.

CHAPTER 2

Analysis of a Cahn-Hilliard-Ladyzhenskaya system with singular potential

Outline

In this chapter we study a model for the evolution of a mixture of two incompressible and (partially) immiscible fluids in a domain of $\mathbb{R}^3$. The model we consider is given by Ladyzhenskaya-Navier-Stokes type equations for the (average) fluid velocity coupled with a convective Cahn-Hilliard equation with a singular (e.g., logarithmic) potential. The former is endowed with no-slip boundary conditions, while the latter is subject to no-flux boundary conditions so that the total mass is conserved. We first prove the existence of a weak solution in three-dimensions and some regularity properties. Then we establish the existence of a weak trajectory attractor for a sufficiently general time-dependent external force. Finally, taking advantage of the validity of the energy identity, we show that the trajectory attractor actually attracts solutions with respect to the strong topology.

We start our mathematical analysis of possible variations on the model H introduced in the previous chapter (see equation (1.1.6) in previous chapter), by considering a special class of non-newtonian fluids. In particular, we investigate the mathematical implications of choosing the following, apparently regularising, constitutive relation for the stress-strain rate relation, which is commonly used to describe shear thickening fluids (e.g. corn starch):

$$\boldsymbol{\tau}(D\mathbf{u}, \psi) \doteq \left(\nu_1(\psi) + \nu_2(\psi)|D\mathbf{u}|^{p-2}\right) D\mathbf{u}. \tag{2.0.1}$$

Here ν_1 and ν_2 are given positive constants and $p > 1$. Moreover, $D\mathbf{u}$ is the symmetrized gradient. This relation, when used in the derivation of Navier-Stokes equations in place of its

standard linear counterpart, $\boldsymbol{\tau}(D\mathbf{u}) \doteq 2\nu(\psi)D\mathbf{u}$, gives rise to the well-known Ladyzhenskaya model (see Ladyzhenskaya (1967)), which has been widely investigated in the case of single fluids (see, e.g., Feireisl and Pražák (2010) and its references). Using this relation in the initial boundary value problem

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \Delta\mu \\ \mu = f(\psi) - \Delta\psi \\ \mathbf{u} = \mathbf{0},\ \partial_{\mathbf{n}}\psi = \partial_{\mathbf{n}}\mu = 0 \qquad \text{on } \partial\Omega\times(0,\infty) \\ \mathbf{u}(0) = \mathbf{u}_0,\ \psi(0) = \psi_0 \qquad \text{in } \Omega \end{cases} \tag{2.0.2}$$

we obtain the system which will be the main objective of our investigation in this chapter. As usual, here $\mathbf{u}$ is the velocity field, ψ is the order parameter field, while π stands for the pressure. In order to simplify notations as much as possible, with respect to system (1.1.6), we took $\varepsilon = M = 1$. Motivated by the above discussion, we will call system (2.0.2) Ladyzhenskaya-Cahn-Hilliard—or LCH—system.

This kind of system has been recently analyzed in Grasselli and Pražák (2011) in the case of regular potentials, periodic boundary conditions, $\mathbf{g}$ time independent and ν_i, $i = 1, 2$, depending on ψ. Well-posedness results and regularity results have been obtained for $p \geqslant \frac{11}{5}$ (see also Kim et al. (2006)). Then, using the short trajectory approach, the existence of global and exponential attractors has been established. Here we want to analyze the singular potential case, namely

$$F(r) \doteq \frac{\theta}{2}\left((1+r)\ln(1+r) + (1-r)\ln(1-r)\right) - \frac{\theta_c}{2}r^2, \tag{2.0.3}$$

with a non-autonomous external force and no-slip and no-flux boundary conditions as in Abels (2009c).

The plan of our analysis goes as follows. We first establish the existence of a weak solution. Contrary to the case of single fluids (see Bulíček et al. (2010); Feireisl and Pražák (2010)) or regular potentials (cf. Grasselli and Pražák (2011)), uniqueness seems a rather challenging issue. Indeed, observe that, in comparison with the Cahn-Hilliard-Navier-Stokes case (i.e., $\nu_2 = 0$) considered in Abels (2009c), $\partial_t\mathbf{u}$ is less regular. This fact influences, through the convective term, the smoothness of ψ so that, even in the $2D$ case, the Korteweg force is not always as smooth as needed to guarantee uniqueness when p is large (see also Remark 2.5.1 below). In order to characterize the asymptotic behavior of system (2.0.2) since uniqueness of solution is not known, we resort to the theory of trajectory attractors according to Chepyzhov and Vishik (1997) (cf. Section 1.3.2 and see also Foias and Temam (1987) and Sell (1996) for earlier contributions to

this field). This approach considers as phase space the set of the solutions on the interval $[0, \infty)$ for the system endowed with a suitable topology so that the dynamical system generated by (2.0.2) reduces to a shift operator on this space. Working within this framework, in Sections 2.6 we establish the existence of a trajectory attractor in a suitably chosen weak topology on the space of trajectories. Finally, observing that any weak solution satisfies the energy equality, we can show that the attraction property holds with respect to the strong topology.

2.1 Functional setting

In this chapter Ω is a given bounded domain in $\mathbb{R}^3$ with smooth boundary (say of class $\mathbf{C}^2$). We recall the notation $Q_t \doteq \Omega \times [0,t)$, $Q_{t,s} \doteq \Omega \times [t_1, t_2)$ introduced in Section 1.4.1 for parabolic domains.

To study the velocity field, we introduce the usual space of solenoidal test functions

$$\mathcal{V}_0 \doteq \{\phi \in \mathbf{C}_c^\infty(\Omega; \mathbb{R}^n) \mid \nabla \cdot \phi = 0\}$$

as well as the distribution spaces $\mathbf{L}^2_{0,\mathrm{div}}(\Omega)$, $\mathbf{H}^s_{0,\mathrm{div}}(\Omega)$ and $\mathbf{W}^{s,r}_{0,\mathrm{div}}(\Omega)$ (cf. Section 1.4.2). Moreover, to simplify notation we also define

$$\mathbf{V}_r(\Omega) \doteq \mathbf{W}^{1,r}_{0,\mathrm{div}}(\Omega).$$

As far as the order parameter is concerned, on account of mass conservation, we use Sobolev spaces with fixed mean value as $L^2_{(m)}(\Omega)$, $H^s_{(m)}(\Omega)$ and $W^{s,p}_{(m)}(\Omega)$. Moreover, we use a similar notation for dual spaces whenever it makes sense. Consistently with Section 1.4.2, we define

$$H^{-1}_{(0)}(\Omega) \doteq (H^1_{(0)}(\Omega))^*.$$

We end this section by recalling a simple result, which will be used in the proofs below (see also (Colli et al., 2012, Lemma 1)).

Lemma 2.1.1. *Let $\Omega \subset \mathbb{R}$ be an open subset (not necessarily bounded) and let $\{f_n\} \subset L^\infty(\Omega)$ be a sequence such that $|f_n|_\infty \leqslant C$ and $f_n \to f$ strongly in $L^2(\Omega)$. Let $\{g_n\} \subset L^p(\Omega)$ be another sequence such that $g_n \rightharpoonup g$ weakly in $L^p(\Omega)$. Then $f_n g_n \rightharpoonup fg$ weakly in $L^p(\Omega)$.*

Proof. The statement can be easily proved using the density of $\mathbf{C}_0^\infty(\Omega)$ in $L^2(\Omega)$ and the estimate

$$|f_n g_n|_p \leqslant |f_n|_\infty |g_n|_p.$$

□

2.2 Main assumptions and weak formulation

Here we list some properties of the stress tensor that will be assumed in this chapter. In particular, $\boldsymbol{\tau}(\mathbf{S}, \psi)$ will be a function acting on $\mathbb{S} \times \mathbb{R}$ with values in $\mathbb{S}$ (here $\mathbb{S}$ is the space of symmetric 3×3 tensors) such that

$$\begin{aligned}
&\boldsymbol{\tau}(\mathbf{0}, \varphi) = \mathbf{0} \\
&(\boldsymbol{\tau}(\mathbf{S}_1, \varphi) - \boldsymbol{\tau}(\mathbf{S}_2, \varphi)) : (\mathbf{S}_1 - \mathbf{S}_2) \geqslant \nu_* \left(1 + |\mathbf{S}_1| + |\mathbf{S}_2|\right)^{p-2} |\mathbf{S}_1 - \mathbf{S}_2|^2 \\
&|\boldsymbol{\tau}(\mathbf{S}_1, \varphi) - \boldsymbol{\tau}(\mathbf{S}_2, \varphi)| \leqslant C\nu^* \left(1 + |\mathbf{S}_1| + |\mathbf{S}_2|\right)^{p-2} |\mathbf{S}_1 - \mathbf{S}_2| \\
&|\boldsymbol{\tau}(\mathbf{S}, \varphi_1) - \boldsymbol{\tau}(\mathbf{S}, \varphi_2)| \leqslant C\nu^{\#} \left(1 + |\mathbf{S}|\right)^{p-1} |\varphi_1 - \varphi_2|
\end{aligned}$$

for all φ, $\varphi_i \in \mathbb{R}$, $i = 1, 2$ and for all $\mathbf{S}$, $\mathbf{S}_i \in \mathbb{S}$, $i = 1, 2$, where ν_*, ν^*, $\nu^{\#} \in \mathbb{R}$ are strictly positive constants and where p is assumed to be greater than 2. Under these assumptions, $\boldsymbol{\tau}$ induces an operator, still denoted by $\boldsymbol{\tau}$, acting on $\mathbf{L}^p(\Omega) \times \mathcal{M}(\Omega)$ with values in $\mathbf{L}^{p'}(\Omega)$ (here $\mathcal{M}(\Omega)$ is the space of measurable functions on Ω). Moreover, the operator $\boldsymbol{\tau}(\,\cdot\,, \psi)$ is hemicontinuous from $\mathbf{L}^p(\Omega)$ into $\mathbf{L}^{p'}(\Omega)$ for any fixed $\psi \in \mathcal{M}(\Omega)$.

In the case of the constitutive law (2.0.1), all the above properties are implied by the assumption

$$\nu_i \in \mathbf{C}^1(\mathbb{R}, \mathbb{R})$$

by setting

$$\min_{y \in \mathbb{R}} |\nu_i(y)| \geqslant \nu_* > 0, \quad \max_{y \in \mathbb{R}} |\nu_i(y)| \leqslant \nu^*, \quad \max_{y \in \mathbb{R}} |\nu_i'(y)| \leqslant \nu^{\#}$$

The reader is referred to Bulíček et al. (2010) or (Feireisl and Pražák, 2010, Section 7.1.1) for a more thorough discussion of the above assumptions and their possible generalisations.

As far as the potential F is concerned, following Abels (2009c), we will assume that $F \in \mathbf{C}([-1, 1]) \cap \mathbf{C}^2((-1, 1)))$ and

$$\begin{aligned}
&F(s) = F_0(s) - \frac{\beta}{2} s^2 + \gamma s \\
&F_0(0) = f_0(0) = 0 \\
&\lim_{t \to \pm 1} F(t) \in \mathbb{R} \\
&\lim_{t \to \pm 1} f(t) = \pm\infty.
\end{aligned}$$

for some $\beta \geqslant 0$, $\gamma \in \mathbb{R}$.

Remark 2.2.1. We observe that the logarithmic double-well potential (2.0.3) satisfies the above assumptions.

Let us now introduce the total energy associated with our system:

$$E(\psi, \mathbf{u}) \doteq E_P(\psi) + \frac{1}{2} \int_\Omega |\mathbf{v}(\mathbf{x})|^2 \, d\mathbf{x},$$

where $E_P(\psi)$ is the potential energy for the Cahn-Hilliard equation as given in Section 1.1.1 (cf. equation (1.1.1))

$$E_P(\psi) \doteq \frac{1}{2}\int_\Omega |\nabla\psi(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x} + \int_\Omega F(\psi(\mathbf{x}))\,\mathrm{d}\mathbf{x}.$$

We can now give the definition of weak solution to problem (2.0.2).

Definition 2.2.1. Let $(\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1_{(0)}(\Omega)$ and let $T > 0$ be given. A triplet $(\mathbf{u}, \psi, \mu)$ such that

$$\begin{aligned}
\mathbf{u} &\in L^p(0,T;\mathbf{V}_p) \cap W^{1,p'}(0,T;\mathbf{V}_p^*)\\
\psi &\in L^\infty(0,T;H^1_{(0)}(\Omega)) \cap H^1(0,T;H^{-1}_{(0)}(\Omega))\\
f(\psi) &\in L^2(0,T;L^2(\Omega))\\
\mu &\in L^2(0,T;H^1(\Omega))
\end{aligned}$$

is called a weak solution to (2.0.2) on $(0,T)$ if

$$\begin{aligned}
&\langle \partial_t \mathbf{u}, \mathbf{v}\rangle_{Q_T} + \langle (\mathbf{u}\cdot\nabla)\mathbf{u}, \mathbf{v}\rangle_{Q_T} + \langle \boldsymbol{\tau}(D\mathbf{u}, \psi), D\mathbf{v}\rangle_{Q_T}\\
=&\langle \mu\nabla\psi, \mathbf{v}\rangle_{Q_T} + \langle \mathbf{g}, \mathbf{v}\rangle_{Q_T}, \quad \forall \mathbf{v} \in \mathbf{C}^\infty([0,T);\mathcal{V})\\
&\langle \partial_t\psi, \phi\rangle_{Q_T} + \langle \mathbf{u}\cdot\nabla\psi, \phi\rangle_{Q_T} = -(\nabla\mu, \nabla\phi)_{Q_T}\\
&(\mu, \xi)_{Q_T} = (f(\psi), \xi)_{Q_T} + (\nabla\psi, \nabla\xi)_{Q_T}
\end{aligned} \tag{2.2.1}$$

for all ϕ and ξ in $\mathbf{C}^\infty([0,T);H^1(\Omega))$ and if the energy inequality

$$\begin{aligned}
E(\psi(t), \mathbf{u}(t)) + \|\nabla\mu\|^2_{L^2(Q_{t_0,t})} + C\nu_1\|\nabla\mathbf{u}\|^2_{L^2(Q_{t_0,t})} + C\nu_2\|\nabla\mathbf{u}\|^p_{L^p(Q_{t_0,t})}&\\
\leqslant E(\psi(t_0), \mathbf{u}(t_0)) + C\|\mathbf{g}\|^2_{L^2(\mathbf{H}^{-1})}&
\end{aligned}$$

holds for a.e. $t_0 \in [0,T)$ and all $t \in [t_0, T)$.

Remark 2.2.2. Note that any weak solution is such that $\mathbf{u} \in \mathbf{C}([0,T];\mathbf{L}^2_{0,\mathrm{div}}(\Omega))$. Moreover, it is easy to deduce that $\psi \in L^2(0,T;H^2(\Omega))$. Furthermore, we will see that $\psi \in \mathbf{C}([0,T];H^1_{(0)}(\Omega))$.

Remark 2.2.3. We observe that due to the assumptions on the singular potential F (namely $\lim_{t\to\pm1} f(t) = \pm\infty$), the requirement $f(\psi) \in L^2(0,T;L^2(\Omega))$ in the definition of weak solutions immediately implies that $|\psi| < 1$ a.e. in Q_T.

Remark 2.2.4. Since the Cahn-Hilliard equation with homogeneous Neumann boundary conditions on the chemical potential μ conserves the total mass of the order parameter $\int_\Omega \psi\,\mathrm{d}^3\mathbf{x}$, a suitable shift in the values of the order parameter field is sufficient to ensure that

$$\int_\Omega \psi(t)\,\mathrm{d}^3\mathbf{x} = 0 \qquad \forall t \geqslant 0 \tag{2.2.2}$$

holds as soon as $\int_\Omega \psi_0 \, \mathrm{d}^3\mathbf{x} = 0$. This choice for the values of the order parameter can always be made compatible with the above assumptions on the potential F (namely $F_0(0) = 0$ and $f_0(0) = 0$) by suitably adjusting the constant γ in the decomposition of the potential F and by adding an uninfluential constant to F itself. Therefore, in the remaining part of this chapter we will assume that (2.2.2) holds true.

In this chapter, C will always be a generic constant, which may change from line to line or from passage to passage, depending only on the domain Ω, and on the physical parameters of the model (ν_1, ν_0 and on the potential F). In particular C will always be assumed independent of time.

2.3 The convective Cahn-Hilliard equation

Here we report a result from Abels (2009c) on the convective Cahn-Hilliard equation. Let us consider the following problem

$$\begin{cases} \partial_t \psi + (\mathbf{v}(t) \cdot \nabla)\psi = \Delta \mu & \text{in } \Omega \times (0, \infty) \\ \mu = f(\psi) - \Delta \psi & \text{in } \Omega \times (0, \infty) \\ \partial_{\mathbf{n}} \psi = \partial_{\mathbf{n}} \mu = 0 & \text{on } \partial\Omega \\ \psi(0) = \psi_0 & \text{in } \Omega \end{cases} \tag{2.3.1}$$

where the velocity field $\mathbf{v}$ is given.

Definition 2.3.1. Let $\psi_0 \in H^1_{(0)}(\Omega)$ and let $T > 0$ be given. A pair (ψ, μ) such that

$$\psi \in L^\infty(0, T; H^1_{(0)}(\Omega)) \qquad \partial_t \psi \in L^2(0, T; H^{-1}_{(0)}(\Omega))$$
$$\mu \in L^2(0, T; H^1(\Omega))$$
$$F(\psi(t)) \in L^1(\Omega) \qquad \text{q.o. } t \in [0, T]$$

is a weak solution on the interval $[0, T]$ to (2.3.1) if, for a.e. $t \in [0, T]$, it satisfies

$$\langle \partial_t \psi, \phi \rangle + \langle (\mathbf{v}(t) \cdot \nabla)\psi, \phi \rangle + (\nabla \mu, \nabla \phi) = 0 \qquad \forall \phi \in H^1(\Omega)$$
$$(\mu, \eta) = (f(\psi), \eta) + (\nabla \mu, \nabla \eta) \qquad \forall \eta \in H^1(\Omega)$$
$$\psi(0) = \psi_0$$

Under rather general assumptions problem (2.3.1) is well posed. Indeed we have

Theorem 2.3.1 ((Abels, 2009c, Theorem 6))**.** *Let Ω be a regular domain in $\mathbb{R}^3$ and let $\mathbf{v} \in L^2_{\mathrm{loc}}([0, \infty); \mathbf{V}_2) \cap L^\infty([0, \infty); \mathbf{L}^2_{0,\mathrm{div}}(\Omega))$. Then for any $\psi_0 \in H^1_{(0)}(\Omega)$ with $E_P(\psi_0) < \infty$ there is a*

unique weak solution ψ of the Cahn-Hilliard system (2.3.1) with $\psi \in \mathrm{BC}([0,\infty); H^1_{(0)}(\Omega))$. This solution satisfies the energy equality

$$E_P(\psi(t)) + \int_{Q_t} |\nabla \mu|^2 \, d\mathbf{x}dt = E_P(\psi_0) - \int_{Q_t} \mu(\mathbf{v}\cdot\nabla)\psi \, d\mathbf{x}dt \qquad \forall t \geqslant 0 \tag{2.3.2}$$

and the energy estimates

$$\begin{aligned}
&\|\psi\|^2_{L^\infty([0,\infty);H^1_{(0)})} + \|\partial_t\psi\|^2_{L^2_{\mathrm{loc}}([0,\infty);H^{-1}_{(0)})} + \|\nabla\mu\|^2_{L^2_{\mathrm{loc}}([0,\infty);\mathbf{L}^2)} \\
\leqslant& C\left(E_P(\psi_0) + \|\mathbf{v}\|^2_{L^2_{\mathrm{loc}}([0,\infty);\mathbf{L}^2)}\right), \\
&\|\psi\|^2_{L^2_{\mathrm{loc}}([0,\infty);W^{2,r}_{(0)})} + \|f(\psi)\|^2_{L^2_{\mathrm{loc}}([0,\infty);L^r)} \leqslant C\left(E_P(\psi_0) + \|\mathbf{v}\|^2_{L^2_{\mathrm{loc}}([0,\infty);\mathbf{L}^2)} + 1\right)
\end{aligned}$$

where the constants C do not depend on either $\mathbf{v}$ or ψ_0. Also, it fulfills the regularity properties

$$\psi \in Y \doteq L^2_{\mathrm{loc}}([0,\infty); W^{2,6}(\Omega)) \cap H^1_{\mathrm{loc}}([0,\infty); H^{-1}_{(0)}(\Omega)).$$

Moreover, the solution depends continuously on the data $(\phi_0, \mathbf{v})$ in $H^1(\Omega)\times L^2_{\mathrm{loc}}([0,\infty); \mathbf{L}^2_{0,\mathrm{div}}(\Omega))$ such that $E_P(\psi_0) + \|\mathbf{v}\|_{L^2([0,\infty);H^1)} \leqslant R$, with respect to the weak topology of Y and the strong topology of $H^1(\Omega) \times L^2_{\mathrm{loc}}([0,\infty); \mathbf{L}^2_{0,\mathrm{div}}(\Omega))$.

2.4 Some results on the Ladyzhenskaya model

In this section we summarize some of the results known on the well-posedness of the Ladyzhenskaya model. We start by recalling that the Ladyzhenskaya model for non-Newtonian fluids is

$$\begin{cases}
\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u})) + \mathbf{f}(t) & \text{in } \Omega\times(0,\infty) \\
\nabla\cdot\mathbf{u} = 0 & \text{in } \Omega\times(0,\infty) \\
\mathbf{u} = \mathbf{0} & \text{on } \partial\Omega \\
\mathbf{u}(0) = \mathbf{u}_0 & \text{in } \Omega
\end{cases} \tag{2.4.1}$$

where $\boldsymbol{\tau}$ is given by (2.0.1).

The well posedness of system (2.4.1) has been extensively studied in the literature. In the shear-thickening case (i.e. $p \geqslant 2$), existence and uniqueness of solutions have been obtained as soon as $p \geqslant \frac{11}{5}$ (see, for instance, Feireisl and Pražák (2010) and references therein). Although we will not use directly the results of this section in our results, we observe that the same mathematical difficulties (i.e. uniqueness is an open issue for $p < \frac{11}{5}$) hold both for the Ladyzhenskaya model as well as for the coupled model we are studying.

Definition 2.4.1. Let $\mathbf{u}_0 \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega)$ and let $T > 0$ be given. A function $\mathbf{u}$ such that

$$\mathbf{u} \in L^p(0,T;\mathbf{V}_p(\Omega)) \qquad \partial_t\mathbf{u} \in L^{p'}(0,T;(\mathbf{V}_p(\Omega))^*)$$

is a *weak solution* on the interval $[0,T]$ to problem (2.4.1) if for a.e. $t \in [0,T]$

$$\langle \partial_t \mathbf{u}, \boldsymbol{\phi} \rangle + \langle (\mathbf{u}\cdot\nabla)\mathbf{u}, \boldsymbol{\phi} \rangle + (\boldsymbol{\tau}(D\mathbf{u}), D\boldsymbol{\phi}) + \langle \mathbf{f}(t), \boldsymbol{\phi} \rangle \qquad \forall \boldsymbol{\phi} \in \mathbf{V}_p(\Omega)$$
$$\mathbf{u}(0) = \mathbf{u}_0.$$

Definition 2.4.2. A function $\mathbf{u}$ such that

$$\mathbf{u} \in L^p_{\mathrm{loc}}([0,\infty); \mathbf{V}_p(\Omega)) \qquad \partial_t \mathbf{u} \in L^{p'}_{\mathrm{loc}}([0,\infty); (\mathbf{V}_p(\Omega))^*)$$

is a *global weak solution* to problem (2.4.1) if it is a weak solution on $[0,T]$ for any $T > 0$.

Then, thanks to the results in (Feireisl and Pražák, 2010, Chapter 7.1) (see also Málek et al. (2001) for some more detailed results), we have

Theorem 2.4.1. *Let $p \geqslant \frac{11}{5}$. If $\mathbf{f} \in H^1_{\mathrm{loc}}([0,\infty); \mathbf{H}^{-1}(\Omega))$. Then there exists a unique global weak solution $\mathbf{u}$ to problem (2.4.1) which satisfies*

$$\mathbf{u} \in L^\infty([0,\infty); \mathbf{L}^2_{0,\mathrm{div}}(\Omega)) \cap L^p_{\mathrm{loc}}([0,\infty); \mathbf{V}_p) \cap W^{1,p'}_{\mathrm{loc}}([0,\infty); \mathbf{V}_p^*).$$

Moreover $\mathbf{u}$ also satisfies the following energy equality

$$\frac{1}{2}\frac{d}{dt}|\mathbf{u}|_2^2 + \int_\Omega \boldsymbol{\tau}(D\mathbf{u}) : D\mathbf{u}\,\mathrm{d}\mathbf{x} = \int_\Omega \mathbf{f}\cdot\mathbf{u}\,\mathrm{d}\mathbf{x}.$$

2.5 Weak solutions and energy estimates

Here we prove the existence of a weak solution to problem (2.0.2) revisiting the fixed-point argument devised in (Abels, 2009c, Theorem 9).

Theorem 2.5.1. *Let $p > \frac{11}{5}$ and let $\mathbf{g} \in L^{p'}_{\mathrm{loc}}([0,\infty); \mathbf{V}_p^*)$. Then, for any given $T > 0$, there exists a weak solution $(\mathbf{u}, \psi, \mu)$ to problem (2.0.2). In addition, $\psi \in C([0,T]; H^1_{(0)}(\Omega))$.*

Proof. We will first prove the existence of solutions for the following approximated problem:

$$\begin{cases} \partial_t \mathbf{u} + (\Phi_\epsilon \mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\pi + \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) - \nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t) \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi = \Delta\mu \\ \mu = f(\psi) - \Delta\psi \\ \mathbf{u} = \mathbf{0},\ \partial_{\mathbf{n}}\psi = \partial_{\mathbf{n}}\mu = 0 \qquad \text{on } \partial\Omega\times(0,\infty) \\ \mathbf{u}(0) = \mathbf{u}_0,\ \psi(0) = \psi_0 \qquad \text{in } \Omega. \end{cases} \tag{2.5.1}$$

The operator Φ_ϵ appearing above is a suitable regularization defined as

$$\Phi_\epsilon \mathbf{w} = P_p(\phi_\epsilon * \mathbf{w})$$

where $\phi_\epsilon(\mathbf{x}) = \epsilon^{-3}\phi(\mathbf{x}/\epsilon) \in \mathbf{C}^\infty(\mathbb{R}^3)$, $\epsilon > 0$ is a smoothing kernel and where P_p is the bounded analogue of the Leray's projector from the spaces $\mathbf{L}^p(\Omega)$ to $\mathbf{V}_p$ (see the results on the Helmholtz decomposition in (Fabes et al., 1998, Section 11)). The definition of weak solution for the approximated system (2.5.1) reads as Definition 2.2.1 with the only slight change in (2.2.1) due to the introduction of the regularization.

The existence of weak solutions for the approximated problem can be shown by a fixed point argument. We will consider

$$X = L^p(0,T;\mathbf{V}_p) \cap W^{1,p'}(0,T;\mathbf{V}_p^*)$$

and

$$Y = L^2(0,T;W^{2,6}_{(0)}(\Omega)) \cap H^1(0,T;H^{-1}_{(0)}(\Omega))$$

as functional spaces for the velocity and the order parameter field respectively. The fixed point map $\Psi\colon X \to X$ is defined by first finding the solution ψ to problem (2.3.1), where the velocity field $\mathbf{v}$ is assumed to be known, and then by determining the solution $\mathbf{u}$ to the system

$$\begin{cases} \partial_t \mathbf{u} - \nabla\cdot(\boldsymbol{\tau}(D\mathbf{u},\psi)) = -\nabla p + \mathbf{h}(t) & \text{in } Q_T \\ \nabla\cdot\mathbf{u} = 0 & \text{in } Q_T \\ \mathbf{u} = \mathbf{0} & \text{on } \partial\Omega\times[0,T) \\ \mathbf{u}(0) = \mathbf{u}_0 & \text{in } \Omega. \end{cases} \tag{2.5.2}$$

with

$$\mathbf{h}(t) = -(\Phi_\epsilon\mathbf{v}\cdot\nabla)\mathbf{v} - \nabla\cdot(\nabla\psi\otimes\nabla\psi) + \mathbf{g}(t).$$

The map Ψ is the operator associating to the velocity field $\mathbf{v}$ the solution $\mathbf{u}$ of (2.5.2), i.e. $\Psi\colon \mathbf{v} \mapsto \mathbf{u}$.

Theorem 2.3.1 ensures that $\mathcal{S}_{CH} : \mathbf{v} \mapsto \psi$ is strong-weak continuous from X to Y. On the other hand, by Aubin-Lions' lemma, we have that

$$Y \subset\subset L^2(0,T;\mathbf{C}^1(\overline{\Omega})).$$

Using Theorem 2.3.1 again, we obtain that $\mathcal{S}_{CH}$ is bounded with values in $Y \cap L^\infty(0,T;H^1_{(0)}(\Omega))$ so that $\nabla\psi = \nabla\mathcal{S}_{CH}(\mathbf{v}) \in L^4(0,T;\mathbf{L}^4(\Omega))$ and $\nabla\psi\otimes\nabla\psi \in L^2(0,T;\mathbf{L}^2(\Omega))$. From this we also deduce that the mapping

$$\mathbf{v} \mapsto -\nabla\cdot(\nabla\psi\otimes\nabla\psi) - (\Phi_\epsilon\mathbf{v}\cdot\nabla)\mathbf{v}$$

is continuous and compact from X into $L^{p'}(0,T;\mathbf{V}_p^*)$. Since $\boldsymbol{\tau}(D\mathbf{u},\psi)$ is uniformly monotone and hemicontinuous (w.r.t. $\psi \in \mathcal{M}(\Omega)$) a standard application of the theory of monotone operators

(see Lions (1969)) shows that the solution operator to problem (2.5.2) $\mathcal{S}_P\colon (\mathbf{h}(t),\psi)\mapsto \mathbf{u}$ is well defined and continuous from $L^{p'}(0,T;\mathbf{V}_p^*)\times L^2(0,T;L^2_{(0)}(\Omega))$ into X.

By the above discussion we conclude that the operator

$$\Psi(\mathbf{v})=\mathcal{S}_P\circ\mathcal{S}_{CH}(\mathbf{v}).$$

is continuous being a composition of continuous mappings and is precompact thanks to Aubin-Lions' lemma as shown above.

In order to apply the Leray-Schauder fixed point theorem and conclude our proof we still need a suitable a priori bound on the solutions of the equation

$$s\Psi(\mathbf{u})=\mathbf{u}\qquad s\in[0,1].$$

By multiplying the above equation by $\mathbf{u}$ and integrating over Ω, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}|_2^2+C\nu_1|\nabla\mathbf{u}|_2^2+C\nu_2|\nabla\mathbf{u}|_p^p\leqslant s^2C\|\mathbf{g}\|^{p'}_{\mathbf{V}_p^*}-sC\left((\nabla\psi\otimes\nabla\psi),\nabla\mathbf{u}\right).$$

Recalling the useful vector identity

$$\langle(\mathbf{u}\cdot\nabla)\psi,\mu\rangle=((\nabla\psi\otimes\nabla\psi),\nabla\mathbf{u}) \tag{2.5.3}$$

and energy equality (2.3.2), we get

$$\begin{aligned}&sE(\psi,\mathbf{u})+s\|\nabla\mu\|^2_{L^2(Q_T)}+|\mathbf{u}(T)|_2^2+C\nu_*\|\nabla\mathbf{u}\|^2_{L^2(Q_T)}+C\nu_*\|\nabla\mathbf{u}\|^p_{L^p(Q_T)}\\ \leqslant&E(\psi_0,\mathbf{u}_0)+s^2C\|\mathbf{g}\|^p_{L^{p'}(\mathbf{V}_p)},\end{aligned}$$

which in particular entails an a priori estimate on $\|\nabla\mathbf{u}\|_{L^p(\mathbf{V}_p)}$ which is uniform with respect to s and independent of ϵ.

Thanks to Theorem 2.3.1 we can also obtain uniform estimates for $\nabla\psi$ in $L^\infty(L^2(\Omega))$ and in $L^2(L^\infty(\Omega))$. Thus $\|\partial_t\mathbf{u}\|_{L^{p'}((\mathbf{V}_p)^*)}$ can be uniformly (w.r.t. s) bounded as follows

$$\begin{aligned}\|\partial_t\mathbf{u}\|_{L^{p'}((\mathbf{V}_p)^*)}\leqslant C\|\mathbf{u}\|^{\frac{5p-9}{5p-6}}_{L^\infty(\mathbf{L}^2)}\|\mathbf{u}\|^{\frac{3}{5p-6}}_{L^{2p'\frac{3}{5p-6}}(\mathbf{V}_p)}\|\Phi_\epsilon\mathbf{u}\|^{\frac{5p-9}{5p-6}}_{L^\infty(\mathbf{L}^2)}\|\Phi_\epsilon\mathbf{u}\|^{\frac{3}{5p-6}}_{L^{2p'\frac{3}{5p-6}}(\mathbf{V}_p)}\\ +C\nu^*\|\mathbf{u}\|^{p-1}_{L^p(\mathbf{V}_p)}+C\|\nabla\psi\|^{\frac{2}{p'}}_{L^\infty(\mathbf{L}^2)}\|\psi\|^{\frac{2}{p}}_{L^{2\frac{p'}{p}}(W^{2,3})}+\|\mathbf{g}\|_{L^{p'}((\mathbf{V}_p)^*)}.\end{aligned}$$

as soon as

$$2p'\frac{3}{5p-6}\leqslant p\qquad\text{i.e.}\qquad p\geqslant\frac{11}{5}.$$

Moreover we observe that this bound is uniform also in ϵ for $p\geqslant\frac{11}{5}$. This concludes the proof of the existence of solutions for the approximate problem (2.5.1).

We now want to pass to the limit for $\epsilon\to0$ and recover solutions for the original model as soon as $p\geqslant\frac{11}{5}$. By considering the weak solutions to problem (2.5.1) $(\mathbf{u}_\epsilon,\psi_\epsilon,\mu_\epsilon)$ on the time

interval $[0, T_\epsilon)$, $T_\epsilon = \frac{1}{\epsilon}$ and extended to zero for times greater than T_ϵ, the above discussion gives a sequence $\epsilon_k \to 0$ such that

$$\begin{aligned}
\mathbf{u}_\epsilon &\rightharpoonup \mathbf{u} \text{ in } L^p_{\text{loc}}([0,\infty); \mathbf{V}_p) \\
\mathbf{u}_\epsilon &\overset{*}{\rightharpoonup} \mathbf{u} \text{ in } L^\infty_{\text{loc}}([0,\infty); \mathbf{L}^2_{0,\text{div}}(\Omega)) \\
\partial_t \mathbf{u}_\epsilon &\rightharpoonup \partial_t \mathbf{u} \text{ in } L^{p'}_{\text{loc}}([0,\infty); \mathbf{V}_p^*) \\
\boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi) &\rightharpoonup \chi \text{ in } L^{p'}_{\text{loc}}([0,\infty); \mathbf{V}_p^*) \\
\psi_\epsilon &\rightharpoonup \psi \text{ in } L^2_{\text{loc}}([0,\infty); W^{2,6}_{(0)}(\Omega)) \\
\psi_\epsilon &\overset{*}{\rightharpoonup} \psi \text{ in } L^\infty([0,\infty); L^2(\Omega)) \\
\nabla \mu_\epsilon &\rightharpoonup \nabla \mu \text{ in } L^2_{\text{loc}}([0,\infty); \mathbf{L}^2(\Omega)).
\end{aligned}$$

Moreover, Aubin-Lions' lemma implies that $\mathbf{u}_\epsilon \to \mathbf{u}$ strongly in $L^p_{\text{loc}}([0,\infty); \mathbf{L}^q_{0,\text{div}}(\Omega))$ for all $q < \frac{3p}{3-p}$ so that

$$(\Phi_\epsilon \mathbf{u}_\epsilon \cdot \nabla)\mathbf{u}_\epsilon \rightharpoonup (\mathbf{u} \cdot \nabla)\mathbf{u} \qquad \text{in } L^{p'}_{\text{loc}}([0,\infty); \mathbf{V}_p^*)$$

as soon as $p > \frac{11}{5}$. By using Aubin-Lions' lemma once more, we also have that $\psi_\epsilon \to \psi$ strongly in $L^2_{\text{loc}}([0,\infty); H^1_{(0)}(\Omega))$. This in turn implies strong convergence of ψ_ϵ to ψ in $L^4_{\text{loc}}([0,\infty); L^4_{(0)}(\Omega))$ and

$$\nabla \psi_\epsilon \otimes \nabla \psi_\epsilon \to \nabla \psi \otimes \nabla \psi \text{ in } L^2_{\text{loc}}([0,\infty); \mathbf{L}^2(\Omega)),$$

In order to pass to the limit in the stress term, we observe that for all $\mathbf{v} \in \mathbf{V}_p$ we have

$$\langle \nabla \cdot (\boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi_\epsilon)), \mathbf{v} \rangle = \langle \nabla \cdot (\boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi_\epsilon) - \boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi)), \mathbf{v} \rangle + \langle \nabla \cdot (\boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi)), \mathbf{v} \rangle$$

By the assumptions on $\boldsymbol{\tau}$ we have

$$\int_0^T |\langle \nabla \cdot (\boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi_\epsilon) - \boldsymbol{\tau}(D\mathbf{u}_\epsilon, \psi)), \mathbf{v} \rangle| \leqslant \int_{\Omega \times [0,T]} |\psi_\epsilon - \psi| \left(1 + |D\mathbf{u}_\epsilon|\right)^{p-1} |\nabla \mathbf{v}|, \tag{2.5.4}$$

which is easily seen to converge to 0 by using Lemma 2.1.1 up to a subsequence after noting that $(1+|D\mathbf{u}_\epsilon|)^{p-1}$ is bounded in $L^{p'}(0,T; \mathbf{V}^*_{p'})$, that ψ converges strongly to ψ in $L^2(0,T; L^2_{(0)}(\Omega))$ for any $T > 0$ and that $|\psi_\epsilon| \leqslant 1$ a.e. in $\Omega \times [0,\infty)$. Using again a standard monotonicity argument (see (Lions, 1969, Chapter 2)), we can now identify the limit χ with $\boldsymbol{\tau}(D\mathbf{u}, \psi)$ and pass to the limit in all the terms in the linear momentum equation.

We can also easily pass to the limit in the Cahn-Hilliard equation thanks to the continuous dependence results in Theorem 2.3.1 and to the strong convergence of $\mathbf{u}_\epsilon$ in $L^2_{\text{loc}}([0,\infty); \mathbf{L}^2_{0,\text{div}}(\Omega))$ obtaining therefore that ψ and μ satisfy the order parameter equation with convective term $\mathbf{u} \cdot \nabla \psi$. This proves that $(\mathbf{u}, \psi, \mu)$ satisfies system (2.0.2) in a weak sense.

In order to have a weak solution we still have to show that our candidate solution $(\mathbf{u}, \psi, \mu)$ satisfies the energy inequality. However this easily follows by noting that the approximate solutions $(\mathbf{u}_\epsilon, \psi_\epsilon, \mu_\epsilon)$ satisfy an analogous equality and that from the strong convergence of $\mathbf{u}_\epsilon$ in

$L^2_{\mathrm{loc}}([0,\infty);\mathbf{L}^2_{0,\mathrm{div}}(\Omega))$ and of ψ_ϵ in $L^2_{\mathrm{loc}}([0,\infty);H^1_{(0)}(\Omega))$ we have strong convergence of $\mathbf{u}_\epsilon(t)$ in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega)$ and of $\psi_\epsilon(t)$ in $H^1_{(0)}(\Omega)$ for almost every positive t. Finally we conclude thanks to the weak lower semicontinuity of norms. □

As a consequence (cf. also Remark 2.2.2), we can say that there exists a global weak solution to problem (2.0.2) (i.e. defined on $(0,\infty)$). We now show that any (global) weak solution satisfies an energy equality. This fact will play a basic role in the subsequent analysis of the longtime behavior (see the next sections).

Theorem 2.5.2. *Any weak solution $(\mathbf{u},\psi,\mu)$ to problem (2.0.2) satisfies the following (differential) energy equality, for a.e. $t>0$:*

$$\frac{d}{dt}E(\psi,\mathbf{u})+\int_\Omega \boldsymbol{\tau}(D\mathbf{u},\psi):D\mathbf{u}\,\mathrm{d}\mathbf{x}+\int_\Omega f(\psi)\psi\,\mathrm{d}\mathbf{x}+|\nabla\mu|_2^2+|\nabla\psi|_2^2 = \langle\mathbf{g}(t),\mathbf{u}\rangle+(\mu,\psi)\,. \quad (2.5.5)$$

Proof. Let $(\mathbf{u},\psi,\mu)$ be any (global) weak solution to problem (2.0.2). Before starting, we recall the following identity (see (Colli et al., 2007, Proposition 4.2))

$$\int_\Omega \mu\partial_t\psi=\frac{1}{2}\int_\Omega\frac{\mathrm{d}}{\mathrm{d}t}(2F(\psi)+|\nabla\psi|^2).$$

Testing now the linear momentum balance by $\mathbf{u}$ and the evolution equation for the order parameter by μ, recalling identity (2.5.3) and adding the resulting estimates together, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}E(\mathbf{u},\psi)+\int_\Omega\boldsymbol{\tau}(D\mathbf{u},\psi):D\mathbf{u}\,\mathrm{d}\mathbf{x}+|\nabla\mu|_2^2=\langle\mathbf{g}(t),\mathbf{u}\rangle$$

Multiplying the equation for the chemical potential in (2.0.2) by ψ and integrating over Ω, we also get

$$(\mu,\psi)=|\nabla\psi|_2^2+\int_\Omega f(\psi)\psi\,d\mathbf{x}$$

from which the claim easily follows. □

Corollary 2.5.3 ((Grasselli and Pražák, 2011, Theorem 3.1))**.** *Any global weak solution to problem (2.0.2) satisfies the following dissipative estimate, for a.e. $t>0$:*

$$\frac{d}{dt}E(\psi,\mathbf{u})+cE(\psi,\mathbf{u})+c|\nabla\mathbf{u}|_2^2+c|\nabla\mathbf{u}|_p^p+c|\nabla\mu|_2^2\leqslant C\left(\|\mathbf{g}\|^2_{\mathbf{H}^{-1}_{\mathrm{div}}}+1\right). \quad (2.5.6)$$

where the positive constants c and C depend only on the structural parameters of the model and on Ω.

Proof. The viscous term in (2.5.5) can be estimated from below owing to the monotonicity of $\boldsymbol{\tau}(\,\cdot\,,\psi)$ for fixed ψ. The term arising from potential F can be handled easily as follows

$$\begin{aligned}\int_\Omega f(\psi)\psi\,\mathrm{d}\mathbf{x} &= \int_\Omega f_0(\psi)\psi\,\mathrm{d}\mathbf{x} - \beta\int_\Omega \psi^2\,\mathrm{d}\mathbf{x} + \gamma\int_\Omega \psi\,\mathrm{d}\mathbf{x}\\ &\geqslant \int_\Omega F_0(\psi)\,\mathrm{d}\mathbf{x} - \beta\int_\Omega \psi^2\,\mathrm{d}\mathbf{x} = \int_\Omega F(\psi)\,\mathrm{d}\mathbf{x} - \frac{\beta}{2}\int_\Omega \psi^2\,\mathrm{d}\mathbf{x}\end{aligned}$$

where we used the convexity of F_0 and $F_0(0) = 0$ (see page 40). The dissipativity estimate then follows from Poincaré's inequality. □

Remark 2.5.1. Due to the low time regularity of the acceleration field $\mathbf{u}_t$ for large p, in general we cannot ensure uniqueness even in the 2D case. In particular this lower regularity prevents us from obtaining a suitable time-regularity for the order parameter field (e.g. boundedness of ψ in $L^\infty([0,\infty);W^{1,\infty}_{(0)})$) needed to prove uniqueness of solutions for system (2.0.2). This issue is related to the presence of the singular potential in our model (see Grasselli and Pražák (2011) for a thorough discussion of the regular case).

2.6 A weak trajectory attractor

In this section we define a (trajectory) dynamical system associated with problem (2.0.2) and then we establish the existence of a trajectory attractor by using the general results of Chepyzhov and Vishik (2002).

We start by recalling the main pertinent definitions to our case. The set of all non-autonomous terms appearing in (2.0.2), considered as functions from $\mathbb{R}^+ = [0,\infty)$ into a suitable Banach space Ξ, will be called the *symbol* of the equation and will be denoted by σ (in our case, $\sigma = \mathbf{g}$). The space of all admissible symbols will be called the *symbol space* and will be denoted by Σ. It is possible to define a natural semigroup on the symbol space, the *translation semigroup* $\{T(t)\}_{t\in\mathbb{R}^+}$ that simply translates in time the non-autonomous symbols:

$$[T(t)\sigma](s) = \sigma(t+s) \qquad \forall s > 0.$$

In order to guarantee good asymptotic properties one usually needs the symbol space to be positively translation invariant (i.e. positively invariant under the action of the translation semigroup, $T(t)\Sigma \subset \Sigma\ \forall t \geqslant 0$). In particular we will assume that:

$$\Sigma = \mathcal{H}(\sigma_0) \doteq \overline{\{T(t)\sigma_0 \mid t\in\mathbb{R}^+\}}^{\Xi}$$

where $\sigma_0(s)$ is a suitable translation compact function in Ξ. In our case $\sigma_0 = \mathbf{g}_0$ will be a translation compact function in $L^2_{\mathrm{loc}}(\mathbb{R};\mathbf{H}^{-1}_{\mathrm{div}}(\Omega))$. We recall the following useful proposition.

Proposition 2.6.1 ((Chepyzhov and Vishik, 2002, Proposition V.3.3)). *Let E be a Banach space. A function $\sigma(s)$ is translation compact in $L^p_{\mathrm{loc}}(\mathbb{R};E)$ if and only if:*

1. *for any $h>0$ the set*
$$\left\{\int_t^{t+h}\sigma(s)\,\mathrm{d}s \mid t\in\mathbb{R}\right\}$$
is precompact in E;

2. *there exists a function $\alpha(s)$, $\lim_{s\to 0^+}\alpha(s)=0^+$ such that*
$$\int_t^{t+1}\|\sigma(s)-\sigma(s+l)\|_E^p\,\mathrm{d}s\leqslant\alpha(|l|)\qquad\forall t\in\mathbb{R}.$$

We can now introduce the trajectory space, that is the set of all (weak) solutions to problem (2.0.2) for any given pair $(\mathbf{u}_0,\psi_0)\in\mathbf{L}^2_{0,\mathrm{div}}(\Omega)\times H^1_{(0)}(\Omega)$.

Definition 2.6.1. The set $\mathcal{K}^+_\sigma$, $\sigma\in\Sigma$ given by

$$\begin{aligned}\mathcal{K}^+_\sigma\doteq\{&(\mathbf{u}(\,\cdot\,),\psi(\,\cdot\,),\mu(\,\cdot\,))\mid(\mathbf{u},\psi,\mu)\text{ is a weak solution to (2.0.2) with symbol }\sigma\\&\mathbf{u}\in L^p_{\mathrm{loc}}([0,\infty);\mathbf{V}_p)\cap L^\infty([0,\infty);\mathbf{L}^2_{0,\mathrm{div}}(\Omega))\cap W^{1,p'}([0,\infty);\mathbf{V}_p^*),\\&\psi\in L^\infty_{\mathrm{loc}}([0,\infty);H^1_{(0)}(\Omega))\cap H^1([0,\infty);H^{-1}_{(0)}(\Omega)),\\&f(\psi)\in L^2_{\mathrm{loc}}([0,\infty);L^6(\Omega)),\\&\mu\in L^2_{\mathrm{loc}}([0,\infty);H^1(\Omega))\,\}\end{aligned}$$

is the *trajectory space* to problem (2.0.2) with symbol σ.

Definition 2.6.2. The set
$$\mathcal{K}^+_\Sigma\doteq\bigcup_{\sigma\in\Sigma}\mathcal{K}^+_\sigma$$
is the *united trajectory space* associated with problem (2.0.2).

On account of the previous section, we know that $\mathcal{K}^+_\sigma$ is non-empty for any $\sigma\in\Sigma$. Moreover, $\mathcal{K}^+_\Sigma$ can be embedded in a natural ambient space, namely:

$$\begin{aligned}\mathcal{F}^+_{\mathrm{loc}}\doteq\{&(\mathbf{u}(\,\cdot\,),\psi(\,\cdot\,),\mu(\,\cdot\,))\mid\\&\mathbf{u}\in L^p(0,T;\mathbf{V}_p)\cap L^\infty(0,T;\mathbf{L}^2_{0,\mathrm{div}}(\Omega))\cap W^{1,p'}(0,T;\mathbf{V}_p^*),\forall T>0,\\&\psi\in L^\infty(0,T;H^1_{(0)}(\Omega))\cap H^1(0,T;H^{-1}_{(0)}(\Omega)),\forall T>0,\\&f(\psi)\in L^2(0,T;L^6(\Omega)),\forall T>0,\\&\mu\in L^2(0,T;H^1(\Omega)),\forall T>0\}.\end{aligned}$$

Furthermore we introduce a suitable topology on the enveloping space $\mathcal{F}^+_{\mathrm{loc}}$, which will be inherited by the trajectory space. In this section we consider the following

Definition 2.6.3. The sequence $\{(\mathbf{u}_n, \psi_n, \mu_n)\}_{n\in\mathbb{N}} \subset \mathcal{F}^+_{\mathrm{loc}}$ is said to converge to $(\mathbf{u}, \psi, \mu) \in \mathcal{F}^+_{\mathrm{loc}}$ in the *local weak sequential topology* $\Theta^+_{w,\mathrm{loc}}$ if

$$\begin{aligned}
\mathbf{u}_n &\rightharpoonup \mathbf{u} && \text{in } L^p(0,T;\mathbf{V}_p)\\
\mathbf{u}_n &\overset{*}{\rightharpoonup} \mathbf{u} && \text{in } L^\infty(0,T;\mathbf{L}^2_{0,\mathrm{div}}(\Omega))\\
\partial_t\mathbf{u}_n &\rightharpoonup \partial_t\mathbf{u} && \text{in } L^{p'}(0,T;\mathbf{V}_p^*)\\
\psi_n &\overset{*}{\rightharpoonup} \psi && \text{in } L^\infty(0,T;H^1_{(0)}(\Omega))\\
\partial_t\psi_n &\rightharpoonup \partial_t\psi && \text{in } L^2(0,T;H^{-1}_{(0)}(\Omega))\\
\mu_n &\rightharpoonup \mu && \text{in } L^2(0,T;H^1(\Omega))
\end{aligned}$$

for all $T > 0$.

In what follows we will also assume that the family of trajectory space $\{\mathcal{K}^+_\sigma\}_{\sigma\in\Sigma}$ is *translation coordinated*, i.e. $T(t)\mathcal{K}^+_\sigma \subset \mathcal{K}^+_{T(t)\sigma}$, for all $t \geqslant 0$. This readily follows from the action of time shifts in equation (2.0.2) and from the definition of the translation semigroup $T(\cdot)$. Let us now introduce a notion of closedness in the space of trajectories.

Definition 2.6.4. The family of trajectory spaces $\{\mathcal{K}_\sigma\}_{\sigma\in\Sigma}$ is $(\Theta^+_{w,\mathrm{loc}}, \Sigma)$-*closed* if the set

$$\bigcup_{\sigma\in\Sigma} \mathcal{K}^+_\sigma \times \{\sigma\}$$

is closed in $\Theta^+_{w,\mathrm{loc}} \times \Sigma$ endowed with the standard product topology.

We can prove that our trajectory space is closed. Indeed we have

Lemma 2.6.2. *The trajectory space $\mathcal{K}^+_\sigma$, $\sigma \in \Sigma$ is $(\Theta^+_{w,\mathrm{loc}}, \Sigma)$-closed in $\mathcal{F}^+_{\mathrm{loc}}$.*

Proof. Let $\{(\mathbf{u}_n, \psi_n, \mu_n)\}_{n\in\mathbb{N}}$ be any sequence of solutions of (2.0.2) with symbol $\sigma_n \in \Sigma$ such that $(\mathbf{u}_n, \psi_n, \mu_n) \to (\mathbf{u}, \psi, \mu)$ in $\Theta^+_{w,\mathrm{loc}}$ and $\sigma_n \to \sigma$ in $L^2_{\mathrm{loc}}([0,\infty);\mathbf{H}^{-1}_{\mathrm{div}}(\Omega))$. We only have to show that $(\mathbf{u}, \psi, \mu)$ is a global weak solution to problem (2.0.2) with symbol σ.

Thanks to the regularity results of the previous sections we know that (up to subsequences) ψ_n converges to ψ weakly in $L^2(0,T;W^{2,6}_{(0)})$ and strongly in $L^4(0,T;W^{1,4}_{(0)}(\Omega))$ (see the proof of Theorem 2.5.1). Thus we can pass to the limit in the non-linear coupling term in the momentum equation. Moreover a standard estimate (see, e.g., Bulíček et al. (2010)) shows that

$$\left|\int_T\int_\Omega (\mathbf{u}\cdot\nabla)\mathbf{w}\cdot\boldsymbol{\phi}\,\mathrm{d}\mathbf{x}\mathrm{d}t\right| \leqslant |\boldsymbol{\phi}|_{p,\mathbf{V}_p}|\nabla\mathbf{w}|_{p,p}|\mathbf{u}|_{\frac{p}{p-2},\frac{3p}{4p-6}}.$$

From the weak convergence of $\mathbf{u}_n$ we know that $\{\mathbf{u}_n\}$ is bounded in $L^p(\mathbf{V}_p) \cap L^\infty(\mathbf{L}^2(\Omega))$ and, thanks to Aubin-Lions' lemma, it is also precompact in $L^2(\mathbf{L}^2)$ so that $\mathbf{u}_n \to \mathbf{u}$ strongly in $L^{\frac{p}{p-2}}(\mathbf{L}^{\frac{3p}{4p-6}}(\Omega))$ as soon as $p > \frac{11}{5}$. We can therefore pass to the limit also in the convective term of the momentum equation.

Possibly extracting a further subsequence, we can also assume that $\psi_n \to \psi$ a.e. $\Omega\times\mathbb{R}^+$ so that by the dominated convergence theorem ψ_n converges strongly to ψ in $L^q(L^q_{(0)}(\Omega))$ for all $q \in [1,\infty)$. We can therefore pass to the limit also in the convective term in the order parameter equation. From the equation for μ and the boundedness of μ_n in $L^2(H^1(\Omega))$ and of ψ_n in $L^2(W^{2,6}(\Omega))$, we deduce that $f(\psi_n)$ is bounded in $L^2(L^6(\Omega))$. Therefore, we also have $f(\psi_n) \rightharpoonup \chi$ in $L^2(L^6(\Omega))$ up to a subsequence. We want to show that $\chi = f(\psi)$. From the convergence of ψ_n to ψ a.e in $\Omega \times \mathbb{R}^+$, for a.e. $t > 0$ and any $m \in \mathbb{N}$ we can find a subset of measure $|\Omega| - \frac{1}{2m}$ on which $\psi_n \to \psi$ uniformly. Thanks to the regularity assumed for the potential F, for almost every time t and any $m \in \mathbb{N}$, we can also find $\delta > 0$ and a set of measure $|\Omega| - \frac{1}{2m}$ on which $|\psi| \leqslant 1 - \delta$. Therefore, for a.e. $t > 0$ we can find a subset of Ω of measure $|\Omega| - \frac{1}{m}$ on which $|\psi_n| \leqslant 1 - \frac{\delta}{2}$ definitively so that $f(\psi_n) \to f(\psi)$ a.e except on a set of measure $\frac{1}{m}$. By taking the union of such sets over m we deduce that $f(\psi_n) \to f(\psi)$ a.e. so that $f(\psi) = \chi$ by the uniqueness of weak and pointwise a.e. limits.

We still have to pass to the limit in the viscous part of the linear momentum equation. Thanks to the boundedness of $\boldsymbol{\tau}$ as an operator acting on $L^p(0,T;\mathbf{V}_p)$ into $L^{p'}(0,T;\mathbf{V}_p^*)$ for any $T > 0$, we can assume that $\boldsymbol{\tau}(\mathbf{u}_n,\psi)$ weakly converges to $\chi \in \mathbf{V}_p^*$ up to a subsequence. As in the proof of Theorem 2.5.1, using the continuity of $\boldsymbol{\tau}(D\mathbf{u},\varphi)$ with respect to φ (see estimate (2.5.4)), the uniform (w.r.t. φ) monotonicity of $\boldsymbol{\tau}(\,\cdot\,,\varphi)$ and the convergence of the other nonlinearities previously discussed (see (Lions, 1969, Chapter 2)), we can identify the limit point χ with $\boldsymbol{\tau}(D\mathbf{u},\psi)$ and pass to the limit in all the terms of the equation. Finally, a standard contradiction argument gives the convergence of the whole sequence. □

In addition, a straightforward consequence of the above definition of trajectory space and of the action of the semigroup $\{T(h)\}_{h\geqslant 0}$ on it is

Lemma 2.6.3. *The translation semigroup is continuous on the extended phase space* $\Theta^+_{w,\mathrm{loc}} \times \Sigma$.

Having defined the trajectory space and studied its main topological properties, we now introduce a suitable notion of dissipativity. We start by considering the linear subspace of $\mathcal{F}^+_{\mathrm{loc}}$ of uniformly bounded functions, $\mathcal{F}^+_{\mathrm{b}}$:

$$
\begin{aligned}
\mathcal{F}^+_{\mathrm{b}} \doteq \{&(\mathbf{u}(\,\cdot\,),\psi(\,\cdot\,),\mu(\,\cdot\,)) \mid \\
&\mathbf{u} \in L^p_{\mathrm{b}}([0,\infty);\mathbf{V}_p) \cap L^\infty([0,\infty);\mathbf{L}^2_{0,\mathrm{div}}(\Omega)) \cap W^{1,p'}_{\mathrm{b}}([0,\infty);\mathbf{V}_p^*),\\
&\psi \in L^\infty([0,\infty);H^1_{(0)}(\Omega)) \cap H^1_{\mathrm{b}}([0,\infty);H^{-1}_{(0)}(\Omega)),\\
&\mu \in L^2_{\mathrm{b}}([0,\infty);H^1(\Omega))\}
\end{aligned}
$$

endowed with the norm

$$\begin{aligned}&\|(\mathbf{u},\psi,\mu)\|_{\mathcal{F}^+_{\mathrm{b}}}\\ \doteq&\|\mathbf{u}\|_{L^p_{\mathrm{b}}([0,\infty);\mathbf{V}_p)}+\|\mathbf{u}\|_{L^\infty([0,\infty);\mathbf{L}^2(\Omega))}+\|\mathbf{u}\|_{W^{1,p'}_{\mathrm{b}}([0,\infty);\mathbf{V}^*_p)}\\ &+\|\psi\|_{L^\infty([0,\infty);H^1_{(0)}(\Omega))}+\|\psi\|_{H^1_{\mathrm{b}}([0,\infty);H^{-1}_{(0)}(\Omega))}+\|\mu\|_{L^2_{\mathrm{b}}([0,\infty);H^1(\Omega))}\end{aligned}$$

where we recall (see Section 1.4.2)

$$\|\chi\|_{L^p_{\mathrm{b}}(\mathbb{R}_+;X)}\doteq\sup_{t\geqslant 0}\left(\int_t^{t+1}\|\chi(s)\|_X^p\,\mathrm{d}s\right)^{1/p}.$$

Arguing as in the proof of Lemma 2.6.2 above, we immediately deduce that sets of trajectories bounded in $\mathcal{F}^+_{\mathrm{b}}$ are automatically compact in $\Theta^+_{w,\mathrm{loc}}$.We now introduce the main dissipativity notion for non-autonomous trajectory attractors.

Definition 2.6.5. A set $B_0\subset\Theta$ is *uniformly (w.r.t. $\sigma\in\Sigma$) absorbing* for the family of trajectory spaces $\{\mathcal{K}^+_\sigma\}_{\sigma\in\Sigma}$ in the topology Θ if for any set $B\subset\mathcal{K}^+_\Sigma$ bounded in $\mathcal{F}^+_{\mathrm{b}}$ there exists a time $t_1=t_1(B)>0$ such that $T(t)B\subset B_0$ for all $t\geqslant t_1$.

Lemma 2.6.4. *The set*

$$B_0\doteq\{(\mathbf{u},\psi,\mu)\in\mathcal{K}^+_\Sigma\mid\|(\mathbf{u},\psi,\mu)\|_{\mathcal{F}^+_{\mathrm{b}}}\leqslant R_0\}$$

where

$$R_0=C(\Omega,\beta,\nu)\left(\|\mathbf{g}\|_{L^2_{\mathrm{b}}(\mathbf{H}^{-1}_{\mathrm{div}})}+1\right)$$

is uniformly (w.r.t. $\sigma\in\Sigma$) absorbing for the trajectory space $\mathcal{K}^+_\Sigma$ in $\Theta^+_{w,\mathrm{loc}}$.

Proof. The proof consists in showing that, for a sufficiently large time, all the norm appearing in the definition of $\mathcal{F}^+_{\mathrm{b}}$ are bounded by a constant times $\|\mathbf{g}\|_{L^2_{\mathrm{b}}(\mathbf{H}^{-1}_{\mathrm{div}})}+1$. We start by applying Gronwall's lemma to the energy estimate (2.5.6) getting a suitable bound for $\mathbf{u}\in L^p_{\mathrm{b}}([0,\infty);\mathbf{V}_p)\cap L^\infty([0,\infty);\mathbf{L}^2_{0,\mathrm{div}}(\Omega))$, $\psi\in L^\infty([0,\infty);H^1_{(0)}(\Omega))$, $F(\psi)\in L^\infty([0,\infty);L^1(\Omega))$ and $\mu\in L^2_{\mathrm{b}}([0,\infty);H^1(\Omega))$. From this results we also deduce that also $E_P(\psi)$ is definitely bounded by a constant times $\|\mathbf{g}\|_{L^2_{\mathrm{b}}(\mathbf{H}^{-1}_{\mathrm{div}})}+1$.

Starting now from a sufficiently large time t, which however depends only on the norms of the original initial conditions and on the norm of the forcing term $\mathbf{g}$, Theorem 2.3.1 gives the desired estimates on $\psi\in L^2_{\mathrm{b}}([0,\infty);W^{2,6}_{(0)}(\Omega))\cap H^1_{\mathrm{b}}([0,\infty);H^{-1}_{(0)}(\Omega))$. Finally, directly from the equation for the linear momentum we can control the time derivative of $\mathbf{u}$ obtaining the absorbtion property for $\mathbf{u}\in W^{1,p'}_{\mathrm{b}}([0,\infty);\mathbf{V}^*_p)$. □

Moreover, on account of the preceding analysis, we have

Lemma 2.6.5. *The absorbing set B_0 defined above is positively invariant and compact.*

Proof. The invariance is an immediate consequence of the definition of B_0 and of the translation semigroup. In order to prove the compactness, we can repeat the same argument used in the proof of Lemma 2.6.2 above. □

We can now recall a couple of basic definitions (see Chepyzhov and Vishik (2002))

Definition 2.6.6. A set $B_1 \subset \Theta$ is *uniformly (w.r.t. $\sigma \in \Sigma$) attracting* for the family of trajectory spaces $\{\mathcal{K}_\sigma^+\}_{\sigma\in\Sigma}$ in the topology Θ if for any set $B \subset \mathcal{K}_\Sigma^+$ bounded in $\mathcal{F}_{\rm b}^+$ and for any neighbourhood $\mathcal{O}(B_1)$ of B_1 in Θ, there exists a time $t_1 = t_1(B, \mathcal{O}(B_1)) > 0$ such that $T(t)B \subset \mathcal{O}(B_1)$ for all $t \geqslant t_1$.

Definition 2.6.7. A set $\mathcal{A}_\sigma \subset \mathcal{K}^+$ is the *weak trajectory attractor* for problem (2.0.2) if

1. it is compact in $\Theta_{w,\rm loc}^+$ and bounded in $\mathcal{F}_{\rm b}^+$;
2. it is uniformly (w.r.t. $\sigma \in \Sigma$) attracting in $\Theta_{w,\rm loc}^+$;
3. is strictly invariant, i.e. $T(t)\mathcal{A}_\Sigma = \mathcal{A}_\Sigma$, $\forall t \geqslant 0$.

We can now recall the general existence result for the trajectory attractor of an abstract evolution equation

$$\partial_t u = A_{\sigma(t)}(u), \quad t \in \mathbb{R}. \tag{2.6.1}$$

Theorem 2.6.6 ((Chepyzhov and Vishik, 2002, Theorem XIV.3.1))**.** *Let Σ be a compact metric space and let a continuous translation group $\{T(t)\}_{t\in\mathbb{R}}$ act on Σ, $T(t)\Sigma \subset \Sigma$. Assume that the family of trajectory spaces $\{\mathcal{K}_\sigma^+\}_{\sigma\in\Sigma}$, $\mathcal{K}_\sigma^+ \subset \mathcal{F}_{\rm loc}^+$ corresponding to equation (2.6.1) is translation coordinated and $(\Theta_{w,\rm loc}^+, \Sigma)$-closed. Assume further that there exists a uniformly (w.r.t. $\sigma \in \Sigma$) absorbing set B for $\{\mathcal{K}_\sigma^+\}_{\sigma\in\Sigma}$ in $\Theta_{w,\rm loc}^+$ such that B is compact in $\Theta_{w,\rm loc}^+$ and bounded in $\mathcal{F}_{\rm b}^+$. Then the translation semigroup $\{T(t)\}_{t\geqslant 0}$ acting on $\mathcal{K}_\Sigma^+$ possesses the uniform (w.r.t. $\sigma \in \Sigma$) trajectory attractor $\mathcal{A}_\Sigma \subset \mathcal{K}_\Sigma^+ \cap B$.*

In our case we deduce

Theorem 2.6.7. *Let $\mathbf{g}(t)$ be translation compact in $L^2_{\rm loc}([0,\infty); \mathbf{H}^{-1}_{\rm div}(\Omega))$. Then system (2.0.2) has the uniform (with respect to $\sigma \in \Sigma = \mathcal{H}(\mathbf{g})$) trajectory attractor $\mathcal{A}_\Sigma$.*

Proof. The claim follows from Lemmata 2.6.2, 2.6.3, 2.6.4 and 2.6.5. □

2.7 A strong trajectory attractor

Here we exploit the energy equality (2.5.5) which allows us to use the argument devised in Vishik et al. (2010), to prove that the weak trajectory attractor actually attracts trajectories with respect to the strong topology. More precisely, the attraction property also holds in the strong local convergence topology defined below.

Definition 2.7.1. A sequence $\{(\mathbf{u}_n, \psi_n, \mu_n)\}_{n\in\mathbb{N}} \subset \mathcal{F}^+_{\rm loc}$ converges to $(\mathbf{u}, \psi, \mu) \in \mathcal{F}^+_{\rm loc}$ in the *strong local convergence topology* $\Theta^+_{s,\rm loc}$ if, for any $T > 0$, we have

$$\lim_{n\to\infty} \|\mathbf{u}_n - \mathbf{u}\|_{L^p(0,T;\mathbf{V}_p)} = 0, \qquad \lim_{n\to\infty} \|\partial_t \mathbf{u}_n - \partial_t \mathbf{v}\|_{L^{p'}(0,T;\mathbf{V}^*_p)} = 0$$
$$\lim_{n\to\infty} \|\psi_n - \psi\|_{L^2(0,T;H^1_{(0)}(\Omega))} = 0, \qquad \lim_{n\to\infty} \|\partial_t \psi_n - \partial_t \psi\|_{L^2(0,T;H^{-1}_{(0)}(\Omega))} = 0$$
$$\lim_{n\to\infty} \|\mu_n - \mu\|_{L^2(0,T;H^1(\Omega))} = 0.$$

Indeed, we now prove the following

Theorem 2.7.1. *Let $\mathbf{g}(t)$ be translation compact in $L^2_{\rm loc}([0,\infty);\mathbf{H}^{-1}_{\rm div}(\Omega))$. Then the uniform (w.r.t. $\sigma \in \Sigma = \mathcal{H}(\mathbf{g})$) trajectory attractor $\mathcal{A}_\Sigma$ is the strong uniform (w.r.t. $\sigma \in \Sigma = \mathcal{H}(\mathbf{g})$) trajectory attractor, i.e. it attracts trajectories in the strong topology $\Theta^+_{s,\rm loc}$.*

Proof. In order to prove this result it is sufficient to show that, whenever $\{(\mathbf{u}_n, \psi_n, \mu_n)\}_{n\in\mathbb{N}} \subset B_0$ is a weakly convergent sequence of solutions of equation (2.0.2), then it also converges strongly for sufficiently large times. Indeed, if this is true, the weak compactness of the attractor implies its compactness in the strong topology $\Theta^+_{s,\rm loc}$ and the weak attraction property is carried over to the strong topology as well.

Therefore, the proof reduces to showing that, whenever $\{(\mathbf{u}_n, \psi_n, \mu_n)\}_{n\in\mathbb{N}} \subset B_0 \cap \mathcal{K}^+_\Sigma$ weakly converges to $(\widehat{\mathbf{u}}, \widehat{\psi}, \widehat{\mu})$, then $T(1)(\mathbf{u}_n, \psi_n, \mu_n) \to T(1)(\widehat{\mathbf{u}}, \widehat{\psi}, \widehat{\mu})$ strongly on any bounded interval sufficiently far from the origin. In the computations below for the sake of simplicity we will consider the time interval $[1, 2]$.

We now multiply (2.5.5) by the time t and integrate it from 0 to 2 obtaining, for all $n \in \mathbb{N}$,

$$2E(\psi_n(2), \mathbf{u}_n(2)) - \frac{1}{2}\int_0^2 |\mathbf{u}_n|_2^2 \,\mathrm{d}t - \frac{1}{2}\int_0^2 |\nabla\psi_n|_2^2 \,\mathrm{d}t - \int_0^2\int_\Omega F(\psi_n)\,\mathrm{d}\mathbf{x}\mathrm{d}t$$
$$+ \int_0^2 t\langle \boldsymbol{\tau}(D\mathbf{u}_n, \psi_n), D\mathbf{u}_n\rangle \,\mathrm{d}t + \int_0^2\int_\Omega t f(\psi_n)\psi_n \,\mathrm{d}\mathbf{x}\mathrm{d}t + \int_0^2 t|\nabla\mu_n|_2^2 \,\mathrm{d}t$$
$$+ \int_0^2 t|\nabla\psi_n|_2^2 \,\mathrm{d}t = \int_0^2 t\langle \mathbf{g}_n(t), \mathbf{u}_n\rangle \,\mathrm{d}t + \int_0^2 t\,(\mu_n, \psi_n)\,\mathrm{d}t. \quad (2.7.1)$$

We observe that the limit solution $(\widehat{\mathbf{u}}, \widehat{\psi}, \widehat{\mu})$ satisfies an analogous identity.

We now want to pass to the limit in (2.7.1). We recall that, on account of the regularity of weak solutions, using Aubin-Lions' compactness lemma and the dominated convergence theorem,

the first three integrals on the left hand side of (2.7.1) converge to their limiting counterparts. Arguing as in the proof of Lemma 2.6.2 we deduce that $f(\psi_n)$ is bounded in $L^2(L^6)$. By the strong convergence of ψ_n in $L^2(L^2)$ we see that we can also pass to the limit in the other term arising from the potential F. By compactness we can also easily pass to the limit in the two terms on the right hand side of (2.7.1). Therefore, only the following four terms are left

$$|\mathbf{u}_n(2)|_2^2, \qquad |\nabla\psi_n(2)|_2^2, \qquad \int_0^2 t|\nabla\mu_n|_2^2\,\mathrm{d}t, \qquad \int_0^2 t\,\langle\boldsymbol{\tau}(D\mathbf{u}_n,\psi_n),D\mathbf{u}_n\rangle\,\mathrm{d}t.$$

Thanks to the monotonicity of $\boldsymbol{\tau}$ we have for a.e. $(\mathbf{x},t)\in\Omega\times[0,2]$

$$(\boldsymbol{\tau}(D\mathbf{u}_n,\psi_n)-\boldsymbol{\tau}(D\hat{\mathbf{u}},\psi_n)):(D\mathbf{u}_n-D\hat{\mathbf{u}})\geqslant 0.$$

Multiplying by t, integrating on $\Omega\times[0,2]$ and using Lemma 2.1.1, we deduce

$$\int_0^2 t\left\langle\boldsymbol{\tau}(D\hat{\mathbf{u}},\widehat{\psi}),D\hat{\mathbf{u}}\right\rangle\,\mathrm{d}t\leqslant\liminf_{n\to\infty}\int_0^2 t\,\langle\boldsymbol{\tau}(D\mathbf{u}_n,\psi_n),D\mathbf{u}_n\rangle\,\mathrm{d}t.$$

Analogously, from the weak lower semicontinuity of norms we deduce

$$\int_0^2 t|\nabla\widehat{\mu}|_2^2\,\mathrm{d}t\leqslant\liminf_{n\to\infty}\int_0^2 t|\nabla\mu_n|_2^2\,\mathrm{d}t$$

$$|\hat{\mathbf{u}}(2)|_2^2\leqslant\liminf_{n\to\infty}|\mathbf{u}_n(2)|_2^2$$

$$|\nabla\widehat{\psi}(2)|_2^2\leqslant\liminf_{n\to\infty}|\nabla\psi_n(2)|_2^2$$

In order to conclude the proof we need the following elementary lemma

Lemma 2.7.2. *Let $\{a_n\}_{n\in\mathbb{N}}$ and $\{b_n\}_{n\in\mathbb{N}}$ be sequences of real numbers such that*

$$a\leqslant\liminf_{n\to\infty}a_n\qquad b\leqslant\liminf_{n\to\infty}b_n$$

and

$$\lim_{n\to\infty}a_n+b_n=a+b.$$

Then

$$\lim_{n\to\infty}a_n=a,\qquad\lim_{n\to\infty}b_n=b.$$

Applying this result to the sum

$$|\mathbf{u}_n(2)|_2^2+|\nabla\psi_n(2)|_2^2+\int_0^2 t|\nabla\mu_n|_2^2\,\mathrm{d}t+\int_0^2 t\,\langle\boldsymbol{\tau}(D\mathbf{u}_n,\psi_n),D\mathbf{u}_n\rangle\,\mathrm{d}t$$

appearing on the left hand side of (2.7.1) we deduce

$$\lim_{n\to\infty}|\mathbf{u}_n(2)|_2^2=|\hat{\mathbf{u}}(2)|_2^2$$

$$\lim_{n\to\infty}|\nabla\psi_n(2)|_2^2=|\nabla\widehat{\psi}(2)|_2^2$$

$$\lim_{n\to\infty}\|\nabla\mu_n\|_{L^2_t(0,2;\mathbf{L}^2(\Omega))}=\|\nabla\mu\|_{L^2_t(0,2;\mathbf{L}^2(\Omega))}$$

$$\lim_{n\to\infty}\int_0^2 t\,\langle\boldsymbol{\tau}(D\mathbf{u}_n,\psi_n),D\mathbf{u}_n\rangle\,\mathrm{d}t=\int_0^2 t\left\langle\boldsymbol{\tau}(D\hat{\mathbf{u}},\widehat{\psi}),D\hat{\mathbf{u}}\right\rangle\,\mathrm{d}t.$$

The last limit and the assumptions on the stress tensor, combined again with Lemma 2.1.1 (see Bulíček et al. (2010)), give

$$\int_0^2 t|\nabla \mathbf{u}_n - \nabla \hat{\mathbf{u}}|_p^p \, dt \leqslant \int_{\Omega\times[0,2]} t(\boldsymbol{\tau}(D\mathbf{u}_n, \psi_n) - \boldsymbol{\tau}(D\hat{\mathbf{u}}, \widehat{\psi})) : (D\mathbf{u}_n - D\hat{\mathbf{u}}) \, \mathrm{d}\mathbf{x} \, dt$$
$$+ \int_{\Omega\times[0,2]} t(\boldsymbol{\tau}(D\hat{\mathbf{u}}, \widehat{\psi}) - \boldsymbol{\tau}(D\hat{\mathbf{u}}, \psi_n)) : (D\mathbf{u}_n - D\hat{\mathbf{u}}) \, \mathrm{d}\mathbf{x} \, dt$$

where the right hand side converges to zero as $n \to \infty$. Thus, on account of the uniform convexity of the Bochner spaces involved (see, e.g., (Brezis, 2011, Proposition 3.32) we can deduce the desired strong convergences on the time interval $[0, 2]$ with weight t. However, we note that this weight is nondegenerate on $[1, 2]$ so that the strong convergence holds in the original un-weighted space on the interval of interest $[1, 2]$. Finally, by the arbitrariness of $t = 2$ as upper bound in the time integration, we also infer the strong convergence of $\mathbf{u}_n$ in $L^\infty_{\mathrm{loc}}(1, \infty; \mathbf{L}^2_{0,\mathrm{div}}(\Omega))$ thanks to the continuous injection $L^p(\mathbf{V}_p) \cap L^{p'}(\mathbf{V}_p^*) \hookrightarrow \mathbf{C}(\mathbf{L}^2_{0,\mathrm{div}}(\Omega))$. Also we can immediately deduce the strong convergence and of ψ_n in $L^2_{\mathrm{loc}}(1, \infty; H^1_{(0)}(\Omega))$. □

Remark 2.7.1. Actually, one can show a slightly stronger convergence for the order parameter field. Indeed, by recalling the results of the previous section we know that the trajectory attractor attracts the ψ component of solutions also in the weak-$*$ topology of $L^\infty([0, \infty); H^1_{(0)})$. By standard interpolation results we have

$$\|\psi_n - \psi\|_{L^p(H^1_{(0)})} \leqslant C\|\psi_n - \psi\|^{\frac{2}{p}}_{L^2(H^1_{(0)})} \|\psi_n - \psi\|^{\frac{p-2}{p}}_{L^\infty(H^1_{(0)})}$$

so that strong attraction in $L^p_{\mathrm{loc}}([0, \infty); H^1_{(0)})$ for any $p \in [2, \infty)$ for the order parameter field ψ is easily seen to hold.

Remark 2.7.2. A more subtle question seems to be whether the attraction of the order parameter field holds also in the strong topology of $L^\infty([0, \infty); H^1_{(0)})$ or not. This would be implied by some additional time-regularity (e.g. Hölder continuity) of the order parameter field seen as a continuous function of time with values in $H^1_{(0)}$. However, this regularity seems to be out of reach on account of our present knowledge.

This chapter has been dedicated to the study of a particular variation on the model H, accounting for non-Newtonian fluid dynamics of the fluid mixture described. As discussed, the incomplete knowledge on the uniqueness of weak solutions led us to using trajectory attractors theory in order to give a description of the long term behaviour of solutions of system (2.0.2). We now wish to bring our attention back to the original model H on a bounded domain in $\mathbb{R}^2$ and study the behaviour of its solutions under the action of non-autonomous forcing bulk force. In doing this we will assume a regular double-well potential and we will pay special care in dealing with its growth at infinity. This will lead us to the use of the theory of exponential pullback attractors, which will also be reviewed in the next chapter.

Bibliography

Abels, H. (2009). On a diffuse interface model for two-phase flows of viscous, incompressible fluids with matched densities. *Arch. Ration. Mech. Anal.*, 194(2):463–506.

Brezis, H. (2011). *Functional analysis, Sobolev spaces and partial differential equations*. Universitext. Springer.

Bulíček, M., Ettwein, F., Kaplický, P., & Pražák, D. (2010). On uniqueness and time regularity of flows of power-law like non-Newtonian fluids. *Math. Methods Appl. Sci.*, 33(16):1995–2010.

Chepyzhov, V. V. & Vishik, M. I. (1997). Evolution equations and their trajectory attractors. *J. Math. Pures Appl. (9)*, 76(10):913–964.

Chepyzhov, V. V. & Vishik, M. I. (2002). *Attractors for equations of mathematical physics*, volume 49 of *American Mathematical Society Colloquium Publications*. American Mathematical Society.

Colli, P., Frigeri, S., & Grasselli, M. (2012). Global existence of weak solutions to a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Math. Anal. Appl.*, 386(1):428–444.

Colli, P., Krejčí, P., Rocca, E., & Sprekels, J. (2007). Nonlinear evolution inclusions arising from phase change models. *Czechoslovak Math. J.*, 57(132)(4):1067–1098.

Fabes, E., Mendez, O., & Mitrea, M. (1998). Boundary layers on Sobolev-Besov spaces and Poisson's equation for the Laplacian in Lipschitz domains. *J. Funct. Anal.*, 159(2):323–368.

Feireisl, E. & Pražák, D. (2010). *Asymptotic behavior of dynamical systems in fluid mechanics*, volume 4 of *AIMS Series on Applied Mathematics*. American Institute of Mathematical Sciences (AIMS), Springfield, MO.

Foias, C. & Temam, R. (1987). The connection between the navier-stokes equations, dynamical systems, and turbulence theory. *Directions in partial differential equations*, pages 55–73.

Grasselli, M. & Pražák, D. (2011). Longtime behavior of a diffuse interface model for binary fluid mixtures with shear dependent viscosity. *Interfaces Free Bound.*, 13:507–530.

Kim, N., Consiglieri, L., & Rodrigues, J. F. (2006). On non-Newtonian incompressible fluids with phase transitions. *Math. Methods Appl. Sci.*, 29(13):1523–1541.

Ladyzhenskaya, O. (1967). New equations for the description of the motions of viscous incompressible fluids, and global solvability for their boundary value problems. *Trudy Matematicheskogo Instituta im. VA Steklova*, 102:85–104.

Lions, J.-L. (1969). *Quelques méthodes de résolution des problèmes aux limites non linéaires*. Dunod.

Málek, J., Nečas, J., & Ružička, M. (2001). On weak solutions to a class of non-Newtonian incompressible fluids in bounded three-dimensional domains: the case $p \geqslant 2$. *Adv. Differential Equations*, 6(3):257–302.

Sell, G. R. (1996). Global attractors for the three-dimensional Navier-Stokes equations. *J. Dynam. Differential Equations*, 8(1):1–33.

Vishik, M. I., Zelik, S. V., & Chepyzhov, V. V. (2010). A strong trajectory attractor for a dissipative reactor-diffusion system. *Dokl. Akad. Nauk*, 435(2):155–159.

CHAPTER 3

Pullback exponential attractors for a Cahn-Hilliard-Navier-Stokes system in $2D$

Outline

We consider a model for the evolution of a mixture of two incompressible and partially immiscible Newtonian fluids in a two dimensional bounded domain. More precisely, we address the well-known model H consisting of the Navier-Stokes equation with non-autonomous external forcing term for the (average) fluid velocity, coupled with a convective Cahn-Hilliard equation with polynomial double-well potential describing the evolution of the relative density of atoms of one of the fluids. We study the long term behavior of solutions and prove that the system possesses a pullback exponential attractor. In particular, the regularity estimates we obtain depend on the initial data only through fixed powers of their norms and these powers are uniform with respect to the growth of the polynomial potential considered in the Cahn-Hilliard equation.

We started the previous chapter by introducing a possible variation on the model H, useful to describe shear-thickening fluids. We ended our analysis of the system considered there by proving the existence of trajectory attractors in a suitable sense. Resort to this technique was motivated by partial knowledge on the well-posedness of the system and in particular by the lack of definite information concerning the uniqueness of weak solutions to the system considered.

We now take a break from the flow of "variations" on the model H. In this chapter we want to

give some insight on a different possible approach to the description of the long-term dynamics of an evolution system. In particular, we are interested in studying the Cahn-Hilliard-Navier-Stokes equations with a non-autonomous forcing term. In doing this, we will use the theory of pullback exponential attractors. This is a new instrument recently introduced in the literature (see Langa et al. (2010)). The related theory combines both the advantages of pullback attractors for non-autonomous dynamical systems (cf. Section 1.3.4 for a quick overview on this approach and Carvalho et al. (2013) for a comprehensive introduction to the theory of pullback attractors) and of the exponential attractors in Banach spaces in their most general form known today (see Efendiev et al. (2000) and cf. Section 1.3.3).

More precisely, given a bounded and smooth domain $\Omega \subset \mathbb{R}^2$, assuming that the viscosity of the mixture is a constant $\nu > 0$, we will consider the system (cf. equation (1.1.6))

$$\begin{cases} \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = \nabla \pi + \mu \nabla \psi + \mathbf{g}, & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = 0, & \text{in } \Omega, \\ \partial_t \psi + (\mathbf{u} \cdot \nabla)\psi = M \Delta \mu, & \text{in } \Omega, \\ \mu = -\varepsilon \Delta \psi + \frac{1}{\varepsilon} f(\psi), & \text{in } \Omega. \end{cases} \tag{3.0.1}$$

As in Chapter 1, here μ is the so called chemical potential with constant mobility $M \geqslant 0$, $\mathbf{g}$ is a time-dependent bulk force, f is the derivative of a double-well potential F while π is the pressure. In particular, as we discussed in Section 1.1, ϵ is related with the small but not negligible thickness of the interface.

As usual, we complement this system with homogeneous Dirichlet boundary conditions on the velocity field, no flux boundary conditions on the order parameter field and chemical potential, namely,

$$\mathbf{u} = \mathbf{0}, \quad \partial_{\mathbf{n}} \psi = 0 \quad \text{and} \quad \partial_{\mathbf{n}} \mu = 0, \qquad \text{on } \partial\Omega. \tag{3.0.2}$$

Being the problem non-autonomous, we specify the initial values at a given time $\tau \in \mathbb{R}$ for the state variables, that is,

$$\mathbf{u}(\tau) = \mathbf{u}_0, \qquad \psi(\tau) = \psi_0, \qquad \text{in } \Omega$$

and assume that (3.0.1) holds in $Q_{\tau,T}$ for $T > \tau$ (with T possibly equal to $+\infty$). We recall that, in this model, the chemical potential of the binary mixture μ is given by the variational derivative of the free energy functional for the Cahn-Hilliard equation (cf. equation (1.1.1))

$$E_P(\psi) \doteq \int_\Omega \left(\frac{\varepsilon}{2} |\nabla \psi(\mathbf{x})|^2 + \frac{1}{\varepsilon} F(\psi(\mathbf{x})) \right) \mathrm{d}\mathbf{x},$$

where $F(\psi)$ is a suitable double-well potential characterizing the phase decomposition of the mixture. Since $F' = f$, the fourth equation in (3.0.1) follows.

In the original setting of spinodal decomposition and coarsening during quenching of alloys, the thermodynamically consistent double-well potential F appearing in the Cahn-Hilliard equation is naturally seen to be logarithmic (see Cahn (1961) and references therein). However, this singular form for the potential causes major difficulties in the numerical and theoretical study of the Cahn-Hilliard system so that in applications it is often replaced by a polynomial approximation like

$$F(\psi) = C(1-\psi^2)^2.$$

In this context, a possible approach to deal with the physically relevant case consists in suitably approximating the singular potential by polynomials of increasing order (see Frigeri and Grasselli (2012a,b) for an application of this technique to a system closely related to the model H). In this chapter we consider a polynomial potential F of arbitrary order $p+3$, for $p \geqslant 1$ (in fact, lower order growth are much easier to analyse) and focus on the dependence on the exponent p of the a priori estimates relevant for system (3.0.1).

The main result in this chapter is the proof of existence of a pullback exponential attractor for the system (3.0.1)-(3.0.2). As a byproduct, we derive several regularity estimates for the solutions to the Cahn-Hilliard-Navier-Stokes system. These have an interest of their own due to their uniform structure with respect to the growth of the double-well potential F. Indeed, if the potential $f(\psi)$ is assumed to satisfy $|f(\psi)| \leqslant C(|\psi|^{p+2}+1)$, we are able to control the solutions only by suitable powers of the norms of the initial data independent of p. This is not an easy task since the computations repeatedly involve $f(\psi)$ and its derivatives, which are naturally estimated as

$$|f(\psi)|_q \leqslant C(|\psi|_\infty^{p+2}+1) \leqslant C(|\psi|_2^{(p+2)/2}|\Delta\psi|_2^{(p+2)/2}+1),$$

carrying the polynomial character of F directly into play. This obstacle is circumvented by suitably handling the nonlinear terms so that the dependence on the "shape" of the potential is confined to the multiplicative constants appearing in our results.

Therefore, these estimates can be seen as a preliminary step forwards an effective approximating procedure able to deal with the more physically relevant case given by the singular potential.

The plan of the chapter goes as follows. In Section 3.1 we introduce the functional setting required to study system (3.0.1) and the main results obtained in this chapter. After recalling the theory of pullback exponential attractors in Section 3.2, we first derive basic energy estimates (Section 3.3) and then higher order regularity estimates (Section 3.4): in particular, our results are uniform w.r.t. the shape of F in the sense made precise above. We then derive continuity results and time regularity for solutions in Sections 3.5 and 3.6. Finally, in Section 3.7 we are able to check for system (3.0.1) all the assumptions of the abstract results of Section 3.2, thus concluding the proof of our main theorem.

3.1 Functional setting and main results

In this chapter, Ω will be a smooth bounded domain of $\mathbb{R}^2$. In order to study the velocity field $\mathbf{u}$ we introduce the usual space of divergence-free test functions

$$\mathcal{V}_0 \doteq \{\boldsymbol{\phi} \in \mathbf{C}_c^\infty(\Omega;\mathbb{R}^2) \mid \nabla\cdot\boldsymbol{\phi} = 0\}.$$

and the related distribution spaces $\mathbf{L}^2_{0,\mathrm{div}}(\Omega)$ and $\mathbf{H}^1_{0,\mathrm{div}}(\Omega)$ (cf. Section 1.4.2. We also introduce the Leray projector $\mathbb{P}\colon \mathbf{L}^2(\Omega) \to \mathbf{L}^2_{0,\mathrm{div}}(\Omega)$ mapping every element of $\mathbf{L}^2(\Omega)$ to its divergence-free part. Furthermore, we will indicate by $\mathbf{H}^{-1}_{\mathrm{div}}(\Omega)$ the dual space of $\mathbf{H}^1_{0,\mathrm{div}}(\Omega)$. In $H^1_0(\Omega)$ and $\mathbf{H}^1_{0,\mathrm{div}}(\Omega)$ we will consider the following norms

$$\|f\|^2_{H^1_0(\Omega)} \doteq |\nabla f|_2^2 = \sum_{i=1}^n \int_\Omega |f_{,i}|^2 \,\mathrm{d}\mathbf{x} \qquad \|\mathbf{f}\|^2_{\mathbf{H}^1_{0,\mathrm{div}}(\Omega)} \doteq |\nabla \mathbf{f}|_2^2 = \sum_{i,j=1}^n \int_\Omega |\mathbf{f}_{i,j}|^2 \,\mathrm{d}\mathbf{x}.$$

Since the second equation in (3.0.1) together with the boundary condition imply that the bulk integral of the order parameter is preserved by the evolution, we need to suitably account for this feature. We recall from Section 1.4.2 the notation for the mean value of f over the domain Ω

$$\langle f\rangle \doteq \frac{1}{|\Omega|}\int_\Omega f \,\mathrm{d}\mathbf{x},$$

and the definition of its mean free part

$$\overline{f} \doteq f - \langle f\rangle.$$

Without loss of generality, only a shift of the order parameter field being required, we can always assume that the mean of ψ is zero at the initial time and, due to the conservation of mass enforced by the Neumann boundary conditions, this will remain true for all positive times. Then the order parameter will belong to the spaces $L^p_{(0)}(\Omega)$ and $H^k_{(0)}(\Omega)$ consisting of functions with zero mean.

We will use Poincaré's inequality (and some of its variants) at several stages when estimating the Sobolev norms of ψ. Indeed, the boundary conditions and the above definitions imply that

$$\int_\Omega \psi = 0, \quad \partial_{\mathbf{n}}\psi = 0 \text{ on } \partial\Omega, \quad \int_\Omega \Delta\psi = \int_{\partial\Omega} \partial_{\mathbf{n}}\psi = 0, \quad \partial_{\mathbf{n}}\Delta\psi = 0 \text{ on } \partial\Omega.$$

Therefore, all the norms $\|\psi\|_{H^j}$, $j = 1,\dots,4$ are equivalent to the L^2-norms of the derivatives of order j. Moreover, Korn's inequality holds. Thus we have

$$\|\psi\|_{H^1} \sim |\nabla\psi|_2, \quad \|\psi\|_{H^2} \sim |\Delta\psi|_2, \quad \|\psi\|_{H^3} \sim |\nabla\Delta\psi|_2, \quad \|\psi\|_{H^4} \sim |\Delta^2\psi|_2.$$

Finally, the functional spaces for the whole solution $(\mathbf{u},\psi)$ are

$$\mathcal{H}_0 \doteq \mathbf{L}^2_{\mathrm{div}}(\Omega) \times H^1_{(0)}(\Omega) \qquad \mathcal{H}_1 \doteq \mathbf{H}^1_{0,\mathrm{div}}(\Omega) \times H^2_{(0)}(\Omega),$$

which arise naturally in the study of the process generated by the solution of system (3.0.1).

We can now list the assumptions on the potential $F(\psi)$, which will be used in this chapter. We start with some hypotheses concerning its regularity and growth:

(A.1) $F \in \mathbf{C}^5(\mathbb{R})$.

(A.2) $F(y)$ grows at most polynomially fast at infinity, namely

$$|f''(y)| \leqslant C_f(1 + |y|^p),$$

for some positive constants p and C_f.

(A.3) The potential is coercive, i.e. there exist positive real numbers q and c_f such that

$$F(y) \geqslant c_f \left(|y|^{2+q} - 1\right)$$

holds for all $y \in \mathbb{R}$.

Recalling that the potential F appears in system (3.0.1) only through its derivative, without loss of generality we can further assume that

(A.4) the functional F is strictly positive, i.e. $F(y) > 0$, $\forall y \in \mathbb{R}$.

We now give some additional assumptions concerning the shape of the double-well potential F.

(A.5) $F(y)$ is a quadratic perturbation of a regular convex function defined on the whole $\mathbb{R}$, that is,

$$F(y) = F_0(y) - \alpha y^2 + \gamma y + \beta,$$

where $F_0 \in \mathbf{C}^5(\mathbb{R})$ is convex and $\alpha \in \mathbb{R}$ is a positive constant.

(A.6) Up to a suitable choice of the constants β and γ in Assumption (A.5), the convex part of the potential F_0 satisfies:

$$F_0(0) = F_0'(0) = 0.$$

In order to obtain higher order estimates having uniform structure with respect to the growth of f, we will assume that F behaves as a polynomial at infinity. In particular we will suppose

(A.7) The relation $q = p + 1$ holds in Assumptions (A.2) and (A.3). Moreover, for any $k = 0, 1, 2, 3, 4$ there exists a positive constant c_k such that

$$|f^{(k)}(y)| \leqslant c_k[1 + F(y)^{(p+2-k)/(p+3)}], \quad \forall y \in \mathbb{R}. \tag{3.1.1}$$

Remark 3.1.1. We will use Assumption (A.7) in order to estimate the L^r norm of the derivatives of the potential F in terms of some L^s norm of the potential itself. In particular, when dealing with higher order estimates we will often use the immediate consequence of Assumption (A.7)

$$|f^{(k)}(\psi)|^{\frac{(p+3)/(p+2-k)}{p+3}}_{p+2-k} \leqslant C(1+|F(\psi)|_1),$$

for any ψ such that $F(\psi) \in L^1(\Omega)$ and for some constant C depending on k and Ω.

Remark 3.1.2. Throughout this chapter, we will always assume that $p \geqslant 2$, being much easier the case when the potential $F(y)$ grows at most as y^5 at infinity. In particular, all estimates in the following sections hold for $p \geqslant 1$, except for (3.5.5) below. However, note that a suitable estimate for this term can be produced also in the case $p \in [1,2)$ (cf. Remark 3.5.1) under the assumption

$$f^{(iv)}(y) \leqslant C \qquad \forall y \in \mathbb{R}.$$

The case $p = 1$ is particularly relevant for applications since the polynomial potential $F(y) = (y^2-1)^2$, which is often used in numerical simulations, falls in this setting.

Finally, we assume the non-autonomous forcing term (symbol) $\mathbf{g}$ appearing in equation (3.0.1) satisfies the following conditions:

(B.1) $\mathbf{g} \in L^2_{\mathrm{loc}}(\mathbb{R}; \mathbf{L}^2_{\mathrm{div}}(\Omega))$.

(B.2) $\mathbf{g} \in L^2_{\mathrm{uloc}}(-\infty, t; \mathbf{L}^2_{\mathrm{div}}(\Omega))$, for any $t \in \mathbb{R}$, that is,

$$M_{\mathbf{g}}(t) \doteq \sup_{r \leqslant t} \int_{r-1}^{r} |\mathbf{g}(s)|_2^2 \, \mathrm{d}s < \infty, \quad \forall t \in \mathbb{R}.$$

(B.3) There exist $t_0 \in \mathbb{R}$ and $q > 2$ such that $\mathbf{g} \in L^q_{\mathrm{uloc}}(-\infty, t_0; \mathbf{L}^2_{\mathrm{div}}(\Omega))$, namely,

$$M_{\mathbf{g},q}(t_0) \doteq \sup_{r \leqslant t_0} \int_{r-1}^{r} |\mathbf{g}(s)|_2^q \, \mathrm{d}s < \infty.$$

In this chapter we will prove the following main results:

Theorem 3.1.1. *Assume that* $\mathbf{g}$ *satisfies (B.1) and (B.3) and let* $U_{\mathbf{g}}(t,\tau)\colon \mathcal{H}_0 \to \mathcal{H}_0$ *be the solution operator for the system* (3.0.1)*. Then there exists a family* $\widetilde{\mathcal{M}}_{U_{\mathbf{g}}} = \{\widetilde{\mathcal{M}}_{U_{\mathbf{g}}}(t)\colon t \leqslant t_0\}$ *of nonempty compact subsets of* $\mathcal{H}_1$*, which is a pullback exponential attractor for system* (3.0.1) *(see Theorem 3.2.2 below) in the topology of* $\mathcal{H}_1$*.*

Corollary 3.1.2. *Under the same assumptions of Theorem 3.1.1, if, moreover,* $\mathbf{g}$ *satisfies (B.3) uniformly for* $t_0 \in \mathbb{R}$ *(as in (B.2)), then the process* $U_{\mathbf{g}}(t,\tau)\colon \mathcal{H}_1 \to \mathcal{H}_1$ *has a family* $\widetilde{\mathcal{M}}_{U_{\mathbf{g}}} = \{\widetilde{\mathcal{M}}_{U_{\mathbf{g}}}(t)\colon t \in \mathbb{R}\}$ *of nonempty compact subsets of* $\mathcal{H}_1$*, which is a pullback exponential attractor for system* (3.0.1) *(see Theorem 3.2.3 below) in the topology of* $\mathcal{H}_1$*.*

3.2 Exponential pullback attractors

In this section we briefly review the theory of exponential pullback attractors as developed in Langa et al. (2010). Below, $(H, |\cdot|)$ and $(V, \|\cdot\|)$ will be two Banach spaces such that V is compactly embedded in H. Both spaces have a metric structure therefore, given any two nonempty subsets D_1, D_2 of the metric space $X = H, V$, the Hausdorff semidistance and distance are well defined respectively as

$$\mathrm{dist}_X(D_1, D_2) \doteq \sup_{v_1 \in D_1} \inf_{v_2 \in D_2} \|v_1 - v_2\|_X$$

and

$$\mathrm{dist}_X^{\mathrm{sym}}(D_1, D_2) \doteq \max\{\mathrm{dist}_X(D_1, D_2), \mathrm{dist}_X(D_2, D_1)\}.$$

As in the usual case of exponential attractors (cf. Efendiev et al. (2000)) the key point of the argument is the introduction of a set of mappings which enjoy a suitable "smoothing property" (see also Section 1.3.3). This is responsible for the exponential convergence of the trajectories of the system to an exponentially attracting finite-dimensional compact set (an exponential attractor) as soon as the trajectories have entered a sufficiently small neighbourhood of the attractor itself. Let $\delta, K \in \mathbb{R}$ be positive constants and let B be a bounded and closed subset of V. Define $\mathbb{S}_{\delta,K}(B)$ to be the class of mappings $S\colon V \to V$ such that the smoothing property holds on a δ-neighbourhood (in V) of B, i.e.

$$S(\mathcal{O}_\delta(B)) \subset B$$

and

$$\|Sv_1 - Sv_2\| \leqslant K|v_1 - v_2| \qquad \text{for all } v_1, v_2 \in \mathcal{O}_\delta(B),$$

where $\mathcal{O}_\delta(B) \doteq \{v \in V \mid \inf_{w \in B} \|v - w\| < \delta\}$ is a δ-neighbourhood of the set B in V.

We introduce a suitable class of family of mappings, which are the abstract, discrete-time, dynamical system representation of the evolution equations we will be interested in. In particular, let $n_0 \in \mathbb{Z}$ be fixed and consider the class $\mathcal{U}_d(V, n_0)$ of all families $U = \{U(m, n) \mid n, m \in \mathbb{Z}, n \leqslant m \leqslant n_0\}$ of mappings $U(m, n)\colon V \to V$ such that

1. $U(n, n) = Id$ for all $n \leqslant n_0$;
2. $U(m, k)U(k, n) = U(m, n)$ for any $n \leqslant k \leqslant m \leqslant n_0$.

When dealing with pullback attractors, only the evolution of the system up to the "present" time n_0 is of interest. The key question is how perturbations of the system in the past affect the present dynamic and what actually is the state of the system observed. This is the reason why elements belonging to the class $\mathcal{U}_d(V, n_0)$ are defined up to time n_0 and not necessarily beyond.

We can say that element of the discrete time class $\mathcal{U}_d(V, \tau_0)$ possess a discrete time pullback exponential attractor in the sense made precise by the following theorem

Theorem 3.2.1 ((Langa et al., 2010, Theorem 2.1)). *Let $n_0 \in \mathbb{Z}$, $\delta > 0$, $K > 0$ and $B \subset V$ be fixed with B bounded and closed in V. Then, there exist positive constants C_1, C_2, $\overline{\epsilon}$ and α only depending on V, H, δ, K and B, such that, for each $U \in \mathcal{U}_d(V, n_0)$ satisfying*

$$U(n, n-1) \in \mathbb{S}_{\delta,K}(B) \qquad \text{for all } n \leqslant n_0,$$

there exists a family $\mathcal{M}_U = \{\mathcal{M}_U(n) \mid n \leqslant n_0\}$, of nonempty subsets of V, which satisfies

a) $\mathcal{M}_U$ is positively invariant i.e.

$$U(m, n)\mathcal{M}_U(n) \subset \mathcal{M}_U(m) \quad \text{for all } n \leqslant m \leqslant n_0,$$

b) $\mathcal{M}_U(n) \subset B$ is a compact subset of V, with finite fractal dimension estimated by

$$\log_2 N_\epsilon(\mathcal{M}_U(n), V) \leqslant C_1 \log_2 \frac{1}{\epsilon} + C_2 \quad \text{for all } 0 < \epsilon < \overline{\epsilon} \text{ and any } n \leqslant n_0,$$

where $N_\epsilon(\mathcal{M}_U(n), V)$ is the minimal number of ϵ-balls in V, which are necessary to cover $\mathcal{M}_U(n)$,

c) $\mathcal{M}_U$ attracts B exponentially in a pullback sense i.e.

$$\operatorname{dist}_V(U(m, n)B, \mathcal{M}_U(m)) \leqslant C_1 e^{-\alpha(m-n)} \qquad \text{for all } n \leqslant m \leqslant n_0,$$

d) for every integer $k \leqslant 0$

$$\mathcal{M}_U(n + k) = \mathcal{M}_{T_k U}(n) \qquad \text{for all } n \leqslant n_0,$$

where $T_k U(m, n) \doteq U(m + k, n + k)$.

Remark 3.2.1. The results in Langa et al. (2010) also include robustness of a discrete-time exponential pullback attractor w.r.t. to a suitable metric in the space of discrete time processes. For simplicity we do not mention all the pertinent details here. However, we recall that this result is important in deducing the analogue continuous-time theory and, in particular, in obtaining continuity in time of an exponential pullback attractor.

Having in mind the more relevant continuous-time setting, we now introduce a suitable analogue of the class $\mathcal{U}_d(V, n_0)$. Let $t_0 \in \mathbb{R}$ be any time, and consider the class $\mathcal{U}(V, t_0)$ of all families $U = \{U(t, s) \mid s, t \in \mathbb{R}, s \leqslant t \leqslant t_0\}$ of mappings $U(t, s) \colon V \to V$ such that

1. $U(s, s) = Id$ for all $s \leqslant t_0$;

2. $U(t, r)U(r, s) = U(t, s)$ for any $s \leqslant r \leqslant t \leqslant t_0$.

In this setting, a natural way to introduce a smoothing property is to consider only those families $U \in \mathcal{U}(V, t_0)$ such that there exists a positive time span τ_0 for which

$$U(t, t-\tau_0) \in \mathbb{S}_{\delta,K}(B) \tag{3.2.1}$$

holds for all $t \leqslant t_0$. Thanks to Theorem 3.2.1, for any $t \leqslant t_0$ the family $U^t \in \mathcal{U}_d(V, 0)$ given by

$$U^t(m, n) \doteq U(t + m\tau_0, t + n\tau_0) \quad \text{for all } n \leqslant m \leqslant 0$$

possesses a discrete time exponential pullback attractor.

In order to obtain a satisfactory dynamical description of the system also in the continuous-time case, we will need some additional assumptions on the time regularity and continuous dependence of the family $U \in \mathcal{U}(V, t_0)$. In particular we will assume

(H.1) Continuity w.r.t. the forcing terms: there exist real positive constants C_0, ϵ_0 and γ such that $\epsilon_0 \leqslant \tau_0$ and that for all $t \leqslant t_0$, $\tau_0 \leqslant r \leqslant 2\tau_0$, $0 \leqslant s \leqslant \epsilon_0$ and $v \in \mathcal{O}_\delta(B)$

$$\|U(t, t-r)v - U(t-s, t-r-s)v\| \leqslant C_0 |s|^\gamma.$$

(H.2) Past continuous dependence on initial data: there exists a positive constant C_B such that

$$\|U(t, t-s)v - U(t, t-s)w\| \leqslant C_B \|v - w\|$$

for all $v, w \in B$ and any $t \leqslant t_0$, $0 \leqslant s \leqslant 2\tau_0$.

(H.3) Time continuity of solutions: there exist positive constants C_0' and γ' such that for all $t \leqslant t_0$, $\tau_0 \leqslant r \leqslant 2\tau_0$, $0 \leqslant s \leqslant \epsilon_0$ and $v \in B$

$$\|U(t, t-r)v - U(t-s, t-r)v\| \leqslant C_0' |s|^{\gamma'}.$$

We can now state the main result on exponential pullback attractors

Theorem 3.2.2 ((Langa et al., 2010, Theorem 2.2)). *If $U \in \mathcal{U}(V, t_0)$ satisfies (3.2.1) and Assumption (H.2), with $B \subset V$ bounded and closed in V, then the family $\mathcal{M}_U = \{\mathcal{M}_U(t) \mid t \leqslant t_0\}$, defined by*

$$\mathcal{M}_U(t) \doteq \bigcup_{s \in [0, \tau_0]} U(t, t-s-\tau_0) \mathcal{M}_{U^{t-s-\tau_0}}(0) \qquad \text{for all } t \leqslant t_0,$$

satisfies

a) $U(t, \tau)\mathcal{M}_U(\tau) \subset \mathcal{M}_U(t)$ for all $\tau \leqslant t \leqslant t_0$,

b) $\mathcal{M}_{T_{-\tau}U}(t) = \mathcal{M}_U(t - \tau)$ for all $\tau \geqslant 0$ and any $t \leqslant t_0$, where $T_{-\tau}U(t, s) \doteq U(t - \tau, s - \tau)$,

c) for all $\tau \geqslant 0$ *and any* $t \leqslant t_0$

$$\operatorname{dist}_V(U(t, t-\tau)B, \mathcal{M}_U(t)) \leqslant Ce^{-\tilde{\alpha}\tau},$$

d) if, for any $D \subset V$ *bounded, there exists a time* $s_D \geqslant 0$ *such that*

$$U(t, t-s_D)D \subset B \qquad \text{for all } t \leqslant t_0$$

then

$$\operatorname{dist}_V(U(t, t-\tau)D, \mathcal{M}_U(t)) \leqslant Ce^{\tilde{\alpha}s_D}e^{-\tilde{\alpha}\tau} \qquad \text{for all } \tau \geqslant s_D \text{ and any } t \leqslant t_0. \tag{3.2.2}$$

If, moreover, U *also satisfies Assumptions (H.1) and (H.3), then*

e) $\mathcal{M}_U(t)$ *is a compact subset of* V*, with finite fractal dimension, for all* $t \leqslant t_0$*,*

f) for all $0 \leqslant r \leqslant \epsilon_0$ *and any* $t \leqslant t_0$*,*

$$\operatorname{dist}_V^{\mathrm{sym}}(\mathcal{M}_U(t), \mathcal{M}_U(t-r)) \leqslant C|r|^{\tilde{\gamma}}.$$

Finally consider the case of processes on V. Let U be a family $U = \{U(t,s) \mid s,t \in \mathbb{R}, s \leqslant t\}$ of mappings $U(t,s)\colon V \to V$ such that

1. $U(s,s) = Id$ for all $s \in \mathbb{R}$;
2. $U(t,r)U(r,s) = U(t,s)$ for any $s \leqslant r \leqslant t$.

This corresponds to a dynamical system defined not only up to the present time t_0, but also for positive times. Considering processes corresponds to investigating what the eventual fate of the system under scrutiny will be. Therefore, it is interesting to investigate the relation between this eventual fate and the present state of the system, which is itself, in a way of speaking, the outcome of an arbitrary long evolution.

We will need the following additional assumption, which is a slight modification of (H.2)

(H.4) Future continuous dependence on initial data: for any $t > t_0$ and D_1, D_2 bounded subsets of V, there exists a positive constant $L(t, D_1, D_2)$ such that

$$\|U(t,t_0)v - U(t,t_0)w\| \leqslant L(t, D_1, D_2)\|v - w\| \qquad \text{for all } v \in D_1,\ w \in D_2.$$

Theorem 3.2.3 ((Langa et al., 2010, Theorem 2.3))**.** *Assume that* U *is a process on* V *and, for some* $t_0 \in \mathbb{R}$*, the subfamily of* U *given by the operators* $U(t,s)$ *when* $s \leqslant t \leqslant t_0$ *satisfies* (3.2.1)

and Assumption (H.2), with $B \subset V$ bounded and closed in V. Under these assumptions, the family $\widetilde{\mathcal{M}}_U = \{\widetilde{\mathcal{M}}_U(t) \mid t \in \mathbb{R}\}$ defined by

$$\widetilde{\mathcal{M}}_U(t) = \begin{cases} \mathcal{M}_U(t) & \text{if } t \leqslant t_0, \\ U(t,t_0)\mathcal{M}_U(t_0) & \text{if } t > t_0, \end{cases}$$

where $\mathcal{M}_U$ is the family given in Theorem 3.2.2, satisfies:

a) $U(t,\tau)\widetilde{\mathcal{M}}_U(\tau) \subset \widetilde{\mathcal{M}}_U(t)$, for all $\tau \leqslant t$,

b) $\widetilde{\mathcal{M}}_{T_{-\tau}U}(t) = \widetilde{\mathcal{M}}_U(t-\tau)$ for all $\tau \geqslant 0$ and any $t \leqslant t_0$ and

$$\widetilde{\mathcal{M}}_{T_{-\tau}U}(t) \subset \widetilde{\mathcal{M}}_U(t-\tau) \qquad \text{for all } \tau \geqslant 0 \text{ and any } t > t_0,$$

where $T_{-\tau}U(t,s) \doteq U(t-\tau, s-\tau)$.

If in addition (H.4) holds, then

c) if, for any $D \subset V$ bounded, there exists a positive time s_D such that

$$U(t, t-s)D \subset B \qquad \text{for all } s \geqslant s_D \text{ and any } t \leqslant t_0,$$

then $\widetilde{\mathcal{M}}_U$ satisfies (3.2.2) for all $t \leqslant t_0$ and

$$\operatorname{dist}_V(U(t,t-\tau)D, \widetilde{\mathcal{M}}_U(t)) \leqslant \tilde{L}(t, B, \widetilde{\mathcal{M}}_U(t_0))e^{\tilde{\alpha}(s_D+t-t_0)}e^{-\tilde{\alpha}\tau}$$

for all $t > t_0$ and any $\tau \geqslant s_D + t - t_0$.

Moreover, if U also satisfies Assumptions (H.1) and (H.3), then

d) $\widetilde{\mathcal{M}}_U(t)$ is a compact subset of V with finite fractal dimension for all $t \in \mathbb{R}$,

e) for all $0 \leqslant r \leqslant \epsilon_0$ and any $t \leqslant t_0$

$$\operatorname{dist}_V^{\mathrm{sym}}(\widetilde{\mathcal{M}}_U(t), \widetilde{\mathcal{M}}_U(t-r)) \leqslant C|r|^{\tilde{\gamma}}.$$

Remark 3.2.2. We recall that in Langa et al. (2010) also explicit estimates on a fractal dimension of the pullback exponential attractor have been derived. For the sake of simplicity, we neglect them here.

3.3 Existence results and basic energy estimate

In this section we recall some basic energy estimates, which are obtained naturally when proving existence of solution to system (3.0.1). First of all, for the sake of simplicity, we set $\varepsilon = M = 1$ and we write the definition of weak solution to system (3.0.1).

Definition 3.3.1. Let $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{\mathrm{div}}(\Omega) \times H^1_{(0)}(\Omega)$ and let $\tau \in \mathbb{R}$. Then a couple $\mathbf{z} = (\mathbf{u}, \psi)$ such that

$$\mathbf{u} \in L^2(\tau, T; \mathbf{H}^1_{0,\mathrm{div}}(\Omega)) \cap H^1(\tau, T; \mathbf{H}^{-1}_{\mathrm{div}}(\Omega))$$
$$\psi \in L^2(\tau, T; H^3(\Omega)) \cap H^1(\tau, T; H^{-1}(\Omega))$$

is called a *weak solution* to (3.0.1) if

$$\langle \partial_t \mathbf{u}(t), \mathbf{v} \rangle + \langle (\mathbf{u}(t) \cdot \nabla)\mathbf{u}(t), \mathbf{v} \rangle + \langle \nu \nabla \mathbf{u}(t), \nabla \mathbf{v} \rangle = \langle \mu(t) \nabla \psi(t), \mathbf{v} \rangle$$
$$\langle \partial_t \psi(t), \phi \rangle + \langle \mathbf{u}(t) \cdot \nabla \psi(t), \phi \rangle = -\left(\nabla \mu(t), \nabla \phi\right)$$

hold for a.e. $t \in [\tau, T]$, for all $\mathbf{v} \in \mathcal{V}$ and for all ϕ in $\mathbf{C}^\infty(\Omega)$, if

$$\mu(t) = f(\psi(t)) - \Delta \psi(t)$$

holds for a.e. $t \in [\tau, T]$ in $H^1(\Omega)$ with $\mu \in L^2(\tau, T; H^1(\Omega))$ and if

$$\lim_{t \to \tau^+} \mathbf{u}(t) = \mathbf{u}_0 \quad \text{in } \mathbf{L}^2_{\mathrm{div}}(\Omega), \qquad \lim_{t \to \tau^+} \psi(t) = \psi_0 \quad \text{in } H^1_{(0)}(\Omega).$$

The well-posedness for problem (3.0.1)-(3.0.2) is justified in a suitable Galerkin scheme, thanks to the following a priori estimates and the subsequent Lemma 3.5.1(see e.g. Boyer (1999); Gal and Grasselli (2010a)).

Theorem 3.3.1. *Let assumptions (A.1)–(A.6) hold. If* $\mathbf{g}$ *satisfies (B.1) and* $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_0$, *then there exists a unique weak solution* $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ *departing at time* τ *from the initial datum* $\mathbf{z}_0$.

We now obtain the first basic energy estimates that will be the basis for the estimates of the following sections.

Lemma 3.3.2. *If* $\mathbf{g}$ *satisfies (B.1) and* $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ *is the solution departing at time* τ *from the initial datum* $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_0$, *denoting by* $\mu(t)$ *the corresponding chemical potential, there holds*

$$|\mathbf{u}(t)|_2^2 + |\nabla \psi(t)|_2^2 + 2|F(\psi(t))|_1 + \int_\tau^t \left[\nu \|\mathbf{u}(s)\|^2_{\mathbf{H}^1_{0,\mathrm{div}}(\Omega)} + |\nabla \mu(s)|_2^2\right] \mathrm{d}s \tag{3.3.1}$$
$$\leqslant |\mathbf{u}_0|_2^2 + |\nabla \psi_0|_2^2 + 2|F(\psi_0)|_1 + C \int_\tau^t |\mathbf{g}(s)|_2^2 \, \mathrm{d}s.$$

Besides, there hold

$$\int_\tau^t |\nabla \psi(s)|_2^2 \, \mathrm{d}s + \int_\tau^t |F(\psi(s))|_1 \, \mathrm{d}s + \int_\tau^t |\Delta \psi(s)|_2^2 \, \mathrm{d}s \tag{3.3.2}$$
$$\leqslant C \left(|\mathbf{u}_0|_2^2 + |\nabla \psi_0|_2^2 + 2|F(\psi_0)|_1 + \int_\tau^t |\mathbf{g}(s)|_2^2 \, \mathrm{d}s \right) + C(t - \tau)$$

as well as

$$\begin{aligned}&\int_\tau^t |\Delta\psi(s)|_2^4 \,\mathrm{d}s \qquad (3.3.3)\\ \leqslant& C\left(|\mathbf{u}_0|_2^2 + |\nabla\psi_0|_2^2 + 2|F(\psi_0)|_1 + \int_\tau^t |\mathbf{g}(s)|_2^2 \,\mathrm{d}s\right)^2\\ &+ C(t-\tau)\left(|\mathbf{u}_0|_2^2 + |\nabla\psi_0|_2^2 + 2|F(\psi_0)|_1 + \int_\tau^t |\mathbf{g}(s)|_2^2 \,\mathrm{d}s\right).\end{aligned}$$

Proof. In order to obtain our first (dissipative) a priori estimate, we multiply the first equation in (3.0.1) by $\mathbf{u}$ and the third by μ. Recalling the antisymmetric property of the convective term in the Navier Stokes equation and exploiting the useful vector identity

$$\begin{aligned}(\partial_t\psi, \mu) =& -(\partial_t\psi, \Delta\psi) + (f(\psi), \partial_t\psi)\\ =& \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\psi|_2^2 + (f(\psi), \partial_t\psi)\\ =& \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\psi|_2^2 + 2|F(\psi)|_1\right),\end{aligned}$$

we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\psi|_2^2 + 2|F(\psi)|_1\right) + \nu|\nabla\mathbf{u}|_2^2 + |\nabla\mu|_2^2 = (\mathbf{g}, \mathbf{u}). \qquad (3.3.4)$$

Poincaré's inequality for $\mathbf{u}$ and integration with respect to time give (3.3.1).

We now have to "complete the norms" on the left hand side of (3.3.4). From the definition of the chemical potential μ (i.e. from the fourth equation in (3.0.1)) we have

$$(\mu, \psi) = |\nabla\psi|_2^2 + (\psi, f(\psi)).$$

Since, by assumption, ψ is mean free, we also deduce

$$(\mu, \psi) = (\mu - \langle\mu\rangle, \psi) \leqslant \frac{1}{2}|\nabla\mu|_2^2 + C|\psi|_2^2,$$

where C is a constant, which only depends on the domain Ω. From assumption (A.5) on the potential F we further deduce

$$(f(\psi), \psi) = (f_0(\psi), \psi) - 2\alpha|\psi|_2^2,$$

being $f_0 = F_0'$. Taking into account the convexity of F_0 we can also bound the right hand side of this identity from below:

$$(f_0(\psi), \psi) \geqslant |F_0(\psi) - F_0(0)|_1.$$

Putting the last four estimates together and recalling Assumption (A.6), we obtain

$$\begin{aligned}&|\nabla\mu|_2^2 + C|\psi|_2^2\\ \geqslant& |\nabla\psi|_2^2 + |F_0(\psi) - F_0(0)|_1 - 2\alpha|\psi|_2^2\\ =& |\nabla\psi|_2^2 + |F(\psi)|_1 - \alpha|\psi|_2^2.\end{aligned}$$

Therefore we get

$$|\nabla\psi|_2^2 + |F(\psi)|_1 \leqslant |\nabla\mu|_2^2 + C|\psi|_2^2 \leqslant |\nabla\mu|_2^2 + \delta|\psi|_{2+q}^{2+q} + C,$$

where q is a positive real number, δ is a (small) positive constant, which will be determined later, and C is a positive constant, which depends only on the domain Ω and is independent of the exponent q as soon as $q \geqslant \overline{q} > 0$.

Remark 3.3.1. We observe that under assumption (A.7) we immediately have $q \geqslant 2$ so that in our case the constant C really depends only on Ω.

By adding this last estimate and (3.3.4) together, choosing δ small enough, we finally deduce the basic energy estimate for system (3.0.1)-(3.0.2)

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\psi|_2^2 + 2|F(\psi)|_1\right) + C\left(|\nabla\mathbf{u}|_2^2 + |\nabla\psi|_2^2 + 2|F(\psi)|_1 + |\nabla\mu|_2^2\right) \leqslant C\left(1 + |\mathbf{g}|_2^2\right). \quad (3.3.5)$$

Integrating with respect to time from τ to t, we then obtain the first part of estimate (3.3.2). Noticing that

$$\langle\nabla\mu, \nabla\psi\rangle = -\langle\mu, \Delta\psi\rangle = |\Delta\psi|_2^2 - \langle f(\psi), \Delta\psi\rangle = |\Delta\psi|_2^2 + \left\langle f'(\psi)\nabla\psi, \nabla\psi\right\rangle \geqslant |\Delta\psi|_2^2 - 2\alpha|\nabla\psi|_2^2,$$

we have

$$|\Delta\psi|_2^2 \leqslant |\nabla\mu|_2|\nabla\psi|_2 + 2\alpha|\nabla\psi|_2^2, \quad (3.3.6)$$

which, integrated in time, on account of the above estimate (3.3.1), gives the second part of estimate (3.3.2).

In order to prove (3.3.3), we square (3.3.6), obtaining

$$|\Delta\psi|_2^4 \leqslant C(|\nabla\mu|_2^2|\nabla\psi|_2^2 + |\nabla\psi|_2^4) \leqslant C(|\nabla\mu|_2^2|\nabla\psi|_2^2 + |\nabla\psi|_2^2|\Delta\psi|_2^2).$$

By an integration in time, in view of (3.3.1) and (3.3.2) we accomplish our purpose. □

Corollary 3.3.3. *If* $\mathbf{g}$ *satisfies (B.1) and (B.2) and* $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ *is the solution departing at time* τ *from the initial datum* $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_0$*, the following dissipative estimate holds*

$$\begin{aligned} &|\mathbf{u}(t)|_2^2 + |\nabla\psi(t)|_2^2 + 2|F(\psi(t))|_1 \\ &\leqslant \left(|\mathbf{u}_0|_2^2 + |\nabla\psi_0|_2^2 + 2|F(\psi_0)|_1\right)e^{-C(t-\tau)} + C\left(1 + M_{\mathbf{g}}(t)\right), \qquad \forall t \geqslant \tau. \end{aligned} \quad (3.3.7)$$

Proof. The claimed dissipative estimate easily follows from the basic energy estimate (3.3.5) using

Poincaré's and Gronwall's inequalities as well as the known estimate

$$\begin{aligned}
&e^{-Ct}\int_\tau^t e^{Cs}|\mathbf{g}(s)|_2^2\,\mathrm{d}s\\
\leqslant& e^{-Ct}\sum_{n=0}^{\infty}\int_{t-(n+1)}^{t-n} e^{Cs}|\mathbf{g}(s)|_2^2\,\mathrm{d}s \leqslant e^{-Ct}\sum_{n=0}^{\infty} e^{C(t-n)}\sup_{r\leqslant t}\int_{r-1}^{r}|\mathbf{g}(s)|_2^2\,\mathrm{d}s\\
\leqslant& C\sup_{r\leqslant t}\int_{r-1}^{r}|\mathbf{g}(s)|_2^2\,\mathrm{d}s,
\end{aligned}$$

which holds for $\mathbf{g}\in L^2_{\mathrm{uloc}}(-\infty,t;\mathbf{L}^2(\Omega))$. □

Remark 3.3.2. A bound on $\nabla\Delta\psi$ in $L^2(\tau,T;\mathbf{L}^2(\Omega))$ can also be easily deduced by computing the L^2 norm of the gradient of the equation for the chemical potential μ in (3.0.1) thus leading to the regularity of the order parameter field required by Definition 3.3.1. However, this estimate cannot be easily made uniform with respect to the shape of the potential F (and in particular with respect to the growth exponent p).

Remark 3.3.3. From the above computations we deduce the following regularity for weak solutions of system (3.0.1)

$$\begin{aligned}
\mathbf{u}&\in L^\infty(\tau,T;\mathbf{L}^2_{\mathrm{div}}(\Omega))\cap L^2(\tau,T;\mathbf{H}^1_{0,\mathrm{div}}(\Omega))\\
\psi&\in L^\infty(\tau,T;H^1(\Omega))\cap L^4(\tau,T;H^2(\Omega))\\
F(\psi)&\in L^\infty(\tau,T;L^1(\Omega))\\
\nabla\mu&\in L^2(\tau,T;\mathbf{L}^2(\Omega))
\end{aligned}$$

for any $T\in\mathbb{R}$, $T>\tau$.

3.4 Higher regularity estimates

In order to obtain estimates having uniform structure with respect to the growth exponent of f, we henceforth assume that F satisfies (A.7). Although all exponents and norms that appear in this and in the following sections are independent of p, the general constant C will quickly become larger as p grows.

In particular, Assumption (A.7) and Lemma 3.3.2 imply

$$\begin{aligned}
|f^{(k)}(\psi(t))|_{\frac{p+3}{p+2-k}} &\leqslant C(|F(\psi(t))|_1+1)\\
&\leqslant C\left(|\mathbf{u}_0|_2^2+|\nabla\psi_0|_2^2+2|F(\psi_0)|_1+\int_\tau^t|\mathbf{g}(s)|_2^2\,\mathrm{d}s+1\right),
\end{aligned}\tag{3.4.1}$$

being $(\mathbf{u}(t),\psi(t))$ the solution to (3.0.1)-(3.0.2) departing from $(\mathbf{u}_0,\psi_0)\in\mathcal{H}_0$ at time τ.

The goal of this section is to improve "by one order" the basic regularity result already obtained. In particular, under suitable assumptions, we will get to $\mathbf{u}\in L^\infty(\mathbf{H}^1_{0,\mathrm{div}}(\Omega))\cap L^2(\mathbf{H}^2_{0,\mathrm{div}}(\Omega))$ and

$\psi \in L^\infty(H^2(\Omega)) \cap L^2(H^4(\Omega))$. This will be achieved in several steps gaining before spatial regularity for $f(\psi)$ and μ and later time regularity as well: first in Lemma 3.4.1 we will deduce $f(\psi) \in L^2(L^2(\Omega))$ and $\mu \in L^2(L^2(\Omega))$; then $f(\psi) \in L^2(L^q(\Omega))$ and $\Delta\psi \in L^2(L^q(\Omega))$ for any $q \geqslant 1$, as shown in Lemma 3.4.2; this will give $\mu \in L^\infty(L^2(\Omega))$ (cf. Lemma 3.4.3) and the final result (see Lemma 3.4.4).

Notation. In order to simplify notation, we will denote by $A_{t,\tau}$ the quantity

$$A_{t,\tau} \doteq 1 + |\mathbf{u}_0|_2^2 + |\nabla\psi_0|_2^2 + 2|F(\psi_0)|_1 + \int_\tau^t |\mathbf{g}(s)|_2^2 \,\mathrm{d}s,$$

which depends only on the initial data $\mathbf{u}_0$, ψ_0, on the forcing term $\mathbf{g}$ and on the times t and τ. Besides, C stands for a generic positive constant depending only on Ω and possibly on p and is allowed to vary even in the same line.

Lemma 3.4.1. *If $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ is the solution departing at time τ from the initial datum $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_0$, denoting by $\mu(t)$ the corresponding chemical potential, there holds*

$$\int_\tau^t (|f(\psi(s)|_2^2 + |\mu(s)|_2^2) \,\mathrm{d}s \leqslant C A_{t,\tau}^2 + C(t-\tau)A_{t,\tau} \tag{3.4.2}$$

for any $t \geqslant \tau$, $\tau \in \mathbb{R}$.

Proof. Remark 2.1 allows to bound the mean value of $f(\psi)$ as

$$|\langle f(\psi)\rangle| \leqslant C|f(\psi)|_{\frac{p+3}{p+2}} \leqslant C(1 + |F(\psi)|_1),$$

for some $C > 0$ depending on p only through the constant c_0 in Assumption (A.7). Recalling the equation defining the chemical potential in (3.0.1) and estimate (3.3.6), we further deduce

$$|f(\psi) - \langle f(\psi)\rangle|_2^2 \leqslant 2|\mu - \langle\mu\rangle|_2^2 + 2|\Delta\psi|_2^2 \leqslant C|\nabla\mu|_2^2 + 4\alpha|\nabla\psi|_2^2.$$

Therefore, we gain full control on the L^2-norm of $f(\psi)$, bounding its time integral as

$$\begin{aligned}
&\int_\tau^t |f(\psi(s))|_2^2 \,\mathrm{d}s \\
\leqslant& C\int_\tau^t |\nabla\mu(s)|_2^2 \,\mathrm{d}s + 4\alpha\int_\tau^t |\nabla\psi(s)|_2^2 \,\mathrm{d}s + C\int_\tau^t (1 + |F(\psi(s))|_1)^2 \,\mathrm{d}s \\
\leqslant& C A_{t,\tau}^2 + C(t-\tau)A_{t,\tau},
\end{aligned}$$

where we used (3.3.1) and (3.3.2) from Lemma 3.3.2. The second part of estimate (3.4.2) follows from

$$|\mu|_2^2 \leqslant 2(|\Delta\psi|_2^2 + |f(\psi)|_2^2),$$

the above bound and (3.3.2). ∎

As announced before, the integrability of $f(\psi)$ can be further improved in two steps.

Lemma 3.4.2. *If $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ is the solution departing at time τ from the initial datum $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_0$, then, for any $b > 0$ there exists $C_b > 0$ such that*

$$\int_\tau^t \left(|f(\psi(s))|_{b+2}^2 + |\Delta\psi(s)|_{b+2}^2 \right) \mathrm{d}s \leqslant C_b A_{t,\tau}^2 + C_b (t-\tau) A_{t,\tau},$$

meaning that $f(\psi)$, $\Delta\psi \in L^2(\tau, t; L^{b+2}(\Omega))$, for any $b > 0$.

Remark 3.4.1. We note that this estimate extends to singular functional f, without appealing to approximation arguments as in Abels (2009c) but with the same order of control.

Proof. Multiplying the equation for the chemical potential by $f(\psi)|f(\psi)|^b$ and integrating over Ω, we have

$$\left\langle \mu, f(\psi)|f(\psi)|^b \right\rangle = |f(\psi)|_{b+2}^{b+2} - \left\langle \Delta\psi, f(\psi)|f(\psi)|^b \right\rangle. \tag{3.4.3}$$

We now exploit assumption (A.5) on F, proving after an integration by parts

$$-\left\langle \Delta\psi, f(\psi)|f(\psi)|^b \right\rangle = (b+1)\left\langle f'(\psi), |f(\psi)|^b |\nabla\psi|^2 \right\rangle \geqslant -2\alpha(b+1)\left\langle |f(\psi)|^b, |\nabla\psi|^2 \right\rangle.$$

Replacement of this estimate in (3.4.3) above leads to

$$|f(\psi)|_{b+2}^{b+2} \leqslant 2\alpha(b+1)\left\langle |f(\psi)|^b, |\nabla\psi|^2 \right\rangle + \left\langle |\mu|, |f(\psi)|^{b+1} \right\rangle.$$

Hölder's and Young's inequalities then provide

$$|f(\psi)|_{b+2}^{b+2} \leqslant 2\alpha(b+1)|f(\psi)|_{b+2}^b |\nabla\psi|_{b+2}^2 + |\mu|_{b+2}|f(\psi)|_{b+2}^{b+1} \leqslant \frac{1}{2}|f(\psi)|_{b+2}^{b+2} + C_b\left(|\nabla\psi|_{b+2}^{b+2} + |\mu|_{b+2}^{b+2} \right).$$

Recalling that from standard interpolation the inequality

$$|h|_{b+2}^{b+2} \leqslant C_b |h|_2^2 \|h\|_{H^1}^b,$$

holds, we end up with

$$|f(\psi)|_{b+2}^{b+2} \leqslant C_b\left(|\nabla\psi|_2^2 |\Delta\psi|_2^b + |\mu|_2^2 \|\mu\|_{H^1}^b \right). \tag{3.4.4}$$

A further application of Young's inequality then gives

$$\begin{aligned} |f(\psi)|_{b+2}^2 &\leqslant C_b\left(|\nabla\psi|_2^{4/(b+2)} |\Delta\psi|_2^{2b/(b+2)} + |\mu|_2^{4/(b+2)} |\nabla\mu|_2^{2b/(b+2)} + |\mu|_2^2 \right) \\ &\leqslant C_b\left(|\nabla\psi|_2^2 + |\Delta\psi|_2^2 + |\mu|_2^2 + |\nabla\mu|_2^2 \right). \end{aligned}$$

Finally, integration with respect to time, leads to

$$\int_\tau^t |f(\psi(s))|_{b+2}^2 \,\mathrm{d}s \leqslant C_b \int_\tau^t \left(|\nabla\psi(s)|_2^2 + |\Delta\psi(s)|_2^2 + |\mu(s)|_2^2 + |\nabla\mu(s)|_2^2 \right) \mathrm{d}s,$$

thus Lemmata 3.3.2 and 3.4.1 provide the first part of the desired estimate. To complete our argument, it is sufficient to exploit the equation for the chemical potential μ and this last estimate together with Lemmata 3.3.2 and 3.4.1:

$$|\Delta\psi|_{b+2}^2 \leqslant 2\left(|\mu|_{b+2}^2 + |f(\psi)|_{b+2}^2\right) \leqslant 2\left(|\mu|_2^2 + |\nabla\mu|_2^2 + |f(\psi)|_{b+2}^2\right). \qquad \square$$

Remark 3.4.2. Provided that F satisfies (A.7), estimates (3.3.1) and (3.1.1) entail (cf. Remark 3.1.1)

$$f(\psi) \in L^\infty(\tau, t; L^{(p+3)/(p+2)}(\Omega)).$$

Besides, the above Lemma 3.4.2 implies $f(\psi) \in L^2(\tau, t; L^{b+2}(\Omega))$ for any $b > 0$. Being $(p+3)/(p+2) > 1$, by the interpolation inequality

$$|h|_2 \leqslant |h|_{\frac{p+3}{p+2}}^{\theta} |h|_{b+2}^{1-\theta}, \quad \text{where } \theta = \frac{b(p+3)}{2(bp+2b+p+1)},$$

we deduce that, when $4(1-\theta) = 4\dfrac{(b+2)(p+1)}{2(bp+2b+p+1)} = 2$, that is, $b = 1+p$,

$$\begin{aligned}\int_\tau^t |f(\psi(s))|_2^4 \,\mathrm{d}s \leqslant & \|f(\psi)\|^2_{L^\infty(\tau,t;L^{\frac{p+3}{p+2}}(\Omega))} \int_\tau^t |f(\psi(s)|_{p+3}^2 \,\mathrm{d}s \\ \leqslant & CA_{t,\tau}^4 + C(t-\tau)A_{t,\tau}^3.\end{aligned}$$

On account of (3.1.1), Lemmata 3.3.2 and 3.4.2, it thus follows $f(\psi) \in L^4(\tau, t; L^2(\Omega))$ and, in particular,

$$\|f(\psi)\|^4_{L^4(\tau,t;L^2(\Omega))} \leqslant CA_{t,\tau}^4 + C(t-\tau)A_{t,\tau}^3.$$

Lemma 3.4.3. *If $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ is the solution departing at time τ from any initial datum $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_1$ so that $\mu_0 \doteq f(\psi_0) - \Delta\psi_0 \in L^2(\Omega)$, then there exists $C > 0$ depending only on p such that the chemical potential μ is bounded in $L^\infty(\tau, T; L^2(\Omega)) \cap L^2(\tau, T; H^2(\Omega))$ for all $T > \tau$ and there hold*

$$|\mu(t)|_2^2 \leqslant C\left(|\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right) e^{C(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3)}$$

and

$$\int_\tau^t |\Delta\mu(s)|_2^2 \,\mathrm{d}s \quad \leqslant \quad C\left(|\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3\right) e^{C\left(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3\right)}.$$

Proof. The evolution of the chemical potential μ is governed by

$$\partial_t\mu = f'(\psi)\Delta\mu - f'(\psi)(\mathbf{u}\cdot\nabla)\psi - \Delta^2\mu + \Delta((\mathbf{u}\cdot\nabla)\psi),$$

as can be seen by formally differentiating with respect to time the last equation in (3.0.1) and by taking into account the third one. The product of this equality by μ gives rise to three terms

from the right hand side: in order to exploit the lower bound on f', the first one can be written as

$$\begin{aligned}
&\left\langle f'(\psi)\Delta\mu,\mu\right\rangle\\
=&-\left\langle f'(\psi)\nabla\mu,\nabla\mu\right\rangle-\left\langle f''(\psi)\nabla\psi,\mu\nabla\mu\right\rangle\\
=&-\left\langle f'(\psi)\nabla\mu,\nabla\mu\right\rangle-\frac{1}{2}\left\langle f''(\psi)\nabla\psi,\nabla(\mu^2)\right\rangle\\
=&-\left\langle f'(\psi)\nabla\mu,\nabla\mu\right\rangle+\frac{1}{2}\left\langle f''(\psi)\Delta\psi,\mu^2\right\rangle+\frac{1}{2}\left\langle f'''(\psi)\left|\nabla\psi\right|^2,\mu^2\right\rangle.
\end{aligned}$$

Thanks to the incompressibility condition, the second one reads as

$$-\left\langle f'(\psi)(\mathbf{u}\cdot\nabla)\psi,\mu\right\rangle=\left\langle f(\psi),\mathbf{u}\cdot\nabla\mu\right\rangle.$$

Finally, noticing that the third equation in (3.0.1) and the boundary conditions (3.0.2) imply $\partial_{\mathbf{n}}(\Delta\mu-\mathbf{u}\cdot\nabla\psi)=\partial_{\mathbf{n}}\partial_t\psi=0$ on $\partial\Omega$, the last term is

$$-\left\langle\Delta^2\mu-\Delta(\mathbf{u}\cdot\nabla\psi),\mu\right\rangle=-|\Delta\mu|_2^2+\left\langle\mathbf{u}\cdot\nabla\psi,\Delta\mu\right\rangle.$$

These computations lead us to

$$\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\mu|_2^2+|\Delta\mu|_2^2\\
&\qquad=-\left\langle f'(\psi)\nabla\mu,\nabla\mu\right\rangle+\frac{1}{2}\left\langle f''(\psi)\Delta\psi,\mu^2\right\rangle+\frac{1}{2}\left\langle f'''(\psi)\left|\nabla\psi\right|^2,\mu^2\right\rangle+\left\langle f(\psi)\mathbf{u},\nabla\mu\right\rangle\\
&\qquad\qquad+\left\langle(\mathbf{u}\cdot\nabla)\psi,\Delta\mu\right\rangle. \qquad (3.4.5)
\end{aligned}$$

By Assumption (A.5) on the potential F, the first term on the right hand side of identity (3.4.5) is easily controlled by $2\alpha|\nabla\mu|_2^2$ while the last one can be bounded by

$$\begin{aligned}
&|\left\langle(\mathbf{u}\cdot\nabla)\psi,\Delta\mu\right\rangle|\\
\leqslant&|\mathbf{u}|_4|\nabla\psi|_4|\Delta\mu|_2\\
\leqslant&C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\nabla\psi|_2^{1/2}|\Delta\psi|_2^{1/2}|\Delta\mu|_2\\
\leqslant&\frac{1}{8}|\Delta\mu|_2^2+C|\mathbf{u}|_2|\nabla\mathbf{u}|_2|\nabla\psi|_2|\Delta\psi|_2.
\end{aligned}$$

We are left to consider the other terms in (3.4.5). Having in mind (3.4.1), we prove

$$\begin{aligned}
&\frac{1}{2}\left|\left\langle f''(\psi)\Delta\psi,\mu^2\right\rangle\right|\\
\leqslant&\frac{1}{2}|f''(\psi)|_{\frac{p+3}{p}}|\Delta\psi|_{p+3}|\mu|_{p+3}^2\\
\leqslant&C|f''(\psi)|_{\frac{p+3}{p}}|\Delta\psi|_{p+3}\|\mu\|_{H^1}^2\\
\leqslant&C|f''(\psi)|_{\frac{p+3}{p}}|\Delta\psi|_{p+3}(|\mu|_2^2+|\mu|_2|\Delta\mu|_2)\\
\leqslant&\frac{1}{8}|\Delta\mu|_2^2+C\left(|f''(\psi)|_{\frac{p+3}{p}}^2+1\right)(|\Delta\psi|_{p+3}^2+1)|\mu|_2^2.
\end{aligned}$$

Analogously we have

$$\begin{aligned}
&\frac{1}{2}\left|\left\langle f'''(\psi)|\nabla\psi|^2,\mu^2\right\rangle\right|\\
\leqslant&\frac{1}{2}|f'''(\psi)|_{\frac{p+3}{p-1}}|\nabla\psi|_{p+3}^2|\mu|_{p+3}^2\\
\leqslant&C|f'''(\psi)|_{\frac{p+3}{p-1}}|\Delta\psi|_2^2\|\mu\|_{H^1}^2\\
\leqslant&C|f'''(\psi)|_{\frac{p+3}{p-1}}|\Delta\psi|_2^2(|\mu|_2^2+|\mu|_2|\Delta\mu|_2)\\
\leqslant&\frac{1}{8}|\Delta\mu|_2^2+C(|f'''(\psi)|_{\frac{p+3}{p-1}}^2+1)(|\Delta\psi|_2^4+1)|\mu|_2^2.
\end{aligned}$$

There also holds

$$\begin{aligned}
&|\langle f(\psi),\mathbf{u}\cdot\nabla\mu\rangle|\\
\leqslant&|f(\psi)|_{\frac{p+3}{p+2}}|\mathbf{u}|_{2(p+3)}|\nabla\mu|_{2(p+3)}\\
\leqslant&C|f(\psi)|_{\frac{p+3}{p+2}}|\nabla\mathbf{u}|_2\|\bar{\mu}\|_{H^2}\\
\leqslant&\frac{1}{8}|\Delta\mu|_2^2+C|\nabla\mu|_2^2+C|f(\psi)|_{\frac{p+3}{p+2}}^2|\nabla\mathbf{u}|_2^2.
\end{aligned}$$

Collecting the above estimates and recalling (3.4.1), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}|\mu|_2^2+|\Delta\mu|_2^2\leqslant h|\mu|_2^2+g, \tag{3.4.6}$$

where

$$\begin{aligned}
h&=C(1+|F(\psi)|_1)^2(1+|\Delta\psi|_2^4+|\Delta\psi|_{p+3}^2)\\
g&=C|\nabla\mu|_2^2+C|\mathbf{u}|_2|\nabla\mathbf{u}|_2|\nabla\psi|_2|\Delta\psi|_2+C(1+|F(\psi)|_1)^2|\nabla\mathbf{u}|_2^2.
\end{aligned}$$

In view of (3.3.3), Lemmata 3.3.2 and 3.4.2, h and g are integrable quantities. Indeed, we have

$$\begin{aligned}
\int_\tau^t h(s)\,\mathrm{d}s&\leqslant C\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right),\\
\int_\tau^t g(s)\,\mathrm{d}s&\leqslant C\left(A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right).
\end{aligned}$$

By Gronwall's lemma we further deduce

$$|\mu(t)|_2^2\leqslant\left(|\mu(\tau)|_2^2+\int_\tau^t g(s)ds\right)\exp\left(\int_\tau^t h(s)ds\right)$$

that is,

$$|\mu(t)|_2^2\leqslant C\left(|\mu(\tau)|_2^2+A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right)e^{C(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3)}.$$

Moreover, integrating (3.4.6), from the estimates above we also deduce

$$\begin{aligned}
&\int_\tau^t|\Delta\mu(s)|_2^2\,\mathrm{d}s\\
\leqslant&|\mu(\tau)|_2^2+\int_\tau^t h(s)|\mu(s)|_2^2\,\mathrm{d}s+\int_\tau^t g(s)\,\mathrm{d}s\\
\leqslant&C\left(|\mu(\tau)|_2^2+A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right)e^{C(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3)}.
\end{aligned}$$

□

Remark 3.4.3. The above Lemma has several consequences. First of all, from the third equation of (3.0.1) we easily obtain $|\partial_t\psi|_2^2 \leqslant C(|\Delta\mu|_2^2 + |\mathbf{u}|_2|\nabla\mathbf{u}|_2|\nabla\psi|_2|\Delta\psi|_2)$. Thus, Lemmata 3.3.2 and 3.4.3 yield

$$\int_\tau^t |\partial_t\psi(s)|_2^2\,\mathrm{d}s \leqslant C\left(|\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3\right)e^{C(A_{t,\tau}^4(t-\tau)A_{t,\tau}^3)}. \quad (3.4.7)$$

Besides, by (3.4.4) with $b = 2$, we have

$$|f(\psi)|_4^4 \leqslant C(|\nabla\psi|_2^2|\Delta\psi|_2^2 + |\mu|_2^4 + |\mu|_2^2|\nabla\mu|_2^2),$$

hence Lemmata 3.4.1 and 3.4.3 entail $f(\psi) \in L^4(\tau, t; L^4(\Omega))$, with

$$\int_\tau^t |f(\psi(s))|_4^4\,\mathrm{d}s \leqslant C\left(|\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^2 + (t-\tau)A_{t,\tau}\right)e^{C(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3)}. \quad (3.4.8)$$

Remark 3.4.4. Actually, even more uniform estimates can be deduced from the above Lemmata. For example, from (3.4.4), using Ladyzhenskaja inequality and interpolation estimates, we deduce

$$\begin{aligned}|f(\psi)|_4^8 &\leqslant C\left(|\nabla\psi|_2^4|\Delta\psi|_2^4 + |\mu|_2^8 + |\mu|_2^4|\nabla\mu|_2^4\right)\\ &\leqslant C\left(|\nabla\psi|_2^4|\Delta\psi|_2^4 + |\mu|_2^8 + |\mu|_2^6|\Delta\mu|_2^2\right),\end{aligned}$$

i.e. $f(\psi) \in L^8(\tau, t; L^4(\Omega))$. In particular,

$$\begin{aligned}\int_{t-1}^t |f(\psi(s))|_4^8\,\mathrm{d}s &\leqslant C\int_{t-1}^t \left(|\nabla\psi(s)|_2^4|\Delta\psi(s)|_2^4 + |\mu(s)|_2^8 + |\mu(s)|_2^6|\Delta\mu(s)|_2^2\right)\mathrm{d}s \quad (3.4.9)\\ &\leqslant C\left(|\mu(t-1)|_2^2 + A_{t,t-1}^3\right)^4 A_{t,t-1}^4 e^{CA_{t,t-1}^4}.\end{aligned}$$

Thanks to our assumptions on f and to the previous results, we can now obtain estimates on the higher norms of the solution, which have uniform structure w.r.t. the shape of the potential. Dependence on the growth of the potential F is limited to the constants C, which appear in the estimate.

Lemma 3.4.4. *Given any initial datum $\mathbf{z}_0 \doteq (\mathbf{u}_0, \psi_0) \in \mathcal{H}_1$ so that $\mu_0 \doteq f(\psi_0) - \Delta\psi_0 \in L^2(\Omega)$, the solution departing at time τ from $\mathbf{z}_0$ satisfies*

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant C\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2 + |\mu_0|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^5 + (t-\tau)A_{t,\tau}^4\right)e^{C\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right)} \quad (3.4.10)$$

for some constant $C > 0$ depending on the exponent p and on the domain Ω but independent on the initial data. Moreover,

$$\int_\tau^t \left(|\Delta^2\psi(s)|_2^2 + |\Delta\mathbf{u}(s)|_2^2\right) \mathrm{d}s \leqslant C\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2 + |\mu_0|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^7 + (t-\tau)A_{t,\tau}^6\right) e^{C\left(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3\right)}.$$

Proof. In this proof, we will exploit the following inequality

$$\left|f'(y)\right| + \left|f''(y)\right| \leqslant C\left(1 + |f(y)|\right), \quad \forall y \in \mathbb{R},$$

which can be easily obtained from Assumptions (A.3), (A.4), (A.5), (A.6) and (A.7) by means of the Young's inequality. In particular, we will take advantage of its straightforward consequence

$$|f'(\psi)|_4 + |f''(\psi)|_4 \leqslant C\left(1 + |f(\psi)|_4\right).$$

Adding together the product of the first equation in (3.0.1) by $2A\mathbf{u} = -2\mathbb{P}\Delta\mathbf{u}$ and of the third one by $2\Delta^2\psi$, we obtain

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2 + |\Delta\psi|_2^2\right) + 2\nu|A\mathbf{u}|_2^2 + 2|\Delta^2\psi|_2^2 \\ =&2\langle\mathbf{g}, A\mathbf{u}\rangle - 2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}, A\mathbf{u}\rangle + 2\langle\mu\nabla\psi, A\mathbf{u}\rangle - 2\left\langle(\mathbf{u}\cdot\nabla)\psi, \Delta^2\psi\right\rangle + 2\left\langle\Delta f(\psi), \Delta^2\psi\right\rangle.\end{aligned} \tag{3.4.11}$$

The first two terms arising from Navier-Stokes equations can be dealt with by writing

$$\begin{aligned}&|-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}, A\mathbf{u}\rangle + 2\langle\mathbf{g}, A\mathbf{u}\rangle| \\ \leqslant& C(|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2|A\mathbf{u}|_2^{3/2} + |\mathbf{g}|_2|A\mathbf{u}|_2) \\ \leqslant& \frac{\nu}{2}|A\mathbf{u}|_2^2 + C|\mathbf{u}|^2|\nabla\mathbf{u}|_2^4 + C|\mathbf{g}|_2^2.\end{aligned}$$

Since $\langle\mu\nabla\psi, A\mathbf{u}\rangle = -\langle\Delta\psi\nabla\psi, A\mathbf{u}\rangle$, from the Agmon's inequality we easily have

$$\begin{aligned}&|2\langle\mu\nabla\psi, A\mathbf{u}\rangle| \\ \leqslant& 2|\Delta\psi|_\infty|\nabla\psi|_2|A\mathbf{u}|_2 \\ \leqslant& C|\Delta\psi|_2^{1/2}|\Delta^2\psi|_2^{1/2}|\nabla\psi|_2|A\mathbf{u}|_2 \\ \leqslant& \frac{\nu}{2}|A\mathbf{u}|_2^2 + \frac{1}{3}|\Delta^2\psi|_2^2 + C|\nabla\psi|_2^4|\Delta\psi|_2^2.\end{aligned}$$

Then, by Ladyzhenskaja inequality and standard estimates

$$\begin{aligned}&\left|2\left\langle(\mathbf{u}\cdot\nabla)\psi, \Delta^2\psi\right\rangle\right| \\ \leqslant& 2|\mathbf{u}|_4|\nabla\psi|_4|\Delta^2\psi|_2 \\ \leqslant& C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\nabla\psi|_2^{1/2}|\Delta\psi|_2^{1/2}|\Delta^2\psi|_2 \\ \leqslant& \frac{1}{3}|\Delta^2\psi|_2^2 + C|\mathbf{u}|_2^2|\nabla\mathbf{u}|_2^2 + C|\nabla\psi|_2^2|\Delta\psi|_2^2.\end{aligned}$$

We are left to consider the last term in (3.4.11), for which we exploit

$$|\Delta\psi|_2|\nabla\Delta\psi|_2 \leqslant C|\nabla\psi|_2|\Delta^2\psi|_2,$$

namely,

$$\begin{aligned}
&2\left|\left\langle \Delta f(\psi), \Delta^2\psi\right\rangle\right| \\
=&\left|2\left\langle f'(\psi)\Delta\psi, \Delta^2\psi\right\rangle + 2\left\langle f''(\psi)|\nabla\psi|^2, \Delta^2\psi\right\rangle\right| \\
\leqslant& C(1+|f(\psi)|_4)(|\Delta\psi|_4 + |\nabla\psi|_\infty|\nabla\psi|_4)|\Delta^2\psi|_2 \\
\leqslant& C(1+|f(\psi)|_4)(|\Delta\psi|_2^{1/2}|\nabla\Delta\psi|_2^{1/2} + |\nabla\psi|_2^{1/2}|\nabla\Delta\psi|_2^{1/2}|\nabla\psi|_2^{1/2}|\Delta\psi|_2^{1/2})|\Delta^2\psi|_2 \\
\leqslant& C(1+|f(\psi)|_4)(|\nabla\psi|_2^{1/2}|\Delta^2\psi|_2^{1/2} + |\nabla\psi|_2^{3/2}|\Delta^2\psi|_2^{1/2})|\Delta^2\psi|_2 \\
\leqslant& \frac{1}{3}|\Delta^2\psi|_2^2 + C(1+|f(\psi)|_4^4)(1+|\nabla\psi|_2^6).
\end{aligned}$$

We finally deduce the differential inequality

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2 + |\Delta\psi|_2^2\right) + \nu|A\mathbf{u}|_2^2 + |\Delta^2\psi|_2^2 \\
\leqslant& C|\mathbf{u}|_2^2|\nabla\mathbf{u}|_2^4 \\
&+ C\left(|\mathbf{u}|_2^2|\nabla\mathbf{u}|_2^2 + (1+|f(\psi)|_4^4)(|\nabla\psi|_2^6+1) + (|\nabla\psi|_2^4+1)|\Delta\psi|_2^2 + |\mathbf{g}|_2^2\right).
\end{aligned} \tag{3.4.12}$$

Introducing

$$\begin{aligned}
h &= C|\mathbf{u}|_2^2|\nabla\mathbf{u}|_2^2 \\
g &= C\left(|\mathbf{u}|_2^2|\nabla\mathbf{u}|_2^2 + (1+|f(\psi)|_4^4)(|\nabla\psi|_2^6+1) + (|\nabla\psi|_2^4+1)|\Delta\psi|_2^2 + |\mathbf{g}|_2^2\right),
\end{aligned}$$

the above differential inequality reads as

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{z}\|_{\mathcal{H}_1}^2 \leqslant h\|\mathbf{z}\|_{\mathcal{H}_1}^2 + g. \tag{3.4.13}$$

Thus Gronwall's lemma gives

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant \left(\|\mathbf{z}(\tau)\|_{\mathcal{H}_1}^2 + \int_\tau^t g(s)\,\mathrm{d}s\right) e^{\int_\tau^t h(s)\,\mathrm{d}s}$$

where, by (3.4.8) and Lemma 3.3.2 we have

$$\begin{aligned}
&\int_\tau^t h(s)\,\mathrm{d}s \leqslant CA_{t,\tau}^2 \\
&\int_\tau^t g(s)\,\mathrm{d}s \leqslant C\left(|\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^5 + (t-\tau)A_{t,\tau}^4\right)e^{C(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3)}
\end{aligned}$$

and the estimate (3.4.10). Moreover, integrating (3.4.12), we also have

$$\begin{aligned}
&\int_\tau^t \left(|\Delta^2\psi(s)|_2^2 + |\Delta\mathbf{u}(s)|_2^2\right)\,\mathrm{d}s \\
&\quad\leqslant C\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2 + |\mu(\tau)|_2^2 + A_{t,\tau}^3 + (t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^7 + (t-\tau)A_{t,\tau}^6\right)e^{C\left(A_{t,\tau}^4 + (t-\tau)A_{t,\tau}^3\right)}. \qquad \square
\end{aligned}$$

In the case of regular initial data, i.e. $\mathbf{z}_0 \in \mathcal{H}_1$, we thus have the sought higher regularity for solutions:

$$\begin{aligned}\mathbf{u} &\in L^\infty(\tau,T;\mathbf{H}^1_{0,\mathrm{div}}(\Omega)) \cap L^2(\tau,T;\mathbf{H}^2_{0,\mathrm{div}}(\Omega))\\ \psi &\in L^\infty(\tau,T;H^2(\Omega)) \cap L^2(\tau,T;H^4(\Omega))\\ \partial_t\psi &\in L^2(\tau,T;L^2(\Omega))\end{aligned}$$

Corollary 3.4.5. *Given any symbol* $\mathbf{g}$ *satisfying (B.1) and (B.2) and any* $t_0 \in \mathbb{R}$*, there exists a positive constant* $C_{\mathbf{g}}(t_0)$ *such that, for any bounded set* $D \subset \mathcal{H}_0$*, there exists* $T = T(|D|) > 0$ *depending only on* $|D| \doteq \max\{1, \sup_{\mathbf{z}\in D}\|\mathbf{z}\|_{\mathcal{H}_0}\}$ *such that*

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1} + |\mu(t)|_2 \leqslant C_{\mathbf{g}}(t_0), \qquad t \leqslant t_0, \quad \tau \leqslant t - 4 - T(|D|),$$

where $\mathbf{z}(t)$ *is the solution to the problem with symbol* $\mathbf{g}$*, departing at time* τ *from the initial datum* $\mathbf{z}_0 \in D$*, and* $\mu(t)$ *is the corresponding chemical potential. Besides, the following integral estimates hold true*

$$\int_{t-1}^{t} |f(\psi(s)|_4^8 \,\mathrm{d}s \leqslant Q(M_{\mathbf{g}}(t_0))$$

for $t \leqslant t_0$*,* $\tau \leqslant t - 4 - T(|D|)$*, and, for* $t \leqslant t_0$*,* $\tau \leqslant t - 5 - T(|D|)$*,*

$$\int_{t-1}^{t} \left(|\Delta\mathbf{u}(s)|_2^2 + |\Delta^2\psi(s)|_2^2\right) \,\mathrm{d}s \leqslant Q(M_{\mathbf{g}}(t_0)),$$

for some nonnegative increasing function Q *depending on* p *only through a multiplicative constant.*

Proof. In order to prove the claim, we divide our argument in several steps. At each step, thanks to the estimates of the previous sections, we will be able to improve the regularity of the solution of (3.0.1)-(3.0.2) by letting the system evolve for a time interval sufficiently large (with the only exception of the initial step, however, all time steps will be taken equal to 1).

Firstly, thanks to Corollary 3.3.3, for any $t_0 \in \mathbb{R}$, any symbol $\mathbf{g}$ as above and any bounded set $D \subset \mathcal{H}_0$, there exists $T = T(|D|) > 0$ such that

$$\|\mathbf{z}(t)\|^2_{\mathcal{H}_0} + 2|F(\psi(t))|_1 \leqslant 1 + C(1 + M_{\mathbf{g}}(t_0)) \leqslant C(1 + M_{\mathbf{g}}(t_0)), \quad t \leqslant t_0, \quad \tau \leqslant t - T,$$

for any $\mathbf{z}_0 \in D$. Moreover integrating (3.3.5) and (3.3.6), for $t \leqslant t_0$

$$\int_{t-1}^{t} \left(\|\mathbf{z}(s)\|^2_{\mathcal{H}_1} + |\nabla\mu(s)|_2^2\right) \,\mathrm{d}s \leqslant C(1 + M_{\mathbf{g}}(t_0)) + \|\mathbf{z}(t-1)\|^2_{\mathcal{H}_0} + 2|F(\psi(t-1))|_1, \quad \tau \leqslant t - 1,$$

so that, provided that $\tau \leqslant t - 1 - T$, we deduce

$$\int_{t-1}^{t} \left(\|\mathbf{z}(s)\|^2_{\mathcal{H}_1} + |\nabla\mu(s)|_2^2\right) \,\mathrm{d}s \leqslant C(1 + M_{\mathbf{g}}(t_0))$$

as well as

$$A_{t,s} \leqslant C(1 + M_{\mathbf{g}}(t_0)), \qquad \tau + T \leqslant t - 1 \leqslant s \leqslant t \leqslant t_0. \tag{3.4.14}$$

It thus follows from Lemmata 3.3.2, 3.4.1 and 3.4.2

$$\int_{t-1}^{t} \left(|\Delta\psi(s)|_2^4 + |\Delta\psi(s)|_{p+3}^2 + |\mu(s)|_2^2 \right) \mathrm{d}s \leqslant C A_{t,t-1}^2 \leqslant C(1 + M_{\mathbf{g}}^2(t_0)), \quad \tau \leqslant t - 1 - T,$$

allowing to prove that the functions h and g in the differential inequality (3.4.6), for $\tau + T < t - 1 < t \leqslant t_0$, satisfy

$$\int_{t-1}^{t} h(s)\mathrm{d}s \leqslant C A_{t,t-1}^4 \leqslant C(1 + M_{\mathbf{g}}^4(t_0)), \qquad \int_{t-1}^{t} g(s)\mathrm{d}s \leqslant C A_{t,t-1}^3 \leqslant C(1 + M_{\mathbf{g}}^3(t_0)).$$

Hence, by the Uniform Gronwall's lemma and (3.4.14), it follows

$$|\mu(t)|_2^2 \leqslant C \left(1 + M_{\mathbf{g}}^3(t_0)\right) e^{C\left(1 + M_{\mathbf{g}}^4(t_0)\right)}, \qquad \tau + T + 2 \leqslant t \leqslant t_0 \tag{3.4.15}$$

as well as

$$\int_{t-1}^{t} |\Delta\mu(s)|_2^2 \mathrm{d}s \leqslant C \left(1 + M_{\mathbf{g}}^7(t_0)\right) e^{C\left(1 + M_{\mathbf{g}}^4(t_0)\right)}, \qquad \tau + T + 3 \leqslant t \leqslant t_0.$$

Then the first claimed integral estimate follows from (3.4.9) and (3.4.15), while the functions h and g in (3.4.13) satisfy

$$\int_{t-1}^{t} h(s)\,\mathrm{d}s \leqslant C \left(1 + M_{\mathbf{g}}^2(t_0)\right) \qquad \int_{t-1}^{t} g(s)\,\mathrm{d}s \leqslant C \left(1 + M_{\mathbf{g}}^8(t_0)\right) e^{C\left(1 + M_{\mathbf{g}}^4(t_0)\right)},$$

provided that $\tau + T + 3 \leqslant t \leqslant t_0$. Therefore, applying the Uniform Gronwall's lemma to (3.4.13) we deduce

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant C_{\mathbf{g}}^2(t_0), \qquad \tau + T + 4 \leqslant t \leqslant t_0,$$

where

$$C_{\mathbf{g}}^2(t_0) \doteq C \left(1 + M_{\mathbf{g}}^8(t_0)\right) e^{C\left(1 + M_{\mathbf{g}}^4(t_0)\right)}.$$

Finally, provided that $\tau \leqslant t - 5 - T$, integrating (3.4.12) over $(t-1, t)$ we obtain

$$\int_{t-1}^{t} \left(|\Delta\mathbf{u}(s)|_2^2 + |\Delta^2\psi(s)|_2^2 \right) \mathrm{d}s \leqslant C \left(1 + M_{\mathbf{g}}^{10}(t_0)\right) e^{C\left(1 + M_{\mathbf{g}}^4(t_0)\right)}. \qquad \square$$

3.5 Continuous dependence

In this section we obtain continuous dependence estimates of the solutions w.r.t. initial data and forcing terms (see Lemmata 3.5.1 and 3.5.2).

In order to address the first issue and to simplify notation, throughout the section we indicate by symbols with no subscripts the difference between quantities denoted by subscripts 1 and 2, i.e.,

$$f \doteq f_1 - f_2.$$

From (3.0.1)-(3.0.2) we easily see that the difference between two solutions $\mathbf{z}_1 = (\mathbf{u}_1, \psi_1)$ and $\mathbf{z}_2 = (\mathbf{u}_2, \psi_2)$ satisfies the system

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}_1 + (\mathbf{u}_2\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} = \mu_1\nabla\psi_1 - \mu_2\nabla\psi_2 + \mathbf{g} \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + \mathbf{u}\cdot\nabla\psi_1 + \mathbf{u}_2\cdot\nabla\psi = \Delta\mu \qquad \text{in} \quad \Omega, \\ \mu = -\Delta\psi + f(\psi_1) - f(\psi_2) \\ \psi(\tau) = \psi_{01} - \psi_{02}, \quad \mathbf{u}(\tau) = \mathbf{u}_{01} - \mathbf{u}_{02} \end{cases} \tag{3.5.1}$$

with the boundary conditions

$$\mathbf{u} = \mathbf{0}, \quad \partial_{\mathbf{n}}\psi = 0, \quad \partial_{\mathbf{n}}\mu = 0, \qquad \text{on } \partial\Omega.$$

Lemma 3.5.1. *Let $\mathbf{z}_{01}, \mathbf{z}_{02} \in \mathcal{H}_0$ be any pair of initial data and let $\mathbf{g}_1, \mathbf{g}_2 \in L^2_{\mathrm{loc}}(-\infty, t; \mathbf{L}^2_{\mathrm{div}}(\Omega))$ be any pair of symbols. Then there exists a constant C such that, if $\mathbf{z}_i(t)$, $i = 1, 2$, are the solutions of (3.0.1)-(3.0.2) with initial data $\mathbf{z}_{0i}$ at time τ and symbol $\mathbf{g}_i$, then the following estimates hold*

$$\|\mathbf{z}(t)\|^2_{\mathcal{H}_0} \leqslant \left(\|\mathbf{z}_0\|^2_{\mathcal{H}_0} + \int_\tau^t |\mathbf{g}(s)|_2^2 \,\mathrm{d}s\right) e^{C\left(\overline{A_{t,\tau}}^6 + (t-\tau)\overline{A_{t,\tau}}^5\right)}$$

and

$$\begin{aligned} &\int_\tau^t \left(|\nabla\mathbf{u}(s)|_2^2 + |\nabla\Delta\psi(s)|_2^2\right) \mathrm{d}s \\ \leqslant & C\left(\|\mathbf{z}_0\|^2_{\mathcal{H}_0} + \int_\tau^t |\mathbf{g}(s)|_2^2 \,\mathrm{d}s\right)\left(\overline{A_{t,\tau}}^6 + (t-\tau)\overline{A_{t,\tau}}^5\right) e^{C\left(\overline{A_{t,\tau}}^6 + (t-\tau)\overline{A_{t,\tau}}^5\right)}, \end{aligned}$$

where $\overline{A_{t,\tau}}$ is defined by $\overline{A_{t,\tau}} \doteq A_{t,\tau(1)} + A_{t,\tau(2)}$ and $A_{t,\tau(i)}$ is the quantity corresponding to the initial datum $\mathbf{z}_i$ and the forcing term $\mathbf{g}_i$, for $i = 1, 2$.

Proof. Recalling that, thanks to the incompressibility assumption on the velocity fields $\mathbf{u}_i$, for $i = 1, 2$, we have

$$\begin{aligned} &\langle \mu_i\nabla\psi_i, \mathbf{u}_i\rangle \\ =& -\langle \Delta\psi_i\nabla\psi_i, \mathbf{u}_i\rangle + \langle f(\psi_i)\nabla\psi_i, \mathbf{u}_i\rangle = -\langle \Delta\psi_i\nabla\psi_i, \mathbf{u}_i\rangle + \langle \nabla F(\psi_i), \mathbf{u}_i\rangle \\ =& -\langle \Delta\psi_i\nabla\psi_i, \mathbf{u}_i\rangle. \end{aligned}$$

Moreover, the product of the first equation in (3.5.1) by $2\mathbf{u}$ gives

$$\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}|_2^2 + 2\nu|\nabla\mathbf{u}|_2^2 + 2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, \mathbf{u}\rangle = -2\langle\Delta\psi\nabla\psi_1, \mathbf{u}\rangle - 2\langle\Delta\psi_2\nabla\psi, \mathbf{u}\rangle + 2\langle\mathbf{g}, \mathbf{u}\rangle. \tag{3.5.2}$$

Noticing that

$$\begin{aligned}
&\langle \Delta\mu, \Delta\psi\rangle \\
=&\langle \Delta[-\Delta\psi + f(\psi_1) - f(\psi_2)], \Delta\psi\rangle \\
=&|\nabla\Delta\psi|_2^2 + \left\langle f'(\psi_1)\Delta\psi, \Delta\psi\right\rangle + \left\langle [f'(\psi_1) - f'(\psi_2)]\Delta\psi_2, \Delta\psi\right\rangle \\
&\quad + \left\langle f''(\psi_1)\nabla\psi(\nabla\psi_1 + \nabla\psi_2), \Delta\psi\right\rangle + \left\langle [f''(\psi_1) - f''(\psi_2)]|\nabla\psi_2|^2, \Delta\psi\right\rangle \\
\geqslant&|\nabla\Delta\psi|_2^2 - 2\alpha|\Delta\psi|_2^2 + \left\langle [f'(\psi_1) - f'(\psi_2)]\Delta\psi_2, \Delta\psi\right\rangle \\
&\quad + \left\langle f''(\psi_1)\nabla\psi(\nabla\psi_1 + \nabla\psi_2), \Delta\psi\right\rangle + \left\langle [f''(\psi_1) - f''(\psi_2)]|\nabla\psi_2|^2, \Delta\psi\right\rangle,
\end{aligned}$$

the product of the third equation in (3.5.1) by $-2\Delta\psi$ yields

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\psi|_2^2 + 2|\nabla\Delta\psi|_2^2 - 2\left\langle (\mathbf{u}\cdot\nabla)\psi_1, \Delta\psi\right\rangle - 2\left\langle (\mathbf{u}_2\cdot\nabla)\psi, \Delta\psi\right\rangle \\
\leqslant&4\alpha|\Delta\psi|_2^2 - 2\left\langle [f'(\psi_1) - f'(\psi_2)]\Delta\psi_2, \Delta\psi\right\rangle \\
&\quad - 2\left\langle f''(\psi_1)\nabla\psi(\nabla\psi_1 + \nabla\psi_2), \Delta\psi\right\rangle - 2\left\langle [f''(\psi_1) - f''(\psi_2)]|\nabla\psi_2|^2, \Delta\psi\right\rangle.
\end{aligned}$$

Adding this last inequality to (3.5.2) we have

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\psi|_2^2\right) + 2\nu|\nabla\mathbf{u}|_2^2 + 2|\nabla\Delta\psi|_2^2 \qquad (3.5.3)\\
\leqslant&4\alpha|\Delta\psi|_2^2 - 2\left\langle [f'(\psi_1) - f'(\psi_2)]\Delta\psi_2, \Delta\psi\right\rangle - 2\left\langle f''(\psi_1)\nabla\psi(\nabla\psi_1 + \nabla\psi_2), \Delta\psi\right\rangle \\
&\quad - 2\left\langle [f''(\psi_1) - f''(\psi_2)]|\nabla\psi_2|^2, \Delta\psi\right\rangle + 2\left\langle (\mathbf{u}_2\cdot\nabla)\psi, \Delta\psi\right\rangle \\
&\quad - 2\left\langle (\mathbf{u}\cdot\nabla)\psi, \Delta\psi_2\right\rangle - 2\left\langle (\mathbf{u}\cdot\nabla)\mathbf{u}_1, \mathbf{u}\right\rangle + 2\left\langle \mathbf{g}, \mathbf{u}\right\rangle.
\end{aligned}$$

Since $|\Delta\psi|_2^2 \leqslant |\nabla\psi|_2|\nabla\Delta\psi|_2$, we immediately obtain

$$4\alpha|\Delta\psi|_2^2 \leqslant 4\alpha|\nabla\psi|_2|\nabla\Delta\psi|_2 \leqslant \frac{1}{5}|\nabla\Delta\psi|_2^2 + C|\nabla\psi|_2^2.$$

Before dealing with the terms arising from the double-well potential F, we introduce some useful estimates for terms of the form $|f^{(k)}(\psi_1) - f^{(k)}(\psi_2)|$. Indeed from the fundamental theorem of calculus and by assumptions (A.7) and (A.5) we have

$$\begin{aligned}
&\left|f^{(k)}(\psi_1) - f^{(k)}(\psi_2)\right| \\
=&\left|\int_{\psi_2}^{\psi_1} f^{(k+1)}(s)\,\mathrm{d}s\right| \leqslant \int_{\psi_1}^{\psi_2}\left|f^{(k+1)}(s)\right|\,\mathrm{d}s \leqslant C\int_{\psi_1}^{\psi_2}\left(1 + F(s)^{(p+1-k)/(p+3)}\right)\,\mathrm{d}s \\
\leqslant&C\left(1 + F(\psi_1)^{(p+1-k)/(p+3)} + F(\psi_2)^{(p+1-k)/(p+3)}\right)|\psi_1 - \psi_2|.
\end{aligned}$$

Moreover, we can estimate suitable L^q norms of this difference as follows

$$
\begin{aligned}
&|f^{(k)}(\psi_1) - f^{(k)}(\psi_2)|_{\frac{p+3}{p+2-k}} \qquad (3.5.4)\\
\leqslant& C\left(\int_\Omega \left(1 + F(\psi_1) + F(\psi_2)\right)^{(p+1-k)/(p+2-k)} |\psi_1 - \psi_2|^{(p+3)/(p+2-k)}\, \mathrm{d}\mathbf{x}\right)^{(p+2-k)/(p+3)}\\
\leqslant& C\left(\int_\Omega \left(1 + F(\psi_1) + F(\psi_2)\right) \mathrm{d}\mathbf{x}\right)^{(p+1-k)/(p+3)} \left(\int_\Omega |\psi_1 - \psi_2|^{p+3}\, \mathrm{d}\mathbf{x}\right)^{1/(p+3)}\\
\leqslant& C\left(1 + |F(\psi_1)|_1^{(p+1-k)/(p+3)} + |F(\psi_2)|_1^{(p+1-k)/(p+3)}\right) |\psi|_{p+3}.
\end{aligned}
$$

In light of this bound, we can now resume the estimation of the terms in the right hand side of (3.5.3). We have

$$
\begin{aligned}
&\left|2\left\langle \left(f'(\psi_1) - f'(\psi_2)\right) \Delta\psi_2, \Delta\psi\right\rangle\right|\\
\leqslant& 2|f'(\psi_1) - f'(\psi_2)|_{\frac{p+3}{p+1}} |\Delta\psi_2|_{p+3} |\Delta\psi|_{p+3}\\
\leqslant& C\left(1 + |F(\psi_1)|_1^{p/(p+3)} + |F(\psi_2)|_1^{p/(p+3)}\right) |\nabla\psi|_2 |\Delta\psi_2|_{p+3} |\nabla\Delta\psi|_2\\
\leqslant& \frac{1}{5}|\nabla\Delta\psi|_2^2 + C\left(1 + |F(\psi_1)|_1^{p/(p+3)} + |F(\psi_2)|_1^{p/(p+3)}\right)^2 |\Delta\psi_2|_{p+3}^2 |\nabla\psi|_2^2.
\end{aligned}
$$

Analogously we also obtain

$$
\begin{aligned}
&\left|-2\left\langle \left(f''(\psi_1) - f''(\psi_2)\right) |\nabla\psi_2|^2, \Delta\psi\right\rangle\right|\\
\leqslant& 2|f''(\psi_1) - f''(\psi_2)|_{\frac{p+3}{p}} |\nabla\psi_2|_{p+3}^2 |\Delta\psi|_{p+3}\\
\leqslant& C\left(1 + |F(\psi_1)|_1^{(p-1)/(p+3)} + |F(\psi_2)|_1^{(p-1)/(p+3)}\right) |\nabla\psi|_2 |\Delta\psi_2|_2^2 |\nabla\Delta\psi|_2\\
\leqslant& \frac{1}{5}|\nabla\Delta\psi|_2^2 + C\left(1 + |F(\psi_1)|_1^{(p-1)/(p+3)} + |F(\psi_2)|_1^{(p-1)/(p+3)}\right)^2 |\Delta\psi_2|_2^4 |\nabla\psi|_2^2.
\end{aligned}
$$

The last term involving the potential F and its derivatives can be dealt with in a similar way. Again the assumptions on F provide

$$
\begin{aligned}
&\left|-2\left\langle f''(\psi_1)\nabla\psi(\nabla\psi_1 + \nabla\psi_2), \Delta\psi\right\rangle\right|\\
\leqslant& 2|f''(\psi_1)|_{\frac{p+3}{p}} |\nabla\psi|_{p+3} \left(|\nabla\psi_1|_{p+3} + |\nabla\psi_2|_{p+3}\right) |\Delta\psi|_{p+3}\\
\leqslant& C\left(1 + |F(\psi_1)|_1^{p/(p+3)}\right) |\Delta\psi|_2 \left(|\Delta\psi_1|_2 + |\Delta\psi_2|_2\right) |\nabla\Delta\psi|_2\\
\leqslant& C\left(1 + |F(\psi_1)|_1^{p/(p+3)}\right) |\nabla\psi|_2^{1/2} |\nabla\Delta\psi|_2^{1/2} \left(|\Delta\psi_1|_2 + |\Delta\psi_2|_2\right) |\nabla\Delta\psi|_2\\
\leqslant& \frac{1}{5}|\nabla\Delta\psi|_2^2 + C\left(1 + |F(\psi_1)|_1^4\right) \left(|\Delta\psi_1|_2^4 + |\Delta\psi_2|_2^4\right) |\nabla\psi|_2^2.
\end{aligned}
$$

We also bound the last four terms on the right hand side of (3.5.3), which arise from the linear

momentum equation. Thanks to Agmon's inequality, we have $|\nabla\psi|_\infty^2 \leqslant C|\nabla\psi|_2|\nabla\Delta\psi|_2$, and thus

$$\begin{aligned}
&|2\langle(\mathbf{u}_2\cdot\nabla)\psi,\Delta\psi\rangle - 2\langle(\mathbf{u}\cdot\nabla)\psi,\Delta\psi_2\rangle|\\
\leqslant&2|\mathbf{u}_2|_2|\nabla\psi|_\infty|\Delta\psi|_2 + 2|\mathbf{u}|_2|\nabla\psi|_\infty|\Delta\psi_2|_2\\
\leqslant&C|\mathbf{u}_2|_2|\nabla\psi|_2|\nabla\Delta\psi|_2 + C|\mathbf{u}|_2|\nabla\psi|_2^{1/2}|\nabla\Delta\psi|_2^{1/2}|\Delta\psi_2|_2\\
\leqslant&\frac{1}{5}|\nabla\Delta\psi|_2^2 + \frac{\nu}{2}|\nabla\mathbf{u}|_2^2 + C(|\mathbf{u}_2|_2^2 + |\Delta\psi_2|_2^4)|\nabla\psi|_2^2
\end{aligned}$$

holds. Finally, by Ladyzhenskaja inequality, it follows

$$\begin{aligned}
&|-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1,\mathbf{u}\rangle + 2\langle\mathbf{g},\mathbf{u}\rangle|\\
\leqslant&C|\mathbf{u}|_4^2|\nabla\mathbf{u}_1|_2 + C|\mathbf{g}|_2|\nabla\mathbf{u}|_2\\
\leqslant&C|\mathbf{u}|_2|\nabla\mathbf{u}|_2|\nabla\mathbf{u}_1|_2 + C|\mathbf{g}|_2|\nabla\mathbf{u}|_2\\
\leqslant&\frac{\nu}{2}|\nabla\mathbf{u}|_2^2 + C|\nabla\mathbf{u}_1|_2^2|\mathbf{u}|_2^2 + C|\mathbf{g}|_2^2.
\end{aligned}$$

Replacing the above estimates in (3.5.3), we see that $\|\mathbf{z}(t)\|_{\mathcal{H}_0}^2 = |\mathbf{u}(t)|_2^2 + |\nabla\psi(t)|_2^2$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{z}\|_{\mathcal{H}_0}^2 + \nu|\nabla\mathbf{u}|_2^2 + |\nabla\Delta\psi|_2^2 \leqslant C|\mathbf{g}|_2^2 + h\|\mathbf{z}\|_{\mathcal{H}_0}^2,$$

where h is given by

$$\begin{aligned}
h \doteq&C\left(1 + |\nabla\mathbf{u}_1|_2^2 + |\nabla\mathbf{u}_2|_2^2\right)\\
&+ C\left(1 + |F(\psi_1)|_1^4 + |F(\psi_2)|_1^4\right)\left(|\Delta\psi_1|_2^4 + |\Delta\psi_2|_2^4 + |\Delta\psi_2|_{p+3}^2\right).
\end{aligned}$$

By the results of the previous section we deduce

$$\int_\tau^t h(s)\,\mathrm{d}s \leqslant C\left(\overline{A_{t,\tau}}^6 + (t-\tau)\overline{A_{t,\tau}}^5\right)$$

so that Gronwall's lemma finally gives the claimed estimates. □

In order to apply the abstract framework described in Section 3.2, we also need the following higher order continuous dependence estimate.

Lemma 3.5.2. *Let $\mathbf{z}_{01},\mathbf{z}_{02}\in\mathcal{H}_1$ be any pair of initial data so that $\mu_{0i}\doteq f(\psi_{0i})-\Delta\psi_{0i}\in L^2(\Omega)$, $i=1,2$ and let $\mathbf{g}_1,\mathbf{g}_2\in L^2_{\mathrm{loc}}(-\infty,t;\mathbf{L}^2_{\mathrm{div}}(\Omega))$ be any pair of symbols. Then there exists a constant C such that, if $\mathbf{z}_i(t)$, $i=1,2$ are the solutions of (3.0.1)-(3.0.2) with initial data $\mathbf{z}_{0i}$ at time τ and symbol $\mathbf{g}_i$, then the following estimate holds*

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant e^{Q(A_{t,\tau},t-\tau)\left(1+\|\mathbf{z}_{01}\|_{\mathcal{H}_1}^2+\|\mathbf{z}_{02}\|_{\mathcal{H}_1}^2+|\mu_{01}|_2^2+|\mu_{02}|_2^2\right)}\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2 + \int_\tau^t|\mathbf{g}(s)|_2^2\,\mathrm{d}s\right),$$

where Q is a nonnegative increasing function of its arguments.

Proof. We start by multiplying the first equation in (3.5.1) by $2A\mathbf{u} = -2\mathbb{P}\Delta\mathbf{u}$, getting

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\mathbf{u}|_2^2 + 2\nu|A\mathbf{u}|_2^2\\ =&-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, A\mathbf{u}\rangle - 2\langle(\mathbf{u}_2\cdot\nabla)\mathbf{u}, A\mathbf{u}\rangle - 2\langle\Delta\psi_1\nabla\psi_1, A\mathbf{u}\rangle + 2\langle\Delta\psi_2\nabla\psi_2, A\mathbf{u}\rangle + 2\langle\mathbf{g}, A\mathbf{u}\rangle.\end{aligned}$$

The product of the third equation in (3.5.1) by $2\Delta^2\psi$, after an integration by parts, provides

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}|\Delta\psi|_2^2 + 2|\Delta^2\psi|_2^2\\ =&-2\left\langle\mathbf{u}\cdot\nabla\psi_1, \Delta^2\psi\right\rangle - 2\left\langle\mathbf{u}_2\cdot\nabla\psi, \Delta^2\psi\right\rangle - 2\left\langle f'(\psi_1)\nabla\Delta\psi, \nabla\Delta\psi\right\rangle\\ &-2\left\langle[f'(\psi_1)-f'(\psi_2)]\nabla\Delta\psi_2, \nabla\Delta\psi\right\rangle - 2\left\langle f''(\psi_1)\nabla\psi\Delta\psi_1, \nabla\Delta\psi\right\rangle\\ &-2\left\langle[f''(\psi_1)-f''(\psi_2)]\nabla\psi_2\Delta\psi_1, \nabla\Delta\psi\right\rangle - 2\left\langle f''(\psi_2)\nabla\psi_2\Delta\psi, \nabla\Delta\psi\right\rangle\\ &-4\left\langle f''(\psi_1)\nabla^2\psi_1\nabla\psi, \nabla\Delta\psi\right\rangle - 4\left\langle(f''(\psi_1)-f''(\psi_2))\nabla^2\psi_1\nabla\psi_2, \nabla\Delta\psi\right\rangle\\ &-4\left\langle f''(\psi_2)\nabla^2\psi\nabla\psi_2, \nabla\Delta\psi\right\rangle - 2\left\langle f'''(\psi_1)\nabla\psi\,|\nabla\psi_1|^2, \nabla\Delta\psi\right\rangle\\ &-2\left\langle f'''(\psi_1)\nabla\psi_2\nabla\psi\cdot(\nabla\psi_1+\nabla\psi_2), \nabla\Delta\psi\right\rangle\\ &-2\langle[f'''(\psi_1)-f'''(\psi_2)]\nabla\psi_2|\nabla\psi_2|^2, \nabla\Delta\psi\rangle.\end{aligned}$$

Adding together the two equations, by Assumption (A.5) we obtain

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\mathbf{u}\|_{\mathbf{H}^1_{0,\mathrm{div}}(\Omega)}^2 + |\Delta\psi|_2^2\right) + 2\nu|A\mathbf{u}|_{\mathbf{L}^2_{\mathrm{div}}(\Omega)}^2 + 2|\Delta^2\psi|_2^2\\ \leqslant&-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, A\mathbf{u}\rangle - 2\langle(\mathbf{u}_2\cdot\nabla)\mathbf{u}, A\mathbf{u}\rangle - 2\langle\Delta\psi\nabla\psi_1, A\mathbf{u}\rangle - 2\langle\Delta\psi_2\nabla\psi, A\mathbf{u}\rangle\\ &+2\langle\mathbf{g}, A\mathbf{u}\rangle - 2\left\langle\mathbf{u}\cdot\nabla\psi_1, \Delta^2\psi\right\rangle - 2\left\langle\mathbf{u}_2\cdot\nabla\psi, \Delta^2\psi\right\rangle + 4\alpha|\nabla\Delta\psi|_2^2\\ &-2\left\langle[f'(\psi_1)-f'(\psi_2)]\nabla\Delta\psi_2, \nabla\Delta\psi\right\rangle - 2\left\langle f''(\psi_1)\nabla\psi\Delta\psi_1, \nabla\Delta\psi\right\rangle\\ &-2\left\langle[f''(\psi_1)-f''(\psi_2)]\nabla\psi_2\Delta\psi_1, \nabla\Delta\psi\right\rangle - 2\left\langle f''(\psi_2)\nabla\psi_2\Delta\psi, \nabla\Delta\psi\right\rangle\\ &-4\left\langle f''(\psi_1)\nabla^2\psi_1\nabla\psi, \nabla\Delta\psi\right\rangle - 4\left\langle(f''(\psi_1)-f''(\psi_2))\nabla^2\psi_1\nabla\psi_2, \nabla\Delta\psi\right\rangle\\ &-4\left\langle f''(\psi_2)\nabla^2\psi\nabla\psi_2, \nabla\Delta\psi\right\rangle - 2\left\langle f'''(\psi_1)\nabla\psi\,|\nabla\psi_1|^2, \nabla\Delta\psi\right\rangle\\ &-2\left\langle f'''(\psi_1)\nabla\psi_2\nabla\psi\cdot(\nabla\psi_1+\nabla\psi_2), \nabla\Delta\psi\right\rangle\\ &-2\left\langle[f'''(\psi_1)-f'''(\psi_2)]\nabla\psi_2|\nabla\psi_2|^2, \nabla\Delta\psi\right\rangle.\end{aligned}$$

We now show that all the eighteen terms on the right hand side of the last inequality can be bounded by

$$h\left(|\nabla\mathbf{u}|_2^2 + |\Delta\psi|_2^2\right),$$

where h is an integrable quantity. Standard computations for the Navier-Stokes equation lead to

$$\begin{aligned}&|-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, A\mathbf{u}\rangle - 2\langle(\mathbf{u}_2\cdot\nabla)\mathbf{u}, A\mathbf{u}\rangle|\\ \leqslant&C|\mathbf{u}|_2^{1/2}|A\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}_1|_2|A\mathbf{u}|_2 + C|\mathbf{u}_2|_2^{1/2}|\nabla\mathbf{u}_2|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|A\mathbf{u}|_2^{3/2}\\ \leqslant&\frac{\nu}{3}|A\mathbf{u}|_2^2 + C|\nabla\mathbf{u}_1|_2^4|\mathbf{u}|_2^2 + C|\mathbf{u}_2|_2^2|\nabla\mathbf{u}_2|_2^2|\nabla\mathbf{u}|_2^2.\end{aligned}$$

Exploiting Agmon's inequality and the interpolation inequality $|\phi|_\infty \leqslant C|\phi|_2^{2/3}\|\phi\|_{H^3}^{1/3}$, we can bound the following three terms

$$\begin{aligned}
&|-2\langle\Delta\psi\nabla\psi_1, A\mathbf{u}\rangle - 2\langle\Delta\psi_2\nabla\psi, A\mathbf{u}\rangle + 2\langle\mathbf{g}, A\mathbf{u}\rangle| \\
\leqslant& 2[|\Delta\psi|_\infty|\nabla\psi_1|_2 + |\Delta\psi_2|_2|\nabla\psi|_\infty + |\mathbf{g}|_2]|A\mathbf{u}|_2 \\
\leqslant& 2[|\Delta\psi|_2^{1/2}|\Delta^2\psi|_2^{1/2}|\nabla\psi_1|_2 + |\Delta\psi_2|_2|\nabla\psi|_2^{2/3}|\Delta^2\psi|_2^{1/3} + |\mathbf{g}|_2]|A\mathbf{u}|_2 \\
\leqslant& \frac{\nu}{3}|A\mathbf{u}|_2^2 + \frac{1}{7}|\Delta^2\psi|_2^2 + C|\nabla\psi_1|_2^4|\Delta\psi|_2^2 + C|\Delta\psi_2|_2^3|\nabla\psi|_2^2 + C|\mathbf{g}|_2^2
\end{aligned}$$

as well as the next two

$$\begin{aligned}
&\left|-2\left\langle\mathbf{u}\cdot\nabla\psi_1, \Delta^2\psi\right\rangle - 2\left\langle\mathbf{u}_2\cdot\nabla\psi, \Delta^2\psi\right\rangle\right| \\
\leqslant& 2|\mathbf{u}|_\infty|\nabla\psi_1|_2|\Delta^2\psi|_2 + 2|\mathbf{u}_2|_2|\nabla\psi|_\infty|\Delta^2\psi|_2 \\
\leqslant& C|\mathbf{u}|_2^{1/2}|A\mathbf{u}|_2^{1/2}|\nabla\psi_1|_2|\Delta^2\psi|_2 + C|\mathbf{u}_2|_2|\nabla\psi|_2^{2/3}|\Delta^2\psi|_2^{4/3} \\
\leqslant& \frac{\nu}{3}|A\mathbf{u}|_2^2 + \frac{1}{7}|\Delta^2\psi|_2^2 + C|\nabla\psi_1|_2^4|\mathbf{u}|_2^2 + C|\mathbf{u}_2|_2^3|\nabla\psi|_2^2.
\end{aligned}$$

The terms arising from the double well potential can be treated using similar techniques. By interpolation, we have

$$4\alpha|\nabla\Delta\psi|_2^2 \leqslant \frac{1}{7}|\Delta^2\psi|_2^2 + C|\Delta\psi|_2^2,$$

while, by (3.5.4), we obtain

$$\begin{aligned}
&\left|-2\left\langle[f'(\psi_1) - f'(\psi_2)]\nabla\Delta\psi_2, \nabla\Delta\psi\right\rangle\right| \\
\leqslant& 2|f'(\psi_1) - f'(\psi_2)|_{\frac{p+3}{p+1}}|\nabla\Delta\psi_2|_{p+3}|\nabla\Delta\psi|_{p+3} \\
\leqslant& C\left(1 + |F(\psi_1)|_1^{p/(p+3)} + |F(\psi_2)|_1^{p/(p+3)}\right)|\nabla\psi|_2|\Delta^2\psi_2|_2|\Delta^2\psi|_2 \\
\leqslant& \frac{1}{7}|\Delta^2\psi|_2^2 + C\left(1 + |F(\psi_1)|_1 + |F(\psi_2)|_1\right)^2|\Delta^2\psi_2|_2^2|\nabla\psi|_2^2.
\end{aligned}$$

Using also Korn's inequality, from Assumptions (A.2) and (A.3) we deduce

$$\begin{aligned}
&\left|-2\left\langle f''(\psi_1)\nabla\psi\Delta\psi_1, \nabla\Delta\psi\right\rangle - 4\left\langle f''(\psi_1)\nabla^2\psi_1\nabla\psi, \nabla\Delta\psi\right\rangle\right| \\
\leqslant& C|f''(\psi_1)|_{\frac{p+3}{p}}|\nabla\psi|_{p+3}|\Delta\psi_1|_{p+3}|\nabla\Delta\psi|_{p+3} \\
\leqslant& C(1 + |F(\psi_1)|_1^{p/(p+3)})|\Delta\psi|_2|\Delta\psi_1|_{p+3}|\Delta^2\psi|_2 \\
\leqslant& \frac{1}{7}|\Delta^2\psi|_2 + C\left(1 + |F(\psi_1)|_1\right)^2|\Delta\psi_1|_{p+3}^2|\Delta\psi|_2^2.
\end{aligned}$$

Arguing as in the proof of Lemma 3.5.1, namely, exploiting (3.5.4) for the first two terms, and

Assumptions (A.2) and (A.3) for the second two, as well as Korn's inequality again, we obtain

$$
\begin{aligned}
&\left|-2\left\langle[f''(\psi_1)-f''(\psi_2)]\nabla\psi_2\Delta\psi_1,\nabla\Delta\psi\right\rangle-4\left\langle\left(f''(\psi_1)-f''(\psi_2)\right)\nabla^2\psi_1\nabla\psi_2,\nabla\Delta\psi\right\rangle\right.\\
&\quad\left.-2\left\langle f''(\psi_2)\nabla\psi_2\Delta\psi,\nabla\Delta\psi\right\rangle-4\left\langle f''(\psi_2)\nabla^2\psi\nabla\psi_2,\nabla\Delta\psi\right\rangle\right|\\
\leqslant&C\left(1+|F(\psi_1)|_1^{(p-1)/(p+3)}+|F(\psi_2)|_1^{(p-1)/(p+3)}\right)|\Delta\psi_2|_2|\Delta\psi_1|_{p+3}|\nabla\psi|_2|\Delta^2\psi|_2\\
&+C\left(1+|F(\psi_2)|_1^{p/(p+3)}\right)|\Delta\psi_2|_2|\nabla\Delta\psi|_2|\Delta^2\psi|_2\\
\leqslant&\frac{1}{7}|\Delta^2\psi|_2^2+C\left(1+|F(\psi_1)|_1^2+|F(\psi_2)|_1^2\right)|\Delta\psi_2|_2^2|\Delta\psi_1|_{p+3}^2|\nabla\psi|_2^2\\
&+C\left(1+|F(\psi_2)|_1^4\right)|\Delta\psi_2|_2^4|\Delta\psi|_2^2.
\end{aligned}
$$

We are left to consider

$$
\begin{aligned}
&\left|-2\left\langle f'''(\psi_1)\nabla\psi|\nabla\psi_1|^2,\nabla\Delta\psi\right\rangle-2\left\langle f'''(\psi_1)\nabla\psi_2\,\nabla\psi\cdot\left(\nabla\psi_1+\nabla\psi_2\right),\nabla\Delta\psi\right\rangle\right.\\
&\quad\left.-2\left\langle[f'''(\psi_1)-f'''(\psi_2)]\nabla\psi_2|\nabla\psi_2|^2,\nabla\Delta\psi\right\rangle\right|\\
\leqslant&C(1+|F(\psi_1)|_1^{(p-1)/(p+3)})(|\Delta\psi_1|_2^2+|\Delta\psi_1|_2||\Delta\psi_2|_2+|\Delta\psi_2|_2^2)|\Delta\psi|_2|\Delta^2\psi|_2\\
&+C\left(1+|F(\psi_1)|_1^{(p-2)/(p+3)}+|F(\psi_2)|_1^{(p-2)/(p+3)}\right)|\Delta\psi_2|_2^3|\nabla\psi|_2|\Delta^2\psi|_2\\
\leqslant&\frac{1}{7}|\Delta^2\psi|_2^2+C(1+|F(\psi_1)|_1^2)(|\Delta\psi_1|_2^4+|\Delta\psi_2|_2^4)|\Delta\psi|_2^2\\
&+C\left(1+|F(\psi_1)|_1^2+|F(\psi_2)|_1^2\right)|\Delta\psi_2|_2^6|\nabla\psi|_2^2.
\end{aligned}
\tag{3.5.5}
$$

Remark 3.5.1. In the case $p\in[1,2)$, under the assumption $f^{(iv)}(y)$ bounded for $y\in\mathbb{R}$ we can still derive the estimate for the term

$$
\left\langle|f'''(\psi_1)-f'''(\psi_2)|\nabla\psi_2|\nabla\psi_2|^2,\nabla\Delta\psi\right\rangle\leqslant C|\nabla\psi|_2|\Delta\psi_2|_2^3|\nabla\Delta\psi|_{p+3},
$$

which gives the same result as above.

From the above inequalities, collecting terms we obtain

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2+|\Delta\psi|_2^2\right)+\nu|A\mathbf{u}|_2^2+|\Delta^2\psi|_2^2\\
\leqslant&C\,|\mathbf{g}|_2^2+C\left(|\nabla\psi_1|_2^4+|\nabla\mathbf{u}_1|_2^4+|\mathbf{u}_2|_2^2|\nabla\mathbf{u}_2|_2^2\right)|\nabla\mathbf{u}|_2^2\\
&+C\left(|\mathbf{u}_2|_2^3+|\Delta\psi_2|_2^3+\left(1+|F(\psi_1)|_1^2+|F(\psi_2)|_1^2\right)\left(|\Delta^2\psi_2|_2^2+|\Delta\psi_2|_2^6+|\Delta\psi_2|_2^2|\Delta\psi_1|_{p+3}^2\right)\right)|\nabla\psi|_2^2\\
&+C\big(1+|\nabla\psi_1|_2^4+\left(1+|F(\psi_1)|_1^2\right)\left(|\Delta\psi_1|_2^4+|\Delta\psi_2|_2^4+|\Delta\psi_1|_{p+3}^2\right)+\left(1+|F(\psi_2)|_1^4\right)|\Delta\psi_2|_2^4)|\Delta\psi|_2^2.
\end{aligned}
$$

Denoting by

$$
\begin{aligned}
h=C&\left(1+|\nabla\psi_1|_2^4+|\mathbf{u}_2|_2^3+|\nabla\mathbf{u}_1|_2^4+|\mathbf{u}_2|_2^2|\nabla\mathbf{u}_2|_2^2+|\Delta\psi_2|_2^3\right.\\
&+\left(1+|F(\psi_1)|_1^2+|F(\psi_2)|_1^2\right)\left(|\Delta^2\psi_2|_2^2+|\Delta\psi_2|_2^6+|\Delta\psi_2|_2^2|\Delta\psi_1|_{p+3}^2\right)\\
&\left.+\left(1+|F(\psi_1)|_1^2\right)\left(|\Delta\psi_1|_2^4+|\Delta\psi_2|_2^4+|\Delta\psi_1|_{p+3}^2\right)+\left(1+|F(\psi_2)|_1^4\right)|\Delta\psi_2|_2^4\right),
\end{aligned}
$$

the above differential inequality reads as

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant h(t)\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 + C|\mathbf{g}(t)|_2^2 \tag{3.5.6}$$

and depends on p only through the constants C included in the definition of h. Therefore, the estimate obtained by Gronwall's lemma below has the structure

$$\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2 \leqslant e^{Q(\overline{A_{t,\tau}},t-\tau)\left(1+\|\mathbf{z}_{01}\|_{\mathcal{H}_1}^2+\|\mathbf{z}_{02}\|_{\mathcal{H}_1}^2+|\mu_{01}|_2^2+|\mu_{02}|_2^2\right)}\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2 + \int_\tau^t |\mathbf{g}(s)|_2^2\,\mathrm{d}s\right)$$

where, for any potential F satisfying the assumptions (A.1)–(A.7), the function Q depends on $\overline{A_{t,\tau}}$ only through some of its powers, which, in particular, do not depend on the growth exponent p (i.e. the shape) of F. □

3.6 Time regularity

In this section we evaluate the distance in $\mathcal{H}_0$ between the solution and the initial datum in terms of the time span (Lemma 3.6.1), and we show a smoothing property for difference of solutions (Lemma 3.6.2). This will be crucial to show that Assumptions (H.1) and (H.3) in Theorems 3.2.2 and 3.2.3 hold true for system (3.0.1).

Lemma 3.6.1. *Given any symbol* $\mathbf{g}$ *satisfying (B.1) and (B.2), there exists a positive constant* C *such that the solution* $\mathbf{z}(t)$*, departing at time* τ *from an arbitrary initial datum* $\mathbf{z}_0 \in \mathcal{H}_1$*, so that* $\mu_0 \in L^2(\Omega)$ *satisfies*

$$\begin{aligned}&\|\mathbf{z}(t)-\mathbf{z}_0\|_{\mathcal{H}_0}^2\\ \leqslant&\sqrt{t-\tau}\,\left(\|\mathbf{z}_0\|_{\mathcal{H}_1}^2+|\mu_0|_2^2+A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^8+(t-\tau)A_{t,\tau}^7\right)e^{C\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right)},\end{aligned}$$

for $\tau \leqslant t \leqslant t_0$.

Proof. The different features of the Navier-Stokes and the Cahn-Hilliard equations force to handle separately the two variables. We preliminarily observe that, denoting the solution and the initial datum as $\mathbf{z}(t) = (\mathbf{u}(t), \psi(t))$ and $\mathbf{z}_0 = (\mathbf{u}_0, \psi_0)$, respectively,

$$|\mathbf{u}(t)-\mathbf{u}_0|_2 \leqslant \int_\tau^t |\partial_t\mathbf{u}(s)|_2\,\mathrm{d}s \leqslant \sqrt{t-\tau}\,\|\partial_t\mathbf{u}\|_{L^2(\tau,t;\mathbf{L}^2_{\mathrm{div}}(\Omega))},$$

meaning that we only need to properly bound the last norm. The product of the first equation in (3.0.1) by $2\partial_t\mathbf{u}$ gives

$$\nu\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\mathbf{u}|_2^2 + 2|\partial_t\mathbf{u}|_2^2 = -2\langle(\mathbf{u}\cdot\nabla)\mathbf{u},\partial_t\mathbf{u}\rangle + 2\langle\mu\nabla\psi,\partial_t\mathbf{u}\rangle + 2\langle\mathbf{g},\partial_t\mathbf{u}\rangle.$$

Here, having observed that

$$|2\langle\mu\nabla\psi,\partial_t\mathbf{u}\rangle| = |2\langle\psi\nabla\mu,\partial_t\mathbf{u}\rangle| \leqslant 2|\nabla\mu|_2|\psi|_\infty|\partial_t\mathbf{u}|_2 \leqslant C|\nabla\mu|_2|\psi|_2^{1/2}|\Delta\psi|_2^{1/2}|\partial_t\mathbf{u}|_2,$$

the right hand side can be controlled as

$$\begin{aligned}&|-2\langle(\mathbf{u}\cdot\nabla)\mathbf{u},\partial_t\mathbf{u}\rangle+2\langle\mu\nabla\psi,\partial_t\mathbf{u}\rangle+2\langle\mathbf{g},\partial_t\mathbf{u}\rangle|\\ \leqslant&|\partial_t\mathbf{u}|_2^2+C|\mathbf{u}|_2|\nabla\mathbf{u}|_2^2|\mathbf{u}|_{\mathbf{H}^2_{0,\mathrm{div}}(\Omega)}+C|\nabla\mu|_2^2|\psi|_2|\Delta\psi|_2+C|\mathbf{g}|_2^2.\end{aligned}$$

Replacing this estimate in the differential equality above, we have

$$\nu\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\mathbf{u}|_2^2+|\partial_t\mathbf{u}|_2^2\leqslant C\left(|\mathbf{u}|_2|\nabla\mathbf{u}|_2^2|\mathbf{u}|_{\mathbf{H}^2_{0,\mathrm{div}}(\Omega)}+|\nabla\mu|_2^2|\psi|_2|\Delta\psi|_2+|\mathbf{g}|_2^2\right),$$

thus, integrating in time over (τ,t), thanks to Lemmata 3.3.2 and 3.4.4, we deduce

$$\begin{aligned}&\int_\tau^t|\partial_t\mathbf{u}(s)|_2^2\,\mathrm{d}s\\ \leqslant&\left(\nu|\nabla\mathbf{u}(\tau)|_2^2+C\int_\tau^t|\mathbf{g}(s)|_2^2\mathrm{d}s+C\int_\tau^t[|\nabla\mu(s)|_2^2\|\psi(s)\|_{H^1}\|\psi(s)\|_{H^2}+|\mathbf{u}(s)|_2^2|\mathbf{u}(s)|^2_{\mathbf{H}^2_{0,\mathrm{div}}(\Omega)}]\,\mathbf{d}s\right)\\ \leqslant&CA_{t,\tau}\left(\|\mathbf{z}(\tau)\|_{\mathcal{H}_1}^2+|\mu(\tau)|_2^2+A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^7+(t-\tau)A_{t,\tau}^6\right)e^{C\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right)},\end{aligned}$$

which provides the desired estimate. We now turn our attention to the order parameter. By interpolation, exploiting (3.4.7) and Lemma 3.4.4 again, we obtain

$$\begin{aligned}&\|\psi(t,\tau)-\psi_0\|_{H^1(\Omega)}^2\\ \leqslant&|\psi(t,\tau)-\psi_0|_2\|\psi(t,\tau)-\psi_0\|_{H^2(\Omega)}\\ \leqslant&C\sqrt{t-\tau}\left(\int_\tau^t|\partial_t\psi(s,\tau)|_2^2\,\mathrm{d}s\right)^{1/2}\sup_{s\in[\tau,t]}\|\psi(s)\|_{H^2(\Omega)}\\ \leqslant&C\sqrt{t-\tau}\left(\|\mathbf{z}(\tau)\|_{\mathcal{H}_1}^2+|\mu(\tau)|_2^2+A_{t,\tau}^3+(t-\tau)A_{t,\tau}\right)\left(A_{t,\tau}^5+(t-\tau)A_{t,\tau}^4\right)e^{C\left(A_{t,\tau}^4+(t-\tau)A_{t,\tau}^3\right)}.\ \square\end{aligned}$$

The following smoothing property is crucial to show that our problem fits in the theoretical setting of Langa et al. (2010), which was presented in Section 3.2.

Lemma 3.6.2. *There exists a positive function $Q(\,\cdot\,,\,\cdot\,)$, increasing in both arguments, such that, given a pair of symbols $\mathbf{g}_1,\mathbf{g}_2$ satisfying (B.1) and (B.2) and any pair of initial data $\mathbf{z}_{01},\mathbf{z}_{02}\in\mathcal{H}_1$ so that $\mu_{0i}\in L^2(\Omega)$, $i=1,2$, there holds*

$$\begin{aligned}&(t-\tau)\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2\\ \leqslant&\left(\|\mathbf{z}_0\|_{\mathcal{H}_0}^2+C(1+t-\tau)\int_\tau^t|\mathbf{g}(s)|_2^2\,\mathrm{d}s\right)e^{Q(\overline{A_{t,\tau}},t-\tau)\left(1+\|\mathbf{z}_{01}\|_{\mathcal{H}_1}^2+\|\mathbf{z}_{02}\|_{\mathcal{H}_1}^2+|\mu_{01}|_2^2+|\mu_{02}|_2^2\right)}\end{aligned}$$

where $\mathbf{z}_i(t)$ stands for the solution to problem (3.0.1)-(3.0.2) corresponding to symbol $\mathbf{g}_i$ originating at time τ from the initial datum $\mathbf{z}_{i0}$.

Proof. Multiplying (3.5.6) by $(t-\tau)$, we obtain the differential inequality

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left((t-\tau)\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2\right)\\ \leqslant&\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2+C(t-\tau)|\mathbf{g}(t)|_2^2+h(t)(t-\tau)\|\mathbf{z}(t)\|_{\mathcal{H}_1}^2,\end{aligned}$$

where the function h is given as in the proof of Lemma 3.5.2. By the second estimate in Lemma 3.5.1, we deduce

$$\int_\tau^t \|\mathbf{z}(s)\|^2_{\mathcal{H}_1}\,\mathrm{d}s \leqslant C\left(\|\mathbf{z}_0\|^2_{\mathcal{H}_0}+\int_\tau^t |\mathbf{g}(s)|_2^2\,\mathrm{d}s\right)\left(\overline{A_{t,\tau}}^6+(t-\tau)\overline{A_{t,\tau}}^5\right)e^{C\left(\overline{A_{t,\tau}}^6+(t-\tau)\overline{A_{t,\tau}}^5\right)},$$

while the integral of h can be bounded as in Lemma 3.5.2. Thus, the Gronwall's lemma entails

$$\begin{aligned}&(t-\tau)\|\mathbf{z}(t)\|^2_{\mathcal{H}_1}\\ \leqslant& C\left(\|\mathbf{z}_0\|^2_{\mathcal{H}_0}+(1+t-\tau)\int_\tau^t |\mathbf{g}(s)|_2^2\,\mathrm{d}s\right)\left(\overline{A_{t,\tau}}^6+(t-\tau)\overline{A_{t,\tau}}^5\right)e^{C\left(\overline{A_{t,\tau}}^6+(t-\tau)\overline{A_{t,\tau}}^5\right)}\\ &e^{Q(\overline{A_{t,\tau}},t-\tau)\left(1+\|\mathbf{z}_{01}\|^2_{\mathcal{H}_1}+\|\mathbf{z}_{02}\|^2_{\mathcal{H}_1}+|\mu_{01}|_2^2+|\mu_{02}|_2^2\right)},\end{aligned}$$

which is, the desired estimate. □

3.7 Proof of the main results

In this section we show how, properly choosing the spaces and the operators, relying on the results of previous sections, we can apply Theorem 3.2.2, and subsequently Theorem 3.2.3, to our system so to prove Theorem 3.1.1 and Corollary 3.1.2.

Let V and H be the spaces $\mathcal{H}_1$ and $\mathcal{H}_0$ respectively. Observe that, whenever the symbol $\mathbf{g}$ satisfies assumptions (B.1) and (B.2), thanks to Theorem 3.3.1 and Lemma 3.5.1 the solution operator associated to system (3.0.1)-(3.0.2) is well-defined and continuous on H. Moreover, thanks to Corollary 3.4.5, in studying the asymptotic behavior of solutions of (3.0.1)-(3.0.2) we can further restrict our attention to the bounded subset of V given by

$$B \doteq \{\mathbf{z}\in V \mid \|\mathbf{z}\|_{\mathcal{H}_1}+|\mu|_2 \leqslant C_{\mathbf{g}}(t_0)\},$$

which is uniformly (w.r.t. the diameter of the set of initial data) absorbing for the solutions of (3.0.1)-(3.0.2). Since the constraint $|\mu|_2 = |f(\psi)-\Delta\psi|_2 \leqslant C$ is closed w.r.t. the topology of V, we can further restrain our attention to the set

$$\mathcal{O}^\mu_\delta(B) \doteq \mathcal{O}_\delta(B)\cap\{|\mu|_2 \leqslant C_{\mathbf{g}}(t_0)\}$$

when discussing the exponential decay of solution towards an exponential pullback attractor.

Let $\tau\in\mathbb{R}$ be given and let $\mathbf{g}$ satisfy (B.1) and (B.3) (so that (B.2) holds true as well for $t\leqslant t_0$, which is enough for our scopes), we denote by $U_{\mathbf{g}}(t,\tau)$ the solution operator to problem (3.0.1)-(3.0.2) at time $t\geqslant\tau$ with symbol $\mathbf{g}$ and initial data in V. Thanks to Lemmata 3.4.4 and 3.5.2 the process $U_{\mathbf{g}}(t,\tau)\colon V\to V$ is well-defined and continuous on $\mathcal{O}^\mu_\delta$. Therefore, if t_0 is the time appearing in assumption (B.3), the restricted family $\{U_{\mathbf{g}}(t,\tau)\colon \quad \tau\leqslant t\leqslant t_0\}$ belongs to the class

$\mathcal{U}(V,t_0)$. Since the set $\mathcal{O}^\mu_\delta$ is uniformly absorbing for the family $\{U_{\mathbf{g}}(t,\tau)\}$, fixing $\delta=1$ and the time span

$$\tau_0 \doteq 5 + T\left(|\mathcal{O}^\mu_1(B)|\right),$$

we deduce by Corollary 3.4.5 and Lemma 3.6.2 that $U_{\mathbf{g}}(t,t-\tau_0)\in\mathcal{S}_{1,L}(B)$, where the constant L depends increasingly on τ_0, $C_{\mathbf{g}}(t_0)$ and $M_{\mathbf{g}}(t_0)$.

In this framework we can now verify assumptions (H.1)–(H.3) for system (3.0.1)-(3.0.2). Indeed, (H.2) is a straightforward consequence of Lemma 3.5.2. The coupling between the Navier-Stokes and the convective Cahn-Hilliard equations makes more involved the validation of assumptions (H.1) and (H.3). In order to avoid further requirements over the symbols but (B.3), we exploit Lemma 3.6.1 and interpolation, thanks to a smoothing in the solution. The technical details of our argument are contained in the following lemma.

Lemma 3.7.1. *Assume that* $\mathbf{g}$ *satisfies (B.1) and (B.3). Then there exists a positive constant* C *depending on the exponent* q *in (B.3) such that, for any initial datum* $\mathbf{z}_0\in\mathcal{O}^\mu_1(B)$*, the solution* $\mathbf{z}(t)=(\mathbf{u}(t),\psi(t))=U_{\mathbf{g}}(t,\tau)\mathbf{z}_0$ *satisfies*

$$\|\mathbf{u}(t)\|_{\mathbf{H}^{(2q-2)/q}_{0,\mathrm{div}}(\Omega)}+\|\psi(t)\|_{H^3}\leqslant C, \tag{3.7.1}$$

for any $t\leqslant t_0-1$ *and* $\tau\leqslant t-1-\tau_0$.

Proof. In this proof, we consider the two equations separately: first, as in Langa et al. (2010), we apply the Giga-Sohr argument (see Giga and Sohr (1991)) to the equation

$$\partial_t\mathbf{u}-\nu\mathbb{P}\Delta\mathbf{u}=\mathbf{h},$$

where

$$\mathbf{h}\doteq-\mathbb{P}\mathbf{u}\cdot\nabla\mathbf{u}+\mathbb{P}\mu\nabla\psi+\mathbf{g}.$$

By Hölder's and Gagliardo-Nirenberg's inequalities, we obtain

$$|\mathbf{u}\cdot\nabla\mathbf{u}|_2\leqslant C|\mathbf{u}|_q|\nabla\mathbf{u}|_{2q/(q-2)}\leqslant C|\nabla\mathbf{u}|_2^{2(q-1)/q}|\Delta\mathbf{u}|_2^{2/q}.$$

Moreover, recalling that $f(\psi)\nabla\psi\in\mathbf{L}^2(\Omega)$ and $f(\psi)\nabla\psi\in\mathbf{L}^2_{\mathrm{div}}(\Omega)^\perp$

$$|\mathbb{P}\mu\nabla\psi|_2\leqslant|\Delta\psi\nabla\psi|_2\leqslant C|\Delta\psi|_2^{2(q-1)/q}|\Delta^2\psi|_2^{2/q},$$

(actually this estimate is not optimal but, due to the previous estimates on the velocity field above, this does not have any influence on the final outcome) then Corollary 3.4.5 and assumption (B.3) ensure

$$\int_{t-2}^t|\mathbf{h}(s)|_2^q\mathrm{d}s\leqslant Q(M_{\mathbf{g},q}(t_0)),\qquad\tau\leqslant t-6-T(|\mathcal{O}^\mu_1(B)|)=t-1-\tau_0,$$

which is identical to (Langa et al., 2010, Equation (84)). From this estimate, arguing as in Langa et al. (2010) we deduce the bound on $\mathbf{u}$

$$\|\mathbf{u}(t)\|_{\mathbf{H}^{(2q-2)/q}_{0,\mathrm{div}}(\Omega)} \leqslant Q(M_{\mathbf{g},q}(t_0)),$$

which is the first part of (3.7.1).

We now turn our attention to the Cahn-Hilliard equation. The product of the third equation in (3.0.1) by $-2\Delta\partial_t\psi$ leads to

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\Delta\psi|_2^2 + 2|\nabla\partial_t\psi|_2^2\\
=&-2\langle\mathbf{u}\cdot\nabla\partial_t\psi,\Delta\psi\rangle + 2\left\langle f'(\psi)\nabla\Delta\psi,\nabla\partial_t\psi\right\rangle + 2\left\langle f''(\psi)\nabla\psi\Delta\psi,\nabla\partial_t\psi\right\rangle\\
&+4\left\langle f''(\psi)\nabla\psi\nabla^2\psi,\nabla\partial_t\psi\right\rangle + 2\left\langle f'''(\psi)\nabla\psi|\nabla\psi|^2,\nabla\partial_t\psi\right\rangle.
\end{aligned}$$

By Ladyzhenskaja inequality and interpolation, the first term on the right hand side can be controlled as

$$\begin{aligned}
&|-2\langle\mathbf{u}\cdot\nabla\partial_t\psi,\Delta\psi\rangle|\\
\leqslant&2|\mathbf{u}|_4|\Delta\psi|_4|\nabla\partial_t\psi|_2\\
\leqslant&C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\Delta\psi|_2^{3/4}|\Delta^2\psi|_2^{1/4}|\nabla\partial_t\psi|_2\\
\leqslant&\frac{1}{4}|\nabla\partial_t\psi|_2^2 + |\Delta^2\psi|_2^2 + C|\mathbf{u}|_2^{4/3}|\nabla\mathbf{u}|_2^{4/3}|\Delta\psi|_2^2
\end{aligned}$$

and, similarly, the second one is

$$\begin{aligned}
&\left|2\left\langle f'(\psi)\nabla\Delta\psi,\nabla\partial_t\psi\right\rangle\right|\\
\leqslant&2|f'(\psi)|_4|\nabla\Delta\psi|_4|\nabla\partial_t\psi|_2\\
\leqslant&C|f'(\psi)|_4|\Delta\psi|_2^{1/4}|\Delta^2\psi|_2^{3/4}|\nabla\partial_t\psi|_2\\
\leqslant&\frac{1}{4}|\nabla\partial_t\psi|_2 + |\Delta^2\psi|_2^2 + C|f'(\psi)|_4^8|\Delta\psi|_2^4.
\end{aligned}$$

Taking advantage also of Agmon's and Korn's inequalities, we compute

$$\begin{aligned}
&\left|2\left\langle f''(\psi)\nabla\psi\Delta\psi,\nabla\partial_t\psi\right\rangle + 4\left\langle f''(\psi)\nabla\psi\nabla^2\psi,\nabla\partial_t\psi\right\rangle\right|\\
\leqslant&2|f''(\psi)|_4|\nabla\psi|_\infty|\Delta\psi|_4|\nabla\partial_t\psi|_2 + 4|f''(\psi)|_4|\nabla\psi|_\infty|\nabla^2\psi|_4|\nabla\partial_t\psi|_2\\
\leqslant&C|f''(\psi)|_4|\nabla\psi|_2^{1/2}|\nabla\Delta\psi|_2^{1/2}|\Delta\psi|_2^{1/2}|\nabla\Delta\psi|_2^{1/2}|\nabla\partial_t\psi|_2\\
\leqslant&C|f''(\psi)|_4|\nabla\psi|_2^{1/2}|\Delta\psi|_2|\Delta^2\psi|_2^{1/2}|\nabla\partial_t\psi|_2\\
\leqslant&\frac{1}{4}|\nabla\partial_t\psi|_2^2 + |\Delta^2\psi|_2^2 + C|f''(\psi)|_4^4|\nabla\psi|_2^2|\Delta\psi|_2^4.
\end{aligned}$$

Finally,

$$\left|2\left\langle f'''(\psi)\nabla\psi|\nabla\psi|^2,\nabla\partial_t\psi\right\rangle\right| \leqslant C|f'''(\psi)|_4|\Delta\psi|_2^3|\nabla\partial_t\psi|_2 \leqslant \frac{1}{4}|\nabla\partial_t\psi|_2^2 + C|f'''(\psi)|_4^2|\Delta\psi|_2^6.$$

Collecting the above estimates, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\Delta\psi|_2^2 \leqslant h,$$

where

$$h = C\left(|\Delta^2\psi|_2^2 + |f'(\psi)|_4^8|\Delta\psi|_2^4 + |\mathbf{u}|_2^{4/3}|\nabla\mathbf{u}|_2^{4/3}|\Delta\psi|_2^2 + |f''(\psi)|_4^4|\nabla\psi|_2^2|\Delta\psi|_2^4 + |f'''(\psi)|_4^2|\Delta\psi|_2^6\right).$$

Having observed that by Assumption (A.6) we have

$$|f'(\psi)|_4 + |f''(\psi)|_4 + |f'''(\psi)|_4 \leqslant |f(\psi)|_4,$$

then Corollary 3.4.5 provides

$$\int_{t-1}^{t} h(s)\mathrm{d}s \leqslant Q(M_{\mathbf{g}}(t_0)), \quad \tau \leqslant t - 5 - T(|\mathcal{O}_1^\mu(B)|),$$

by the Uniform Gronwall's lemma, we deduce

$$|\nabla\Delta\psi(t)|_2^2 \leqslant Q(M_{\mathbf{g}}(t_0)) \quad t \geqslant \tau + 5 + T(|\mathcal{O}_1^\mu(B)|). \qquad \square$$

We can now show that (H.1) holds true. Having fixed $\mathbf{g}$ satisfying (B.1) and (B.3), we denote by C a generic positive constant depending only on $M_{\mathbf{g},q}(t_0)$. Then we observe that by Corollary 3.4.5 there holds

$$\sup_{\mathbf{z}_0\in\mathcal{O}_1^\mu(B)} \|U_{\mathbf{g}}(t,\tau)\mathbf{z}_0\|_{\mathcal{H}_1} \leqslant C$$

for $t \leqslant t_0$ and $\tau \leqslant t - \tau_0$. Besides, Corollary 3.3.3 entails

$$A_{t,\tau} \leqslant C, \qquad t \leqslant t_0, \quad \tau \leqslant t - \tau_0, \quad \forall \mathbf{z}_0 \in \mathcal{O}_1^\mu(B). \tag{3.7.2}$$

Therefore, arguing as in Lemma 3.6.1, for any initial datum $\mathbf{z}_0 \in \mathcal{O}_1^\mu(B)$, we have

$$\|U_{\mathbf{g}}(t,\tau)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,\tau)\mathbf{z}_0\|_{\mathcal{H}_0} \leqslant C\sqrt{s}, \tag{3.7.3}$$

for $t \leqslant t_0 - 1$, $0 \leqslant s \leqslant 1$ and $\tau \leqslant t - \tau_0$. To proceed in our argument, we need to consider the two variable separately: thus, for any initial datum $\mathbf{z}_0 \in \mathcal{O}_1^\mu(B)$, we set $(\mathbf{u}(t,\tau),\psi(t,\tau)) = U_{\mathbf{g}}(t,\tau)\mathbf{z}_0$. Provided that $t \leqslant t_0 - 1$, $0 \leqslant s \leqslant 1$, $\tau_0 \leqslant r \leqslant 2\tau_0$, by interpolation and Lemma 3.7.1, we have

$$\begin{aligned}
&\|\mathbf{u}(t,t-r) - \mathbf{u}(t-s,t-s-r)\|_{\mathbf{H}^1_{0,\mathrm{div}}(\Omega)} \\
\leqslant& C\|\mathbf{u}(t,t-r) - \mathbf{u}(t-s,t-s-r)\|_{\mathbf{L}^2_{\mathrm{div}}(\Omega)}^{(q-2)/(2q-2)}\|\mathbf{u}(t,t-r) - \mathbf{u}(t-s,t-s-r)\|_{\mathbf{H}^{(2q-2)/q}_{0,\mathrm{div}}(\Omega)}^{q/(2q-2)} \\
\leqslant& C\|\mathbf{u}(t,t-r) - \mathbf{u}(t-s,t-s-r)\|_{\mathbf{L}^2_{\mathrm{div}}(\Omega)}^{(q-2)/(2q-2)},
\end{aligned}$$

as well as

$$\begin{aligned}
&\|\psi(t,t-r) - \psi(t-s,t-s-r)\|_{H^2(\Omega)} \\
\leqslant& C\|\psi(t,t-r) - \psi(t-s,t-s-r)\|_{H^1(\Omega)}^{1/2}\|\psi(t,t-r) - \psi(t-s,t-s-r)\|_{H^3(\Omega)}^{1/2} \\
\leqslant& C\|\psi(t,t-r) - \psi(t-s,t-s-r)\|_{H^1(\Omega)}^{1/2}.
\end{aligned}$$

Thus we are left to control a $\mathcal{H}_0$-norm which can be split into two parts as

$$\begin{aligned}
&\|U_{\mathbf{g}}(t,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}\\
\leqslant&\|U_{\mathbf{g}}(t,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0\|_{\mathcal{H}_0} + \|U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}\\
\leqslant&C\sqrt{s} + \|U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0},
\end{aligned}$$

thanks to (3.7.3). In order to control the last term, we observe that, by (3.3.7) with initial datum $U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0$, it follows

$$\begin{aligned}
&A_{t-s,t-r}\\
=&\left(1 + \|\mathbf{z}(t-r,t-s-r)\|^2_{\mathcal{H}_0} + 2|F(\psi(t-r,t-s-r))|_1 + \int_{t-r}^{t-s}|\mathbf{g}(s)|_2^2\,\mathrm{d}s\right)\\
\leqslant&C\left((1 + \|\mathbf{z}_0\|^2_{\mathcal{H}_0} + 2|F(\psi_0)|_1)e^{-Cs} + M_{\mathbf{g}}(t_0)\right)\\
\leqslant&C(1 + M_{\mathbf{g}}(t_0)).
\end{aligned}$$

Exploiting Lemma 3.5.1 with $\mathbf{z}_1 = \mathbf{z}_0$ and $\mathbf{z}_2 = U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0$ together with $\tau_0 \leqslant r \leqslant 2\tau_0$ and (3.7.2), the desired norm can be written as

$$\begin{aligned}
&\|U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}\\
=&\|U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-r)U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}\\
\leqslant&C\|\mathbf{z}_0 - U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}e^{C\left(1+M_{\mathbf{g}}(t_0)^6\right)}.
\end{aligned}$$

Finally, we can use Lemma 3.6.1 and (3.7.2) so to obtain

$$\|\mathbf{z}_0 - U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0} \leqslant C\sqrt{s}\left(|\mu(t-s-r)|_2^2 + A^3_{t-r,t-s-r}\right)A^8_{t-r,t-s-r}e^{CA^4_{t-r,t-s-r}},$$

where the first term on the right hand side is bounded by

$$|\mu(t-r-s)|_2^2 \leqslant C_{\mathbf{g}}^2(t_0)$$

as a consequence of Corollary 3.4.5 and of the absorbing set considered. This together with the Hölder's inequality and (3.7.2) yields the uniform estimate

$$A_{t-r,t-s-r} \leqslant C(1 + M_{\mathbf{g}}(t_0))$$

for all $t \leqslant t_0 - 1$, $0 \leqslant s \leqslant 1$ and $\tau_0 \leqslant r \leqslant 2\tau_0$. We thus obtain

$$\|\mathbf{z}_0 - U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0} \leqslant C\sqrt{s},$$

which, replaced in the above inequalities, gives

$$\begin{aligned}
&\|U_{\mathbf{g}}(t,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_1}\\
\leqslant& C\|U_{\mathbf{g}}(t,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}^{(q-2)/2(q-1)}\\
\leqslant& Cs^{(q-2)/4(q-1)} + C\|\mathbf{z}_0 - U_{\mathbf{g}}(t-r,t-s-r)\mathbf{z}_0\|_{\mathcal{H}_0}^{(q-2)/2(q-1)}\\
\leqslant& Cs^{(q-2)/4(q-1)},
\end{aligned}$$

for any $\mathbf{z}_0 \in \mathcal{O}_1^{\mu}(B)$ and $t \leqslant t_0 - 1$, $0 \leqslant s \leqslant 1 = \epsilon_0$, $\tau_0 \leqslant r \leqslant 2\tau_0$, so that (H.1) holds true.

We now turn our attention to (H.3), whose proof is now straightforward and follows from interpolation, Lemmata 3.7.1 and 3.6.1: indeed, for any $\mathbf{z}_0 \in B$,

$$\|U_{\mathbf{g}}(t,t-r)\mathbf{z}_0 - U_{\mathbf{g}}(t-s,t-r)\mathbf{z}_0\|_{\mathcal{H}_1} \leqslant Cs^{(q-2)/4(q-1)},$$

for any $t \leqslant t_0$, $\tau_0 \leqslant r \leqslant 2\tau_0$, $0 \leqslant s \leqslant 1 = \epsilon_0$. This end the proof of Theorem 3.1.1.

Finally, if (B.3) holds uniformly for $t_0 \in \mathbb{R}$ (exactly as (B.2)), then it is easy to see that the above argument applies for all times to the process $U_{\mathbf{g}}(t,\tau)$. In particular, (H.4) follows from Lemma 3.5.2. This proves Corollary 3.1.2.

In this and in the previous chapter, we studied the large-time behaviour of solutions of a given dynamical system, making use of the theory trajectory attractors or exponential pullback attractors depending on the setting of the problem. In both the case studied, all parameters of the system were considered given and kept fixed. However, in practice, the parameters of a model are only known up to a certain uncertainty. Therefore, a great importance has to be given to the question of the sensitivity on these parameters of the description of the asymptotic behaviour of the systems considered. This study is generally known under the name of "robustness" of the attractors under perturbations of the parameters of the model. We will tackle this problem in a special situation in the next chapter.

Bibliography

Abels, H. (2009). On a diffuse interface model for two-phase flows of viscous, incompressible fluids with matched densities. *Arch. Ration. Mech. Anal.*, 194(2):463–506.

Boyer, F. (1999). Mathematical study of multi-phase flow under shear through order parameter formulation. *Asymptot. Anal.*, 20(2):175–212.

Cahn, J. W. (1961). On spinodal decomposition. *Acta Metallurgica*, 9(9):795 – 801.

Carvalho, A. N., Langa, J. A., & Robinson, J. C. (2013). *Attractors for infinite-dimensional non-autonomous dynamical systems*, volume 182 of *Applied Mathematical Sciences*. Springer.

Efendiev, M., Miranville, A., & Zelik, S. (2000). Exponential attractors for a nonlinear reaction-diffusion system in $\mathbf{R}^3$. *C. R. Acad. Sci. Paris Sér. I Math.*, 330(8):713–718.

Frigeri, S. & Grasselli, M. (2012a). Global and trajectory attractors for a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Dynam. Differential Equations*, 24(4):827–856.

Frigeri, S. & Grasselli, M. (2012b). Nonlocal Cahn-Hilliard-Navier-Stokes systems with singular potentials. *Dyn. Partial Differ. Equ.*, 9(4):273–304.

Gal, C. G. & Grasselli, M. (2010). Asymptotic behavior of a Cahn-Hilliard-Navier-Stokes system in 2D. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(1):401–436.

Giga, Y. & Sohr, H. (1991). Abstract L^p estimates for the Cauchy problem with applications to the Navier-Stokes equations in exterior domains. *J. Funct. Anal.*, 102(1):72–94.

Langa, J. A., Miranville, A., & Real, J. (2010). Pullback exponential attractors. *Discrete Contin. Dyn. Syst.*, 26(4):1329–1357.

CHAPTER 4

A $2D$ hydrodynamic model for chemically reacting binary fluid mixtures

Outline

A $2D$ diffuse interface model for a chemically reacting incompressible binary fluid in a bounded domain is considered. The corresponding evolution system consists of the Navier-Stokes equations for the (averaged) fluid velocity which are nonlinearly coupled with a convective Cahn-Hilliard-Oono type equation for the difference ψ of the two fluid concentrations. The effects of a (reversible) chemical reaction is represented in the latter equation by an additional term of the form $\epsilon(\psi - c_0)$, $\epsilon > 0$. Here c_0 is the stationary spatial average of ψ, provided that, e.g., no-slip and no-flux boundary conditions are considered. The mass is not necessarily conserved unless the spatial average of the initial datum for ψ coincides with c_0. When $\epsilon = 0$ (i.e. in the absence of chemical reaction) the model reduces to the well-known model H. The global dynamic behavior of the system can be shown to be robust with respect to ϵ. More precisely, a family of exponential attractors is constructed, which is continuous with respect to ϵ.

As we saw in Chapter 1, the phase separation of a binary mixture of incompressible and (partially) immiscible fluids (e.g., polymers) can be described through a diffuse interface model (cf., for instance, Anderson et al. (1998) and references therein). If, in addition, a (reversible) chemical reaction takes place, then the model H, usually used in this setting (cf. Section 1.1 and in particular equation (1.1.6) with $M = \varepsilon = 1$) can be modified as

follows (see Huo et al. (2003, 2004) and references therein)

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla\cdot(\nu(\psi)D\mathbf{u}) = \nabla\pi + \mu\nabla\psi \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\psi + (\mathbf{u}\cdot\nabla)\psi + \epsilon(\psi - c_0) = \Delta\mu \\ \mu = -\Delta\psi + f(\psi) \end{cases} \tag{4.0.1}$$

in $\Omega \times (0,\infty)$, Ω being a bounded domain in $\mathbb{R}^2$. Consistently with the notation used elsewhere, $\mathbf{u}$ is the (averaged) velocity of the two fluids, ψ is the difference of the two fluid concentrations, ν is the viscosity and π is the pressure, the symbol $D\mathbf{u}$ denotes the symmetric gradient of $\mathbf{u}$ defined as $D\mathbf{u} \doteq \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$. Moreover, the constant $\epsilon > 0$ is proportional to the reaction rates, while c_0 is the stationary spatial average of ψ. We recall that μ, known as chemical potential, is the first variation of a Ginzburg-Landau functional $E_P(\psi)$ characterized by a double-well potential F whose derivative is f (see equation (1.1.1)). In this chapter, we will assume the potential F to be regular, growing at most polynomially at infinity (see also Section 4.1 below). A physically reasonable set of boundary conditions is given by no-slip for $\mathbf{u}$ and no-flux for the (convective) Cahn-Hilliard-Oono equation, namely,

$$\mathbf{u} = \mathbf{0}, \quad \partial_{\mathbf{n}}\psi = \partial_{\mathbf{n}}\mu = 0 \quad \text{on } \partial\Omega \times (0,\infty). \tag{4.0.2}$$

Observe that, if $\epsilon = 0$, then system (4.0.1) reduces to the well-known model H or Cahn-Hilliard-Navier-Stokes system (1.1.6), which has been widely studied (see also Chapter 3 for some results concerning the asymptotic behaviour of its solutions). Moreover, if we take $\mathbf{u} = \mathbf{0}$ in the last two equations, then (4.0.1) we obtain the so-called Cahn-Hilliard-Oono system (see, e.g., Teramoto and Nishiura (2002); Villain-Guillot (2010) and the discussion in Section 1.2.2).

Some relevant information on the mean of the order parameter field (i.e., on the average composition of the fluid considered), can be easily deduced from (4.0.1). Indeed, integrating the third equation in (4.0.1) over the domain Ω and taking (4.0.2) into account, we obtain the following evolution equation for the (spatial) average $\langle\psi\rangle$ of the order parameter field

$$\partial_t\langle\psi\rangle + \epsilon(\langle\psi\rangle - c_0) = 0, \tag{4.0.3}$$

from which we deduce

$$\langle\psi\rangle(t) = c_0 + e^{-\epsilon t}(\langle\psi_0\rangle - c_0). \tag{4.0.4}$$

Hence, if $\langle\psi_0\rangle = c_0$, then the total mass is conserved as in the classical Cahn-Hilliard equation. Otherwise, we are in the off-critical mixture case, i.e. the order parameter average at steady state differs from $\langle\psi_0\rangle$ (cf. Huo et al. (2003) where numerical simulations are performed in 2D by taking periodic boundary conditions).

System (4.0.1) endowed with (4.0.2) dissipates energy (cf. Theorem 4.1.1 below). However, the set of stationary states can have a complex structure. For instance, if c_0 does not coincide with the pure phases (say $\psi = \pm 1$), then oscillations can be induced between the phases. This happens even in the case $\mathbf{u} = \mathbf{0}$ (see Choksi et al. (2011)). Thus, in case of a binary fluid, the picture might get more complicated (see Remark 4.1.3 below). In particular, it does not seem possible to prove the convergence to a single equilibrium of a given trajectory like in the case $\epsilon = 0$ (cf. Abels (2009c); Gal and Grasselli (2010a); Zhao et al. (2009)), provided that f is real analytic, unless some rather strong restrictions (e.g., on the size of Ω) are imposed.

Nonetheless the global non-transient behavior of (4.0.1)-(4.0.2) can be analyzed within the theory of infinite-dimensional dynamical systems. In particular, it is possible to find sufficiently small (i.e. compact) invariant objects in the phase space which attract all the evolutions of bounded sets of initial data (see, e.g., Miranville and Zelik (2008) and references therein). More precisely, here we establish the existence of the global attractor and of an exponential attractor for (4.0.1)-(4.0.2). As discussed in Section 1.3, the former is fully invariant (hence unique), while the latter is only positively invariant and uniqueness does not hold. However, exponential attractors have finite fractal dimension, they attract solutions exponentially fast and they are robust with respect to perturbations (e.g., of some parameter). In addition, the existence of the global attractor (of finite fractal dimension) follows, as a by-product, from the existence of an exponential attractor.

The existence of exponential attractors for (4.0.1)-(4.0.2) with $\epsilon = 0$ in 2D has been proven in Gal and Grasselli (2010a). We recall that the existence of a robust family of exponential attractors for the Cahn-Hilliard-Oono equation has been obtained in Miranville (2011). Here the main goal is to construct a family of exponential attractors $\{\mathcal{E}_\epsilon\}$ for (4.0.1)-(4.0.2), which is robust (i.e. continuous) with respect to ϵ. In order to achieve this, we need to show first that (4.0.1)-(4.0.2) generates a (nonlinear) semigroup $S_\epsilon(t)$ which acts on a suitable phase-space and possesses a bounded absorbing set. The required existence and the pertinent dissipative estimate are deduced in Section 4.2. This semigroup is also Lipschitz continuous with respect to the initial data and ϵ as shown in Section 4.3. In Section 4.4 we then obtain some higher-order dissipative estimates which entail the existence of a suitable smooth invariant set. Starting from this set, in Section 4.5, we show some further features of $S_\epsilon(t)$ (e.g., the so-called smoothing property). Thanks to a suitable abstract result, such properties allow us to finally prove our main result.

4.1 Functional setting and main results

The aim of this section is to introduce the specific notation, which will be used throughout this chapter, as well as to state the results proven in the following sections (cf. Theorems 4.1.1, 4.1.3 and 4.1.9 below).

We will denote by Ω a smooth bounded domain of $\mathbb{R}^2$. As usual, we will use the standard spaces of solenoidal distributions $\mathbf{L}^2_{0,\mathrm{div}}$ and $\mathbf{H}^1_{0,\mathrm{div}}$ to study the velocity field $\mathbf{u}$ (see Section 1.4.2). We also need the affine subspaces of $L^p(\Omega)$ and $H^k(\Omega)$ consisting of functions with prescribed average. We recall the pertinent notation introduced before:

$$L^p_{(c)}(\Omega) \doteq \{v \in L^p(\Omega) \mid \langle v \rangle = c\}, \qquad H^k_{(c)}(\Omega) \doteq \{v \in H^k(\Omega) \mid \langle v \rangle = c\}.$$

In this chapter we will assume that the potential $F(\psi)$, whose derivative $f(\psi) = F'(\psi)$ appears in (4.0.1), is assumed to be a quadratic perturbation of a regular convex function defined on the whole real line $\mathbb{R}$, that is,

$$F(\psi) = F_0(\psi) - \alpha\psi^2$$

where $F_0 \in \mathbf{C}^3(\mathbb{R})$ is convex and $\alpha \in \mathbb{R}$ is a positive constant. We will also assume that F grows at most polynomially fast at infinity, namely

$$|f''(y)| \leqslant C_f(1 + |y|^r)$$

for some positive constants r and C_f. Moreover, the potential will be coercive, i.e. there exist positive real numbers q and c_f such that

$$F(y) \geqslant c_f \left(|y|^{2+q} - 1\right) \tag{4.1.1}$$

holds for all $y \in \mathbb{R}$.

We suppose that the order-parameter-dependent viscosity satisfies the bounds

$$0 < \nu_1 \leqslant \nu(y) \leqslant \nu_2 < +\infty \qquad \forall y \in \mathbb{R}, \tag{4.1.2}$$

with ν_1 and ν_2 strictly positive. In addition, we assume that $\nu \in \mathbf{C}^{1,1}(\mathbb{R})$ with

$$|\nu'(y)| \leqslant \nu^* \qquad \forall y \in \mathbb{R},$$

for some $\nu^* \geqslant 0$.

We can now introduce the definition of weak solution for system (4.0.1) that will be used in this chapter.

Definition 4.1.1. Let $(\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. Then a triplet $(\mathbf{u}, \psi, \mu)$ such that

$$\begin{aligned}
&\mathbf{u} \in L^2(0,T;\mathbf{H}^1_{0,\mathrm{div}}(\Omega)) \cap H^1(0,T;\mathbf{H}^{-1}_{\mathrm{div}}(\Omega))\\
&\psi \in L^2(0,T;H^3(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))\\
&\mu \in L^2(0,T;H^1(\Omega))
\end{aligned}$$

is called a *weak solution* to (4.0.1) if

$$\begin{aligned}
&\langle \partial_t \mathbf{u}(t), \mathbf{v}\rangle + \langle (\mathbf{u}(t)\cdot\nabla)\mathbf{u}(t), \mathbf{v}\rangle + \langle \nu(\psi(t))D\mathbf{u}(t), \nabla\mathbf{v}\rangle = \langle \mu(t)\nabla\psi(t), \mathbf{v}\rangle\\
&\langle \partial_t \psi(t), \phi\rangle + \langle \mathbf{u}(t)\cdot\nabla\psi(t), \phi\rangle + \epsilon\,(\psi(t)-c_0,\phi) = -\,(\nabla\mu(t),\nabla\phi)\\
&(\mu(t),\xi) = (f(\psi(t)),\xi) + (\nabla\psi(t),\nabla\xi)
\end{aligned}$$

hold for a.a. $t \in [0,T]$, for all $\mathbf{v} \in \mathcal{V}$, for all ϕ, ξ in $\mathbf{C}^\infty_c(\Omega)$ and for all $T > 0$ and if

$$\lim_{t\to 0^+} \mathbf{u}(t) = \mathbf{u}_0 \quad \text{in } \mathbf{L}^2_{0,\mathrm{div}}(\Omega), \qquad \lim_{t\to 0^+} \psi(t) = \psi_0 \quad \text{in } H^1(\Omega).$$

In order to study the well-posedness and asymptotic behavior of system (4.0.1) it is convenient to introduce the mean-free component of ψ:

$$\overline{\psi} \doteq \psi - \langle\psi\rangle.$$

Since the behavior of the average of ψ is explicitly known (see equation (4.0.4)) we can rewrite system (4.0.1) as

$$\begin{cases}
\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla\cdot(\nu(\psi)D\mathbf{u}) = \nabla p + \mu\nabla\overline{\psi}\\
\nabla\cdot\mathbf{u} = 0\\
\partial_t\overline{\psi} + (\mathbf{u}\cdot\nabla)\overline{\psi} + \epsilon\overline{\psi} = \Delta\mu\\
\mu = -\Delta\overline{\psi} + f(\psi).
\end{cases} \tag{4.1.3}$$

This formulation is particularly convenient since we can use Poincaré's inequality (and some of its variants) at several stages when estimating the Sobolev norms of $\overline{\psi}$. Indeed, the boundary conditions (4.0.2) and the above definitions imply that

$$\int_\Omega \overline{\psi} = 0, \quad \partial_{\mathbf{n}}\overline{\psi} = 0 \text{ on } \partial\Omega, \quad \int_\Omega \Delta\overline{\psi} = \int_{\partial\Omega} \partial_{\mathbf{n}}\overline{\psi} = 0, \quad \partial_{\mathbf{n}}\Delta\overline{\psi} = 0 \text{ on } \partial\Omega.$$

Therefore, all the norms $\|\overline{\psi}\|_{H^j}$, $j = 1,\dots,4$, are equivalent to the L^2-norms of the derivatives of order j. Moreover, Korn's inequality holds. Thus we have

$$\|\overline{\psi}\|_{H^1} \sim |\nabla\overline{\psi}|_2, \quad \|\overline{\psi}\|_{H^2} \sim |\Delta\overline{\psi}|_2, \quad \|\overline{\psi}\|_{H^3} \sim |\nabla\Delta\overline{\psi}|_2, \quad \|\overline{\psi}\|_{H^4} \sim |\Delta^2\overline{\psi}|_2.$$

The main results we will prove in this chapter are the following.

Theorem 4.1.1. *Let $(\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. Then there exists at least a weak solution $(\mathbf{u}, \psi, \mu)$ to system (4.0.1). Moreover, all weak solutions satisfy the dissipative estimate*

$$\frac{d}{dt}\left(|\mathbf{u}|_2^2 + |\nabla\psi|_2^2 + 2\int_\Omega F(\psi)\right) + C_1\left(|\nabla\mathbf{u}|_2^2 + |\nabla\mu|_2^2 + |\nabla\psi|_2^2 + \int_\Omega F(\psi)\right) \\ \leqslant \epsilon C_2\left(\int_\Omega F(c_0) + (\langle\psi_0\rangle - c_0)^2 + 1\right) + C_2 F(\langle\psi_0\rangle) + C_2, \quad (4.1.4)$$

where the generic positive constants C_1 and C_2 only depend on the domain Ω and on the potential F.

Thanks to the dissipative estimate (4.1.4), weak solutions can always be extended up to any time $T > 0$.

Corollary 4.1.2. *Let $(\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. Then there exists a global weak solution $(\mathbf{u}, \psi, \mu)$ to system (4.0.1) defined for all positive times.*

Remark 4.1.1. Existence of a global weak solution can also be proven in dimension three with some growth restrictions on F (in the case $\epsilon = 0$ see, e.g., Gal and Grasselli (2010b), cf. also Abels (2009c) for singular potentials).

In the following we will assume that the viscosity is constant $\nu(y) \equiv \nu > 0$ for all $y \in \mathbb{R}$. This assumption seems essential in order to obtain uniqueness of (weak) solutions within the present framework. However, the higher order dissipative estimate, from which Lemma 4.1.5 below is deduced, may still be derived even by assuming a nonconstant viscosity. In addition, we will also fix $c_0 \in [-1, 1]$ and let $\epsilon \in [0, 1]$.

Theorem 4.1.3. *Let $(\mathbf{u}_{0,1}, \psi_{0,1})$ and $(\mathbf{u}_{0,2}, \psi_{0,2})$ be two pairs of initial data in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$ and let $\epsilon_1, \epsilon_2 \in [0, 1]$. Then any two weak solutions $(\mathbf{u}_1, \psi_1, \mu_1)$ and $(\mathbf{u}_2, \psi_2, \mu_2)$ satisfying (4.0.1) with initial data $(\mathbf{u}_{0,1}, \psi_{0,1})$ and $(\mathbf{u}_{0,2}, \psi_{0,2})$ and with parameter ϵ equal to ϵ_1 and ϵ_2, respectively, also satisfy the following estimate*

$$|\mathbf{u}_1(t) - \mathbf{u}_2(t)|_2^2 + \|\psi_1(t) - \psi_2(t)\|_{H^1}^2 \\ \leqslant (|\mathbf{u}_{0,1} - \mathbf{u}_{0,2}|_2^2 + \|\psi_{0,1} - \psi_{0,2}\|_{H^1}^2) e^{Ct} + (\epsilon_1 - \epsilon_2)^2 e^{Ct} \int_0^t |\nabla\psi_1(s)|_2^2 \, \mathrm{d}s$$

for all $t \geqslant 0$, where $C \geqslant 0$ depend only on the domain Ω, the potential F, the norms of the initial data and on $\max\{\epsilon_1, \epsilon_2\}$.

We thus deduce uniqueness of weak solutions.

Corollary 4.1.4. *Let $(\mathbf{u}_0, \psi_0) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. Then there exists a unique weak solution $(\mathbf{u}, \psi, \mu)$ to system (4.0.1).*

Thanks to the well-posedness results in Theorems 4.1.1 and 4.1.3, it is possible to define on the phase space $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$ the semigroup $S_\epsilon(t)$ associated with the solution operator of system (4.0.1). The dissipative estimate (4.1.4) shows that there exists a bounded absorbing set in the phase space, which uniformly attracts all solutions. Moreover, it is possible to show that a compact absorbing set exists entailing the existence of the (connected) global attractor for our system. Indeed we have

Lemma 4.1.5. *System (4.0.1) possesses a compact absorbing set B_1 defined as follows*

$$B_1 \doteq \{(\mathbf{u}, \psi) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega) \mid \|\mathbf{u}\|^2_{\mathbf{H}^1} + \|\psi\|^2_{H^2} + \int_\Omega F(\psi) \leqslant \rho_0\}.$$

Moreover, we have:

$$\int_t^{t+1} |\Delta \mathbf{u}(s)|_2^2 \,\mathrm{d}s + \int_t^{t+1} |\Delta^2 \psi(s)|_2^2 \,\mathrm{d}s + \int_t^{t+1} |\partial_t \psi(s)|_2^2 \,\mathrm{d}s \leqslant \rho_0$$

for any time t greater than an entry time t_0 which depends only on the norms of the initial data. Here ρ_0 is a positive constant depending on Ω, F, ν only.

Remark 4.1.2. Note that, in the case $\epsilon = 0$, for any fixed physically significant $c \in [-1, 1]$, the existence of a bounded absorbing set is ensured in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1_{(c)}(\Omega)$ as well.

For every fixed ϵ, Lemma 4.1.5 implies that system (4.0.1) has the global attractor. System (4.0.1) also possesses a robust (w.r.t. ϵ) family of exponential attractors. This can be proved by means of the following abstract results (see (Miranville, 2011, Proposition 5.1) and references therein)

Proposition 4.1.6. *Let H and H_1 be two Banach spaces such that H_1 is compactly embedded in H, let B be a bounded subset of H and let $L_\epsilon \colon B \to B$, $\epsilon \geqslant 0$, be a family of operators such that:*

- *for every $x_1, x_2 \in B$ and every $\epsilon \geqslant 0$*

  $$\|L_\epsilon x_1 - L_\epsilon x_2\|_{H_1} \leqslant C \|x_1 - x_2\|_H$$

  holds, where the constant C is independent of ϵ;

- *for every $\epsilon_1, \epsilon_2 \geqslant 0$, for every $i \in \mathbb{N}$ and every $x \in B$*

  $$\|L^i_{\epsilon_1} x - L^i_{\epsilon_2} x\|_H \leqslant C |\epsilon_1 - \epsilon_2|$$

  holds, where the constant C is independent of ϵ_1 and ϵ_2.

Then, there exists a robust family $\mathcal{M}_\epsilon \subset B$ such that $\mathcal{M}_\epsilon$ is an exponential attractor for the discrete dynamical system generated by L_ϵ i.e.

- *the set $\mathcal{M}_\epsilon$ has finite fractal dimension and is positively invariant*

$$L_\epsilon \mathcal{M}_\epsilon \subset \mathcal{M}_\epsilon;$$

- *the set $\mathcal{M}_\epsilon$ attracts B exponentially fast*

$$\operatorname{dist}_H(L^i B, \mathcal{M}_\epsilon) \leqslant Ce^{-Ci}, \quad i \in \mathbb{N}, C > 0$$

where dist_H denotes the Hausdorff semidistance between sets;

- *the family $\mathcal{M}_\epsilon$ is Hölder continuous at every ϵ, i.e. there exist some $\alpha \in (0,1)$ such that*

$$\operatorname{dist}_{\mathrm{sym},H}(\mathcal{M}_{\epsilon_1}, \mathcal{M}_{\epsilon_2}) \leqslant C|\epsilon_1 - \epsilon_2|^\alpha,$$

where $\operatorname{dist}_{\mathrm{sym},H}$ denotes the Hausdorff symmetric distance between sets.

We note that for our system, the following two lemmata, which will be proved in Section 4.5 hold

Lemma 4.1.7 (Smoothing property)**.** *Let $(\mathbf{u}_{0,1}, \psi_{0,1})$ and $(\mathbf{u}_{0,2}, \psi_{0,2})$ be two pairs of initial data belonging to the absorbing set B_1 defined in Lemma 4.1.5 and let $\epsilon \in [0,1]$ be fixed. Then any two weak solutions $(\mathbf{u}_1, \psi_1, \mu_1)$ and $(\mathbf{u}_2, \psi_2, \mu_2)$ satisfying (4.0.1) with initial data $(\mathbf{u}_{0,1}, \psi_{0,1})$ and $(\mathbf{u}_{0,2}, \psi_{0,2})$ also satisfy the following estimate*

$$|\nabla \mathbf{u}(t_0)|_2^2 + |\nabla \overline{\psi}(t_0)|_2^2 + |\Delta \overline{\psi}(t_0)|_2^2 + \epsilon |\overline{\psi}(t_0)|_2^2 \leqslant C\left(|\mathbf{u}_0|_2^2 + \|\overline{\psi}_0\|_{H^1}^2\right) + \frac{C}{\epsilon}\langle \psi_0 \rangle^2,$$

where $t_0 > 0$ is a fixed positive time and where the constant $C \geqslant 0$ depends only on the domain Ω, the potential F and the norms of the initial data.

Lemma 4.1.8. *Let $(\mathbf{u}, \psi, \mu)$ be any weak solution belonging to the set B_1 for all times. Then for any $T > 0$, $(\mathbf{u}, \psi)\colon [0,T] \to \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$ is an Hölder continuous function with respect to time.*

Using the abstract result contained in Proposition 4.1.6 and the two above Lemmata, we can prove the main result of this chapter.

Theorem 4.1.9. *For every $\epsilon > 0$ the semigroup $S_\epsilon(t)$ acting on $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1$ possesses an exponential attractor $\mathcal{M}_\epsilon$ (i.e. a bounded positively invariant, finite dimensional exponentially attracting subset of the phase space). Moreover, the family $\mathcal{M}_\epsilon$ is robust, i.e.,*

$$\operatorname{dist}_{\mathrm{sym},\mathbf{L}^2_{0,\mathrm{div}} \times H^1}(\mathcal{M}_{\epsilon_1}, \mathcal{M}_{\epsilon_2}) \leqslant C|\epsilon_1 - \epsilon_2|^\alpha, \quad \alpha \in (0,1).$$

Furthermore, if we restrict the phase space to $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1_{(c_0)}$, then the family of exponential attractors $\mathcal{M}_\epsilon$ is also robust at the origin, that is,

$$\operatorname{dist}_{\mathrm{sym},\mathbf{L}^2_{0,\mathrm{div}} \times H^1_{(c_0)}}(\mathcal{M}_\epsilon, \mathcal{M}_0) \leqslant C\epsilon^\alpha, \quad \alpha \in (0,1).$$

Remark 4.1.3. System (4.1.3) can be rewritten into the form (assuming, for simplicity, constant viscosity)

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\Delta\mathbf{u} = \nabla p + \tilde{\mu}\nabla\overline{\psi} - \epsilon(-\Delta)^{-1}(\overline{\psi})\nabla\overline{\psi} \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\overline{\psi} + (\mathbf{u}\cdot\nabla)\overline{\psi} = \Delta\tilde{\mu} \\ \tilde{\mu} = -\Delta\overline{\psi} + f(\psi) + \epsilon(-\Delta)^{-1}(\overline{\psi}) \end{cases}$$

where $(-\Delta)^{-1}$ is the inverse of the laplace operator with homogeneous boundary conditions. This system is formally equivalent to the standard Cahn-Hilliard-Navier-Stokes system but for the additional nonlocal forcing term $\epsilon(-\Delta)^{-1}(\overline{\psi})\nabla\overline{\psi}$. Let us assume that c_0 is not a pure phase and ψ be a solution which does not converge to c_0 as t goes to ∞. Then it cannot converge to a pure phase due to (4.0.4). Moreover, the coupling term in the momentum equation might not vanish and therefore $\mathbf{u}$ might not converge to $\mathbf{0}$ as it happens in the case $\epsilon = 0$. Indeed, the system does not seem to have any Lyapunov functional. From the energy identity (4.2.1) where the term $\int_\Omega(\psi - c_0)f(\psi)$ apparently has no well-defined sign.

4.2 Existence and dissipation

In this section and in the following one, we discuss the proofs of the main results summarized above. We start by proving our an existence result, Theorem 4.1.1. The a priori estimates obtained in our argument will provide a dissipative estimate which will be essential in the following proofs.

Proof of Theorem 4.1.1. In order to prove the existence of solutions to equation (4.0.1), a standard Galerkin scheme may be used. The finite dimensional vector spaces generated by the first eigenfunctions of the Stokes operator constitute suitable approximation spaces for the velocity field. Moreover, equation (4.0.4) suggests to chose a constant function plus a basis of $L^2_{(0)}(\Omega)$ to approximate the order parameter field. In this section we will only derive the a priori bounds needed to justify the convergence of the Galerkin scheme, leaving the straightforward technical details to the interested reader. We only observe that existence of solutions to system (4.0.1) is equivalent to proving the existence of solutions to system (4.1.3). Therefore we will work with the latter, which leads to simpler considerations.

In order to obtain our first (dissipative) a priori estimate, we multiply the first equation

in (4.1.3) by $\mathbf{u}$ and the third by μ. Recalling the useful vector identity

$$\begin{aligned}\int_\Omega \partial_t\overline{\psi}\mu &= -\int_\Omega \partial_t\overline{\psi}\Delta\psi + \int_\Omega f(\psi)\partial_t\overline{\psi}\\ =&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\overline{\psi}|_2^2 + \int_\Omega f(\psi)\partial_t\psi + \epsilon(\langle\psi\rangle - c_0)\int_\Omega f(\psi)\\ =&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\overline{\psi}|_2^2 + 2\int_\Omega F(\psi)\right) + \epsilon(\langle\psi\rangle - c_0)\int_\Omega f(\psi)\end{aligned}$$

we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\overline{\psi}|_2^2 + 2\int_\Omega F(\psi)\right) + \int_\Omega \nu(\psi)\,|D\mathbf{u}|^2 + |\nabla\mu|_2^2 \\ + \epsilon\left(\overline{\psi},\mu\right) + \epsilon(\langle\psi\rangle - c_0)\int_\Omega f(\psi) = 0.$$

From the definition of the chemical potential μ we also have

$$\left(\overline{\psi},\mu\right) = |\nabla\overline{\psi}|_2^2 + \int_\Omega \overline{\psi}f(\psi)$$

which further implies the following energy balance

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\overline{\psi}|_2^2 + 2\int_\Omega F(\psi)\right) + \int_\Omega \nu(\psi)\,|D\mathbf{u}|^2 + |\nabla\mu|_2^2 + \epsilon|\nabla\overline{\psi}|_2^2 \\ + \epsilon\int_\Omega(\psi - c_0)f(\psi) = 0. \quad (4.2.1)$$

In order to obtain the sought dissipative estimate, only the last term in this relation requires some additional care. We observe that this factor represents the interplay between the chemical reacting term, which drives the system towards the $\psi \equiv c_0$ equilibrium, and the phase separation potential F, which pushes the dynamics toward the two pure phases. Thanks to the assumptions on the structure of the potential, by the convexity of F_0, we have

$$F_0(\psi) \leqslant F_0(c_0) + (\psi - c_0)f_0(\psi)$$

and hence

$$F(\psi) \leqslant F(c_0) + (\psi - c_0)f(\psi) + \frac{\alpha}{2}(\psi - c_0)^2.$$

Therefore, recalling also equation (4.1.2), we deduce

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\overline{\psi}|_2^2 + 2\int_\Omega F(\psi)\right) + \nu_1|D\mathbf{u}|_2^2 + |\nabla\mu|_2^2 + \epsilon|\nabla\overline{\psi}|_2^2 + \epsilon\int_\Omega F(\psi) \\ \leqslant \epsilon\int_\Omega F(c_0) + \epsilon\frac{\alpha}{2}|\psi - c_0|_2^2.$$

We can further estimate the last term on the right hand side by resorting to the coercivity assumption (4.1.1) on F and to the known evolution law (4.0.4) for $\langle\psi\rangle$ as follows

$$|\psi - c_0|_2^2 \leqslant 2|\overline{\psi}|_2^2 + 2(\langle\psi\rangle - c_0)^2|\Omega| \leqslant \delta|\overline{\psi}|_{2+q}^{2+q} + C + C(\langle\psi_0\rangle - c_0)^2.$$

Here δ is a small positive constant and all the other constants depend only on the domain Ω and on the features of the potential F. Therefore, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2+|\nabla\overline{\psi}|_2^2+2\int_\Omega F(\psi)\right)+\nu_1|D\mathbf{u}|_2^2+|\nabla\mu|_2^2+\epsilon|\nabla\overline{\psi}|_2^2+\epsilon\int_\Omega F(\psi)$$
$$\leqslant \epsilon C\left(\int_\Omega F(c_0)+(\langle\psi_0\rangle-c_0)^2+1\right).$$

In order to get a dissipative estimate, we still have to "reconstruct the norm" on the left hand side. Testing the fourth equation in (4.1.3) by $\overline{\psi}$ we find

$$\left(\mu,\overline{\psi}\right)=|\nabla\overline{\psi}|_2^2+\left(f(\psi),\overline{\psi}\right).$$

Using the structure of the potential F and arguing as above we can deduce

$$\left(f(\psi),\overline{\psi}\right)+\frac{\alpha}{2}|\overline{\psi}|_2^2+\int_\Omega F(\langle\psi\rangle)\geqslant\int_\Omega F(\psi)$$

so that

$$\int_\Omega F(\psi)+|\nabla\overline{\psi}|_2^2\leqslant\left(\mu,\overline{\psi}\right)+\frac{\alpha}{2}|\overline{\psi}|_2^2+|\Omega|F(\langle\psi\rangle).$$

Since $\overline{\psi}$ has zero mean, we also have

$$\left(\mu,\overline{\psi}\right)=\left(\overline{\mu},\overline{\psi}\right)\leqslant C|\overline{\psi}|_2^2+|\nabla\overline{\mu}|_2^2$$

and hence

$$\int_\Omega F(\psi)+|\nabla\overline{\psi}|_2^2\leqslant C|\overline{\psi}|_2^2+CF(\langle\psi\rangle)+|\nabla\mu|_2^2. \tag{4.2.2}$$

Moreover, we note that

$$|\overline{\psi}|_2^2\leqslant\delta|\overline{\psi}|_{2+q}^{2+q}+C(\Omega,q)$$

where δ is a small constant, which will be chosen later. By substituting in (4.2.2), recalling the coercivity assumptions on the potential F and fixing δ, we finally infer

$$\int_\Omega F(\psi)+|\nabla\overline{\psi}|_2^2\leqslant C\left(1+F(\langle\psi\rangle)+|\nabla\mu|_2^2\right)$$

where all the constants depend only on Ω and on the structural constants of F. Moreover, from the monotonicity of $\langle\psi\rangle$ (see (4.0.4)) and from the regularity assumptions on F, we also have

$$F(\langle\psi\rangle)\leqslant CF(\langle\psi_0\rangle)+C$$

where the constants only depend on the potential F. Putting all these estimates together and recalling Korn's inequality, we finally obtain estimate (4.1.4). □

Besides the existence of global solutions for system (4.0.1), a few further consequences may be deduced from this result. For example, a straightforward use of Gronwall's inequality gives the following lemma.

Lemma 4.2.1. *There exists a constant ρ_2 such that the system (4.0.1) admits an absorbing set $B_0 \subset \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$ defined by:*

$$B_0 \doteq \{(\mathbf{u}, \psi) \in \mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega) \mid |\mathbf{u}|_2^2 + \|\psi\|_{H^1}^2 + \int_\Omega F(\psi) \leqslant \rho_2\}.$$

Moreover we have

$$\int_t^{t+1} |\nabla \mathbf{u}(s)|_2^2 \, \mathrm{d}s + \int_t^{t+1} |\nabla \mu(s)|_2^2 \, \mathrm{d}s \leqslant \rho_2$$

for any time t greater than an entry time t_0 depending only on the norms of the initial data.

Remark 4.2.1. An immediate implication of the above lemma is that

$$\int_t^{t+1} |\Delta \overline{\psi}|_2^2 \, \mathrm{d}s$$

is uniformly bounded for any time t greater than t_0. It suffices to compute the L^2-norm of the last equation in (4.1.3) and observe that the average of μ and $f(\psi)$ over Ω are equal and bounded.

Remark 4.2.2. It is also easy to deduce that

$$\int_t^{t+1} |\nabla \Delta \overline{\psi}|_2^2 \, \mathrm{d}s$$

is uniformly bounded for any time t greater than t_0. This indeed follows straightforwardly by computing the L^2-norm of the gradient of the last equation in (4.1.3).

Remark 4.2.3. More generally, from the above estimates we can deduce that any solution $(\mathbf{u}, \psi)$ to (4.0.1) is uniformly bounded (w.r.t. the norm of the initial conditions) in

$$\mathbf{u} \in L^2(0, T; \mathbf{H}^1_{0,\mathrm{div}}(\Omega)) \cap L^\infty(0, T; \mathbf{L}^2_{0,\mathrm{div}}(\Omega))$$
$$\psi \in L^2(0, T; H^3(\Omega)) \cap L^\infty(0, T; H^1(\Omega))$$

for any $T > 0$.

4.3 Continuous dependence

Having obtained existence of global solutions for system (4.0.1) and uniform bounds on the energy norms of the solutions, we can now prove the continuous dependence result stated in Theorem 4.1.3. Since our main goal is to obtain robustness of the dynamics of system (4.0.1) with respect to perturbations of the parameter ϵ, we will study continuous dependence of solutions not only with respect to the initial data, but also with respect to this kinetic parameter ϵ. We recall that from this section onward the viscosity $\nu(\psi)$ will be considered constant: $\nu(\psi) \equiv \nu > 0$ for all $\psi \in \mathbb{R}$. In order to simplify our argument we will further assume $\nu = 1$.

Remark 4.3.1. We underline that all our results on the asymptotic dynamics for system (4.0.1) remain valid also in the original setting. Indeed, in the general setting, one can prove uniqueness of strong solutions following Boyer (1999). One can easily see by adapting the results of the following section (in particular the proof of Lemma 4.1.5) that the solutions to (4.0.1) regularize (uniformly) in finite time. Therefore, the general robustness results follow by arguing as in the constant viscosity case analyzed here, as soon as the solution semigroup starts from any positive time $t_0 > 0$.

Proof of Theorem 4.1.3. We will denote by $(\mathbf{u}_1, \psi_1)$ and $(\mathbf{u}_2, \psi_2)$ two solutions to system (4.0.1) originating from the initial conditions $(\mathbf{u}_{0,1}, \psi_{0,1})$ and $(\mathbf{u}_{0,2}, \psi_{0,2})$ and satisfying (4.0.1) with ϵ equal to ϵ_1 and ϵ_2 respectively. In order to shorten notation, we will also denote by $\mathbf{u}$ (with no subscript!) the difference between $\mathbf{u}_1$ and $\mathbf{u}_2$ (i.e. $\mathbf{u} \doteq \mathbf{u}_1 - \mathbf{u}_2$). Analogous notation will be used for the other functions appearing in the computations below. Moreover, we will assume ϵ_1 to be greater than ϵ_2 so that $\epsilon \doteq \epsilon_1 - \epsilon_2 \geqslant 0$.

By taking the difference of the "mean-free" equations satisfied by $(\mathbf{u}_1, \psi_1)$ and $(\mathbf{u}_2, \psi_2)$ we obtain

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}_1 + (\mathbf{u}_2\cdot\nabla)\mathbf{u} - \Delta\mathbf{u} = \nabla p + \mu\nabla\overline{\psi}_1 + \mu_2\nabla\overline{\psi} \\ \nabla\cdot\mathbf{u} = 0 \\ \partial_t\overline{\psi} + (\mathbf{u}\cdot\nabla)\overline{\psi}_1 + (\mathbf{u}_2\cdot\nabla)\overline{\psi} + \epsilon\overline{\psi}_1 + \epsilon_2\overline{\psi} = \Delta\mu \\ \mu = -\Delta\overline{\psi} + f(\psi_1) - f(\psi_2). \end{cases} \tag{4.3.1}$$

Before going through the main estimates involving this system, we immediately observe that also the difference $\langle\psi\rangle$ between the average of ψ_1 and of ψ_2 can easily be controlled by equation (4.0.3), which gives

$$\partial_t\langle\psi\rangle + \epsilon_2\langle\psi\rangle = \epsilon(c_0 - \langle\psi_1\rangle).$$

This in turn implies the continuous dependence (indeed stability if ϵ_1 and ϵ_2 are both different from zero) of $\langle\psi\rangle(t)$ with respect to initial data

$$\begin{aligned} \langle\psi\rangle(t) &= e^{-\epsilon_1 t}(c_0 - \langle\psi_{10}\rangle) - e^{-\epsilon_2 t}(c_0 - \langle\psi_{20}\rangle) \\ &= \left(e^{-\epsilon_1 t} - e^{-\epsilon_2 t}\right)(c_0 - \langle\psi_{10}\rangle) + e^{-\epsilon_2 t}\langle\psi_0\rangle. \end{aligned} \tag{4.3.2}$$

We consider now the difference system (4.3.1) and multiply the first equation by $\mathbf{u}$ and the third by $-\Delta\overline{\psi}$ obtaining respectively

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\mathbf{u}|_2^2 + \langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, \mathbf{u}\rangle + |\nabla\mathbf{u}|_2^2 = \langle\mu\nabla\overline{\psi}_1, \mathbf{u}\rangle + \langle\mu_2\nabla\overline{\psi}, \mathbf{u}\rangle$$

and

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\overline{\psi}|_2^2 - \left\langle \mathbf{u}\cdot\nabla\overline{\psi}_1, \Delta\overline{\psi}\right\rangle - \left\langle \mathbf{u}_2\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\right\rangle - \epsilon\left\langle \overline{\psi}_1, \Delta\overline{\psi}\right\rangle + \epsilon_2|\nabla\overline{\psi}|_2^2$$
$$= -\left\langle \Delta\mu, \Delta\overline{\psi}\right\rangle = -|\nabla\Delta\overline{\psi}|_2^2 + \left\langle \nabla(f(\psi_1)-f(\psi_2)), \nabla\Delta\overline{\psi}\right\rangle.$$

Summing these two identities and reordering terms we get

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2 + |\nabla\overline{\psi}|_2^2\right) + |\nabla\mathbf{u}|_2^2 + |\nabla\Delta\overline{\psi}|_2^2 + \epsilon_2|\nabla\overline{\psi}|_2^2 \\ = -\left\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, \mathbf{u}\right\rangle + \left\langle \mu\nabla\overline{\psi}_1, \mathbf{u}\right\rangle + \left\langle \mu_2\nabla\overline{\psi}, \mathbf{u}\right\rangle + \left\langle \mathbf{u}\cdot\nabla\overline{\psi}_1, \Delta\overline{\psi}\right\rangle \\ + \left\langle \mathbf{u}_2\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\right\rangle - \epsilon\left\langle \nabla\overline{\psi}_1, \nabla\overline{\psi}\right\rangle + \left\langle \nabla(f(\psi_1)-f(\psi_2)), \nabla\Delta\overline{\psi}\right\rangle. \quad (4.3.3)\end{aligned}$$

We now have to estimate the seven terms appearing on the right hand side of the last equality. The first estimate is immediate:

$$|\left\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, \mathbf{u}\right\rangle| \leqslant |\mathbf{u}|_4^2|\nabla\mathbf{u}_1|_2 \leqslant C|\mathbf{u}|_2|\nabla\mathbf{u}|_2|\nabla\mathbf{u}_1|_2 \leqslant \frac{1}{8}|\nabla\mathbf{u}|_2^2 + C|\nabla\mathbf{u}_1|_2^2|\mathbf{u}|_2^2.$$

Indeed, recall that, thanks to the results of Lemma 4.2.1, the coefficient $|\nabla\mathbf{u}_1|_2^2$ is integrable. Some more work is needed to estimate the second term in (4.3.3). We have

$$\begin{aligned}|\left\langle \mu\nabla\overline{\psi}_1, \mathbf{u}\right\rangle| = |\left\langle \overline{\psi}_1\nabla\mu, \mathbf{u}\right\rangle| &\leqslant |\nabla\mu|_2|\mathbf{u}|_4|\overline{\psi}_1|_4 \\ &\leqslant |\nabla\mu|_2|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\overline{\psi}_1|_2^{1/2}|\nabla\overline{\psi}_1|_2^{1/2}. \quad (4.3.4)\end{aligned}$$

By the last equation in (4.3.1) we can bound the chemical potential term $|\nabla\mu|_2$ by

$$|\nabla\mu|_2 \leqslant |\nabla\Delta\overline{\psi}|_2 + |\nabla(f(\psi_1)-f(\psi_2))|_2.$$

A direct computation also gives

$$\begin{aligned}\nabla(f(\psi_1)-f(\psi_2)) &= f'(\psi_1)\nabla\psi_1 - f'(\psi_2)\nabla\psi_2 \\ &= f'(\psi_1)\nabla\overline{\psi} + (f'(\psi_2)-f'(\psi_2))\nabla\overline{\psi}_2 = f'(\psi_1)\nabla\overline{\psi} + f''(\xi)\psi\nabla\overline{\psi}_2\end{aligned}$$

where we have used the mean value theorem and ξ is a suitable function bounded by $\max\{\psi_1,\psi_1\}$ from above and by $\min\{\psi_1,\psi_2\}$ from below. We then have

$$\begin{aligned}&|\nabla\mu|_2 \\ \leqslant&|\nabla\Delta\overline{\psi}|_2 + |f'(\psi_1)\nabla\overline{\psi}|_2 + |f''(\xi)\psi\nabla\overline{\psi}_2|_2 \\ \leqslant&|\nabla\Delta\overline{\psi}|_2 + |f'(\psi_1)|_4|\nabla\overline{\psi}|_4 + |\psi|_8|\nabla\overline{\psi}_2|_4|f''(\xi)|_8 \\ \leqslant&|\nabla\Delta\overline{\psi}|_2 + C|f'(\psi_1)|_4|\nabla\overline{\psi}|_2^{3/4}|\nabla\Delta\overline{\psi}|_2^{1/4} \\ &\quad + C|\nabla\overline{\psi}_2|_2^{1/2}|\Delta\overline{\psi}_2|_2^{1/2}|f''(\xi)|_8(|\nabla\overline{\psi}|_2 + \langle\psi\rangle) \\ \leqslant&2|\nabla\Delta\overline{\psi}|_2 + C\left(|f'(\psi_1)|_4^{4/3} + |\nabla\overline{\psi}_2|_2^{1/2}|\Delta\overline{\psi}_2|_2^{1/2}|f''(\xi)|_8\right)|\nabla\overline{\psi}|_2 \\ &\quad + C|\nabla\overline{\psi}_2|_2^{1/2}|\Delta\overline{\psi}_2|_2^{1/2}|f''(\xi)|_8\langle\psi\rangle\end{aligned}$$

Substituting this estimate in (4.3.4) and using Young's inequality, we get

$$\begin{aligned}
&|\langle \mu\nabla\overline{\psi}_1, \mathbf{u}\rangle| \\
\leqslant &\frac{1}{8}|\nabla\mathbf{u}|_2^2 + \frac{1}{10}|\nabla\Delta\overline{\psi}|_2^2 + C\left(|\overline{\psi}_1|_2^2|\nabla\overline{\psi}_1|_2^2\right)|\mathbf{u}|_2^2 \\
&+ C\left(|f'(\psi_1)|_4^{8/3} + |\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2\right)|\nabla\overline{\psi}|_2^2 \\
&+ C\left(|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2\right)\langle\psi\rangle^2
\end{aligned}$$

where all the coefficients enclosed in parenthesis are easily seen to be integrable thanks to Lemma 4.2.1 and where $\langle\psi\rangle$ is a known bounded function of time depending only on $\langle\psi_{10}\rangle$, $\langle\psi_{20}\rangle$, ϵ_1 and on ϵ_2 (see equation (4.3.2)). We can now consider the remaining terms on the right hand side of (4.3.3). The third one gives

$$\begin{aligned}
&|\langle \mu_2\nabla\overline{\psi}, \mathbf{u}\rangle| \\
\leqslant &|\mathbf{u}|_4|\nabla\overline{\psi}|_4|\mu_2|_2 \\
\leqslant &C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\nabla\overline{\psi}|_2^{3/4}|\nabla\Delta\overline{\psi}|_2^{1/4}|\mu_2|_2 \\
\leqslant &\frac{1}{8}|\nabla\mathbf{u}|_2^2 + \frac{1}{10}|\nabla\Delta\overline{\psi}|_2^2 + C|\mu_2|_2^2|\mathbf{u}|_2^2 + C|\mu_2|_2^{4/3}|\nabla\overline{\psi}|_2^2,
\end{aligned}$$

while the fourth and fifth can be estimated as

$$\begin{aligned}
&|\langle \mathbf{u}\cdot\nabla\overline{\psi}_1, \Delta\overline{\psi}\rangle| \\
= &|\langle \mathbf{u}\cdot\nabla\Delta\overline{\psi}, \overline{\psi}_1\rangle| \\
\leqslant &|\mathbf{u}|_4|\nabla\Delta\overline{\psi}|_2|\overline{\psi}_1|_4 \\
\leqslant &C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\nabla\Delta\overline{\psi}|_2|\overline{\psi}_1|_4 \\
\leqslant &\frac{1}{8}|\nabla\mathbf{u}|_2^2 + \frac{1}{10}|\nabla\Delta\overline{\psi}|_2^2 + C|\overline{\psi}_1|_4^4|\mathbf{u}|_2^2
\end{aligned}$$

and

$$\begin{aligned}
&|\langle \mathbf{u}_2\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\rangle| \\
= &|\langle \mathbf{u}_2\cdot\nabla\Delta\overline{\psi}, \overline{\psi}\rangle| \\
\leqslant &|\mathbf{u}_2|_4|\nabla\Delta\overline{\psi}|_2|\overline{\psi}|_4 \\
\leqslant &C|\mathbf{u}_2|_2^{1/2}|\nabla\mathbf{u}_2|_2^{1/2}|\nabla\Delta\overline{\psi}|_2|\nabla\overline{\psi}|_2 \\
\leqslant &\frac{1}{10}|\nabla\Delta\overline{\psi}|_2^2 + \left(|\mathbf{u}_2|_2|\nabla\mathbf{u}_2|_2\right)|\nabla\overline{\psi}|_2^2.
\end{aligned}$$

Moreover we have

$$\epsilon|\langle\nabla\overline{\psi}_1, \nabla\overline{\psi}_2\rangle| \leqslant \epsilon|\nabla\overline{\psi}_1|_2|\nabla\overline{\psi}|_2 \leqslant \epsilon^2|\nabla\overline{\psi}_1|_2^2 + \frac{1}{4}|\nabla\overline{\psi}|_2^2.$$

Arguing as for the second term above, the last term in (4.3.3) is bounded by

$$\begin{aligned}
&|\left\langle \nabla(f(\psi_1)-f(\psi_2)), \nabla\Delta\overline{\psi}\right\rangle|\\
=&|\left\langle f'(\psi_1)\nabla\overline{\psi}+f''(\xi)\psi\nabla\overline{\psi}_2, \nabla\Delta\overline{\psi}\right\rangle|\\
\leqslant&|\nabla\overline{\psi}|_4|f'(\psi_1)|_4|\nabla\Delta\overline{\psi}|_2+|f''(\xi)|_8|\psi|_8|\nabla\overline{\psi}_2|_4|\nabla\Delta\overline{\psi}|_2\\
\leqslant&\frac{1}{10}|\nabla\Delta\overline{\psi}|_2^2+C\left(|f'(\psi_1)|_4^{8/3}+|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2\right)|\nabla\overline{\psi}|_2^2\\
&\quad+C\left(|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2\right)\langle\psi\rangle^2.
\end{aligned}$$

We can now combine all the above estimates in order to infer from (4.3.3) the following inequality

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\mathbf{u}|_2^2+|\nabla\overline{\psi}|_2^2\right)+|\nabla\mathbf{u}|_2^2+|\nabla\Delta\overline{\psi}|_2^2+\epsilon_2|\nabla\overline{\psi}|_2^2\\
\leqslant&C\left(|\nabla\mathbf{u}_1|_2^2+|\overline{\psi}_1|_2^2|\nabla\overline{\psi}_1|_2^2+|\mu_2|_2^2+|\psi_1|_4^4\right)|\mathbf{u}|_2^2\\
&+C\left(|f'(\psi_1)|_4^{8/3}+|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2+|\mu_2|_2^{4/3}+|\mathbf{u}_2|_2|\nabla\mathbf{u}|_2\right)|\nabla\overline{\psi}|_2^2\\
&+C\left(1+|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|f''(\xi)|_8^2\right)\langle\psi\rangle^2\\
&+\epsilon^2|\nabla\overline{\psi}_1|_2^2
\end{aligned}\tag{4.3.5}$$

from which continuous dependence of solutions can easily be deduced. In particular, thanks to Lemma (4.2.1) again, we observe that, for solutions to (4.0.1) starting from the same initial datum with different ϵ's, the continuous dependence estimate reduces to

$$|\mathbf{u}|_2^2+|\nabla\overline{\psi}|_2^2\leqslant\epsilon^2e^{Ct}\int_0^t|\nabla\overline{\psi}_1|_2^2,$$

which will be essential when studying the continuity of the family of exponential attractors as a function of ϵ. □

4.4 Higher-order dissipative estimate

Our next goal will be to obtain suitable higher-order dissipative estimates for system (4.0.1). In particular we will show the existence of a compact absorbing set, which absorbs all the solutions to system (4.0.1) in a finite time depending only on the size of the initial data (see Lemma 4.1.5). As above we will proceed through formal estimates, which can be made rigorous using the approximation scheme given by the Galerkin method on the basis made up by the eigenfunctions of the Stokes operator. We recall that these eigenfunctions $\{\boldsymbol{\varphi}_n\}_{n\in\mathbb{N}}\subset\mathcal{V}$ are regular and that $\Delta\boldsymbol{\varphi}_n$ is divergence-free. Moreover, the identity $\langle\boldsymbol{\varphi}\cdot\nabla\boldsymbol{\varphi},\Delta\boldsymbol{\varphi}\rangle=0$ holds for any function $\mathbf{v}$ in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega)$ for which $\Delta\mathbf{v}$ is also divergence-free as is the case of Stokes eigenfunctions. For the following

estimates to hold, we will also assume that the solution has already entered the absorbing set B_0 introduced in Lemma 4.2.1.

Proof of Lemma 4.1.5. The first step in our argument is to multiply the first equation in (4.1.3) by $-\Delta\mathbf{u}$ and to integrate the resulting equation over Ω. After some integrations by parts, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\mathbf{u}|_2^2 - \langle(\mathbf{u}\cdot\nabla)\mathbf{u},\Delta\mathbf{u}\rangle + \int_\Omega \nu(\psi)|\Delta\mathbf{u}|^2 = -\left\langle\mu\nabla\overline{\psi},\Delta\mathbf{u}\right\rangle - \left\langle\nu'(\psi)\nabla\psi\cdot\nabla\mathbf{u},\Delta\mathbf{u}\right\rangle. \quad (4.4.1)$$

We immediately observe that the convective term vanishes due to the well-known properties of the trilinear form in the case of Dirichlet (or periodic) boundary conditions in $\mathbb{R}^2$ (see, e.g., the proof of (Temam, 1984, Theorem III.3.10)). Next we multiply the third equation in (4.1.3) by $\Delta^2\overline{\psi}$ thus obtaining

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\Delta\overline{\psi}|_2^2 + \left\langle\mathbf{u}\cdot\nabla\overline{\psi},\Delta^2\overline{\psi}\right\rangle + \epsilon|\Delta\overline{\psi}|_2^2 = \left\langle\Delta(-\Delta\overline{\psi}+f(\psi)),\Delta^2\overline{\psi}\right\rangle.$$

Simple computations then give

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\Delta\overline{\psi}|_2^2 + \epsilon|\Delta\overline{\psi}|_2^2 + |\Delta^2\overline{\psi}|_2^2 = -\left\langle\mathbf{u}\cdot\nabla\overline{\psi},\Delta^2\overline{\psi}\right\rangle + \left\langle f''(\psi)|\nabla\overline{\psi}|^2,\Delta^2\overline{\psi}\right\rangle + \left\langle f'(\psi)\Delta\overline{\psi},\Delta^2\overline{\psi}\right\rangle. \quad (4.4.2)$$

Summing (4.4.1) and (4.4.2) together, we get

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2+|\Delta\overline{\psi}|_2^2\right) + \int_\Omega \nu(\psi)\,|\Delta\mathbf{u}|^2 + \epsilon|\Delta\overline{\psi}|_2^2 + |\Delta^2\overline{\psi}|_2^2 \\ = -\left\langle\mu\nabla\overline{\psi},\Delta\mathbf{u}\right\rangle - \left\langle\nu'(\psi)\nabla\psi\cdot\nabla\mathbf{u},\Delta\mathbf{u}\right\rangle - \left\langle\mathbf{u}\cdot\nabla\overline{\psi},\Delta^2\overline{\psi}\right\rangle \\ + \left\langle f''(\psi)|\nabla\overline{\psi}|^2,\Delta^2\overline{\psi}\right\rangle + \left\langle f'(\psi)\Delta\overline{\psi},\Delta^2\overline{\psi}\right\rangle. \quad (4.4.3)\end{aligned}$$

We now only have to estimate the five terms appearing on the right hand side of the last equality. We recall that, thanks to Lemma 4.2.1, ψ is bounded in $H^1(\Omega)$ and $\mathbf{u}$ is bounded in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega)$. Since Lemma 4.2.1 implies

$$\int_\Omega \mu = \int_\Omega \Delta\overline{\psi} + \int_\Omega f(\psi) = \int_\Omega f(\psi) \leqslant C(\psi_0)$$

and since the fourth equation in (4.1.3) gives

$$|\mu|_2 \leqslant |\Delta\overline{\psi}|_2 + |f(\psi)|_2 \leqslant |\nabla\overline{\psi}|_2^{2/3}|\Delta^2\overline{\psi}|_2^{1/3} + C,$$

the first term can be estimated as

$$
\begin{aligned}
&|\langle \mu\nabla\overline{\psi}, \Delta\mathbf{u}\rangle| \\
&\leqslant |\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_4|\mu|_4 \\
&\leqslant C|\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_2^{5/6}|\Delta^2\overline{\psi}|_2^{1/6}|\mu|_2^{1/2}(1+|\nabla\mu|_2^{1/2}) \\
&\leqslant C|\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_2^{7/6}|\Delta^2\overline{\psi}|_2^{1/3} + C|\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_2^{7/6}|\Delta^2\overline{\psi}|_2^{1/3}|\nabla\mu|_2^{1/2} \\
&\quad + C|\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_2^{5/6}|\Delta^2\overline{\psi}|_2^{1/6} + C|\Delta\mathbf{u}|_2|\nabla\overline{\psi}|_2^{5/6}|\Delta^2\overline{\psi}|_2^{1/6}|\nabla\mu|_2^{1/2} \\
&\leqslant \frac{\nu_1}{6}|\Delta\mathbf{u}|_2^2 + \frac{1}{10}|\Delta^2\overline{\psi}|_2^2 + C(1+|\nabla\overline{\psi}|_2^{7/2})(1+|\nabla\mu|_2^{3/2}).
\end{aligned}
$$

Here, the L^2-norm of $\nabla\overline{\psi}$ is already known to be bounded. Moreover the L^2-norm of $\nabla\mu$ is integrable and uniformly bounded

$$
\sup_{t\geqslant t_0}\int_t^{t+1}|\nabla\mu(s)|_2^2\,\mathrm{d}s \leqslant \rho_1.
$$

The next two terms can be easily handled using Hölder's and Young's inequalities

$$
\begin{aligned}
&|\langle \nu'(\psi)\nabla\overline{\psi}\cdot\nabla\mathbf{u}, \Delta\mathbf{u}\rangle| \\
\leqslant&\nu^*|\nabla\overline{\psi}|_\infty|\nabla\mathbf{u}|_2|\Delta\mathbf{u}|_2 \\
\leqslant&C|\nabla\overline{\psi}|_2^{2/3}|\Delta^2\overline{\psi}|_2^{1/3}|\mathbf{u}|_2^{1/2}|\Delta\mathbf{u}|_2^{3/2} \\
\leqslant&\frac{\nu_1}{6}|\Delta\mathbf{u}|_2^2 + \frac{1}{8}|\Delta^2\overline{\psi}|_2^2 + C|\mathbf{u}|_2^6|\nabla\overline{\psi}|_2^8
\end{aligned}
$$

and

$$
\begin{aligned}
&|\langle \mathbf{u}\cdot\nabla\overline{\psi}, \Delta^2\overline{\psi}\rangle| \\
\leqslant&|\Delta^2\overline{\psi}|_2|\nabla\overline{\psi}|_2|\mathbf{u}|_\infty \\
\leqslant&C|\Delta^2\overline{\psi}|_2|\nabla\overline{\psi}|_2|\mathbf{u}|_2^{1/2}|\Delta\mathbf{u}|_2^{1/2} \\
\leqslant&\frac{\nu_1}{6}|\Delta\mathbf{u}|_2^2 + \frac{1}{8}|\Delta^2\overline{\psi}|_2^2 + C|\mathbf{u}|_2^2|\nabla\overline{\psi}|_2^4
\end{aligned}
$$

where the last terms in both the above estimates are bounded for sufficiently large times. The fourth and fifth terms in (4.4.3) thus give

$$
\begin{aligned}
&|\langle f''(\psi)|\nabla\overline{\psi}|^2, \Delta^2\overline{\psi}\rangle| \\
\leqslant&|f''(\psi)|_2|\nabla\overline{\psi}|_\infty^2|\Delta^2\overline{\psi}|_2 \\
\leqslant&C|f''(\psi)|_2|\nabla\overline{\psi}|_2^{4/3}|\Delta^2\overline{\psi}|_2^{5/3} \\
\leqslant&\frac{1}{10}|\Delta^2\overline{\psi}|_2^2 + C|f''(\psi)|_2^6|\nabla\overline{\psi}|_2^8
\end{aligned}
$$

and

$$\begin{aligned}
&|\left\langle f'(\psi)\Delta\overline{\psi}, \Delta^2\overline{\psi}\right\rangle| \\
\leqslant &|f'(\psi)|_4|\Delta\overline{\psi}|_4|\Delta^2\overline{\psi}|_2 \\
\leqslant &C|f'(\psi)|_4|\nabla\overline{\psi}|_2^{1/2}|\Delta^2\overline{\psi}|_2^{3/2} \\
\leqslant &\frac{1}{10}|\Delta^2\overline{\psi}|_2^2 + C|f'(\psi)|_4^4|\nabla\overline{\psi}|_2^2.
\end{aligned}$$

Again the terms on the right hand side of the above estimates can either be reabsorbed in the left hand side of equation (4.4.3) or are bounded by the results of Lemma 4.2.1.

Substituting the above estimates in (4.4.3) and reordering we obtain

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2 + \nu_1|\Delta\overline{\psi}|_2^2\right) + |\Delta\mathbf{u}|_2^2 + \epsilon|\Delta\overline{\psi}|_2^2 + |\Delta^2\overline{\psi}|_2^2 \\
&\qquad \leqslant C(1+|\nabla\overline{\psi}|_2^{7/2})(1+|\nabla\mu|_2^{3/2}) + C|\mathbf{u}|_2^2|\nabla\overline{\psi}|_2^4 + C|\mathbf{u}|_2^6|\nabla\overline{\psi}|_2^8 \\
&\qquad\qquad + C|f''(\psi)|_2^6|\nabla\overline{\psi}|_2^8 + C|\nabla\overline{\psi}|_2^2|f'(\psi)|_4^4
\end{aligned}$$

where all the terms on the right hand side except the first are easily seen to be bounded. Poincaré's inequality implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2 + |\Delta\overline{\psi}|_2^2\right) + C\left(|\nabla\mathbf{u}|_2^2 + |\Delta\overline{\psi}|_2^2\right) \leqslant C|\nabla\mu|_2^2 + C$$

where all the constants C are positive. A standard application of Gronwall's inequality yields the sought higher regularity estimate

$$\begin{aligned}
&|\nabla\mathbf{u}(t)|_2^2 + |\Delta\overline{\psi}(t)|_2^2 \\
&\qquad \leqslant \left(|\nabla\mathbf{u}(t_0)|_2^2 + |\Delta\overline{\psi}(t_0)|_2^2\right)e^{-C(t-t_0)} + C\int_{t_0}^{t}|\nabla\mu(s)|_2^2 e^{-C(t-s)}\,\mathrm{d}s + C.
\end{aligned}$$

Here the integral term involving the chemical potential is bounded since $|\nabla\mu(s)|_2^2$ is translation bounded in time. Thanks to Lemma 4.2.1, we finally deduce the existence of the compact absorbing set B_1 defined above. A simple integration in time from t to $t+1$ finally entails the remaining uniform bound of Lemma 4.1.5 thus concluding our proof. □

Remark 4.4.1. With the results obtained so far, we can conclude that, for fixed $\epsilon > 0$, system (4.0.1) possesses the (compact) global attractor in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. In the case $\epsilon = 0$, we recover the known result in the phase space $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1_{(c_0)}(\Omega)$.

4.5 A robust family of exponential attractors

The final section of this chapter is devoted to the proof of the existence and robustness with respect to ϵ of exponential attractors for system (4.0.1) (Theorem 4.1.9). However, before giving the proof of our main result we prove Lemmata 4.1.7 and 4.1.8.

Proof of Lemma 4.1.7. In order to establish the required smoothing property, we will consider again the approximation scheme given by the Galerkin method on the space generated by the eigenfunctions of the Stokes operator. We start by (formally) multiplying by $-\Delta\mathbf{u}$ the first equation of system (4.3.1) with $\epsilon_1 = \epsilon_2 = \epsilon$ and integrating the resulting identity over Ω. Therefore, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\mathbf{u}|_2^2 - \langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1, \Delta\mathbf{u}\rangle - \langle(\mathbf{u}_2\cdot\nabla)\mathbf{u}, \Delta\mathbf{u}\rangle + |\Delta\mathbf{u}|_2^2 = -\left\langle\mu_1\nabla\overline{\psi}, \Delta\mathbf{u}\right\rangle - \left\langle\mu\nabla\overline{\psi}_2, \Delta\mathbf{u}\right\rangle. \quad (4.5.1)$$

Then we consider the third equation in (4.3.1), we multiply it by $-\Delta\overline{\psi}$ and we integrate once again over Ω getting

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\overline{\psi}|_2^2 - \left\langle\mathbf{u}_1\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\right\rangle - \left\langle\mathbf{u}\cdot\nabla\overline{\psi}_2, \Delta\overline{\psi}\right\rangle + \epsilon|\nabla\overline{\psi}|_2^2 = \left\langle\Delta\mu, \Delta\overline{\psi}\right\rangle.$$

Thanks to the fourth equation in (4.3.1), we can rewrite the forcing term in the right hand side of the last identity as

$$-\left\langle\Delta\mu, \Delta\overline{\psi}\right\rangle = \left\langle\nabla\mu, \nabla\Delta\overline{\psi}\right\rangle = -|\nabla\Delta\overline{\psi}|_2^2 + \left\langle f'(\psi_1)\nabla\psi_1 - f'(\psi_2)\nabla\psi_2, \nabla\Delta\overline{\psi}\right\rangle$$

thus obtaining

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\nabla\overline{\psi}|_2^2 + \epsilon|\nabla\overline{\psi}|_2^2 + |\nabla\Delta\psi|_2^2 = \left\langle\mathbf{u}_1\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\right\rangle + \left\langle\mathbf{u}\cdot\nabla\overline{\psi}_2, \Delta\overline{\psi}\right\rangle + \left\langle f'(\psi_1)\nabla\psi_1 - f'(\psi_2)\nabla\psi_2, \nabla\Delta\overline{\psi}\right\rangle. \quad (4.5.2)$$

Considering the third equation in (4.3.1) once more, multiplying it by $\partial_t\overline{\psi}$ this time and integrating over Ω, we further deduce

$$|\partial_t\overline{\psi}|_2^2 + \left\langle\mathbf{u}_1\cdot\nabla\overline{\psi}, \partial_t\overline{\psi}\right\rangle + \left\langle\mathbf{u}\cdot\nabla\overline{\psi}_2, \partial_t\overline{\psi}\right\rangle + \frac{\epsilon}{2}|\overline{\psi}|_2^2 = \left\langle\Delta\mu, \partial_t\overline{\psi}\right\rangle. \quad (4.5.3)$$

Using once more the definition of the chemical potential μ (see the last equation in (4.3.1)) we see that the right hand side of the last equation can be rewritten as follows

$$\begin{aligned}\left\langle\Delta\mu, \partial_t\overline{\psi}\right\rangle = \left\langle\mu, \Delta\partial_t\overline{\psi}\right\rangle &= -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\Delta\overline{\psi}|_2^2 + \left\langle f(\psi_1) - f(\psi_2), \Delta\partial_t\overline{\psi}\right\rangle \\ &= -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\Delta\overline{\psi}|_2^2 + \left\langle\Delta f(\psi_1) - \Delta f(\psi_2), \partial_t\overline{\psi}\right\rangle.\end{aligned}$$

Summing the three above identities (4.5.1), (4.5.2) and (4.5.3), after reordering of the terms

and some computations, we get

$$\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2+|\nabla\overline{\psi}|_2^2+|\Delta\overline{\psi}|_2^2+\epsilon|\overline{\psi}|_2^2\right)+|\Delta\mathbf{u}|_2^2+|\nabla\Delta\overline{\psi}|_2^2+|\partial_t\overline{\psi}|_2^2+\epsilon|\nabla\overline{\psi}|_2^2\\
=&\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1,\Delta\mathbf{u}\rangle+\langle(\mathbf{u}_2\cdot\nabla)\mathbf{u},\Delta\mathbf{u}\rangle-\left\langle\mu_1\nabla\overline{\psi},\Delta\mathbf{u}\right\rangle-\left\langle\mu\nabla\overline{\psi}_2,\Delta\mathbf{u}\right\rangle\\
&+\left\langle\mathbf{u}_1\cdot\nabla\overline{\psi},\Delta\overline{\psi}\right\rangle+\left\langle\mathbf{u}\cdot\nabla\overline{\psi}_2,\Delta\overline{\psi}\right\rangle\\
&+\left\langle(f'(\psi_1)-f'(\psi_2))\nabla\overline{\psi}_1,\nabla\Delta\overline{\psi}\right\rangle+\left\langle f'(\psi_2)\nabla\overline{\psi},\nabla\Delta\overline{\psi}\right\rangle\\
&+\left\langle\mathbf{u}_1\cdot\nabla\overline{\psi},\partial_t\overline{\psi}\right\rangle+\left\langle\mathbf{u}\cdot\nabla\overline{\psi}_2,\partial_t\overline{\psi}\right\rangle+\left\langle(f''(\psi_1)-f''(\psi_2))|\nabla\overline{\psi}_1|^2,\partial_t\overline{\psi}\right\rangle\\
&+\left\langle f''(\psi_2)\nabla\overline{\psi}_1\cdot\nabla\overline{\psi},\partial_t\overline{\psi}\right\rangle+\left\langle f''(\psi_2)\nabla\overline{\psi}\cdot\nabla\overline{\psi}_2,\partial_t\overline{\psi}\right\rangle\\
&+\left\langle(f'(\psi_1)-f'(\psi_2))\Delta\overline{\psi}_1,\partial_t\overline{\psi}\right\rangle+\left\langle f'(\psi_2)\Delta\overline{\psi},\partial_t\overline{\psi}\right\rangle. \qquad (4.5.4)
\end{aligned}$$

We now have to bound the 15 terms appearing on the right hand side of this last identity. For brevity, we will refer to them with the roman numbers I to XV estimating them according to the order specified above. The bounds obtained will always be of the form:

$$\delta|\Delta\mathbf{u}|_2^2+\delta|\nabla\Delta\overline{\psi}|_2^2+\delta|\partial_t\overline{\psi}|_2^2+C(t)|\nabla\mathbf{u}|_2^2+C(t)|\nabla\overline{\psi}|_2^2+C(t)|\Delta\overline{\psi}|_2^2+C(t)\langle\psi\rangle^2$$

where the δ's are suitable small positive constants and where the time-dependent constants are integrable. The first four terms can be estimated as follows

$$\begin{aligned}
|\mathrm{I}|&=|\langle(\mathbf{u}\cdot\nabla)\mathbf{u}_1,\Delta\mathbf{u}\rangle|\\
&\leqslant|\mathbf{u}|_\infty|\nabla\mathbf{u}_1|_2|\Delta\mathbf{u}|_2\\
&\leqslant C|\mathbf{u}|_2^{1/2}|\nabla\mathbf{u}_1|_2|\Delta\mathbf{u}|_2^{3/2}\\
&\leqslant\frac{1}{8}|\Delta\mathbf{u}|_2^2+C|\nabla\mathbf{u}_1|_2^4|\nabla\mathbf{u}|_2^2,
\end{aligned}$$

$$\begin{aligned}
|\mathrm{II}|&=|\langle(\mathbf{u}_2\cdot\nabla)\mathbf{u},\Delta\mathbf{u}\rangle|\\
&\leqslant|\mathbf{u}_2|_4|\nabla\mathbf{u}|_4|\Delta\mathbf{u}|_2\\
&\leqslant C|\mathbf{u}_2|_2^{1/2}|\nabla\mathbf{u}_2|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\Delta\mathbf{u}|_2^{3/2}\\
&\leqslant\frac{1}{8}|\Delta\mathbf{u}|_2^2+C|\mathbf{u}_2|_2^2|\nabla\mathbf{u}_2|_2^2|\nabla\mathbf{u}|_2^2,
\end{aligned}$$

$$\begin{aligned}
|\mathrm{III}|&=|\left\langle\mu_1\nabla\overline{\psi},\Delta\mathbf{u}\right\rangle|\\
&\leqslant|\mu_1|_4|\nabla\overline{\psi}|_4|\Delta\mathbf{u}|_2\\
&\leqslant C|\mu_1|_2^{1/2}\|\mu_1\|_{H^1}^{1/2}|\nabla\overline{\psi}|_2^{3/4}|\nabla\Delta\overline{\psi}|_2^{1/4}|\Delta\mathbf{u}|_2\\
&\leqslant\frac{1}{8}|\Delta\mathbf{u}|_2^2+\frac{1}{8}|\nabla\Delta\overline{\psi}|_2^2+C|\mu_1|_2^{4/3}\|\mu_1\|_{H^1}^{4/3}|\nabla\overline{\psi}|_2^2,
\end{aligned}$$

$$
\begin{aligned}
|\mathrm{IV}| &= |\left\langle \mu\nabla\overline{\psi}_2, \Delta\mathbf{u}\right\rangle| \\
&\leqslant |\mu|_2|\nabla\overline{\psi}_2|_\infty|\Delta\mathbf{u}|_2 \\
&\leqslant C\left(|f(\psi_1)-f(\psi_2)|_2+|\Delta\overline{\psi}|_2\right)|\nabla\overline{\psi}_2|_2^{1/2}|\nabla\Delta\overline{\psi}_2|_2^{1/2}|\Delta\mathbf{u}|_2 \\
&\leqslant C\left(|f(\xi)|_\infty|\psi|_2+|\nabla\overline{\psi}|_2^{1/2}|\nabla\Delta\overline{\psi}|_2^{1/2}\right)|\nabla\overline{\psi}_2|_2^{1/2}|\nabla\Delta\overline{\psi}_1|_2^{1/2}|\Delta\mathbf{u}|_2 \\
&\leqslant \frac{1}{8}|\Delta\mathbf{u}|_2^2+\frac{1}{8}|\nabla\Delta\overline{\psi}|_2^2+C|\nabla\overline{\psi}_2|_2^2|\nabla\Delta\overline{\psi}_2|_2^2|\nabla\overline{\psi}|_2^2 \\
&\quad + C|f(\xi)|_\infty^2|\nabla\overline{\psi}_2|_2|\nabla\Delta\overline{\psi}_2|_2\langle\psi\rangle^2+C|f(\xi)|_\infty^2|\nabla\overline{\psi}_2|_2|\nabla\Delta\overline{\psi}_2|_2|\nabla\overline{\psi}|_2^2
\end{aligned}
$$

where ξ is a function bounded by $\max\{\psi_1,\psi_2\}$ from above and by $\min\{\psi_1,\psi_2\}$ from below. As far as the fifth to the twelfth are concerned we have

$$
\begin{aligned}
|\mathrm{V}| &= |\left\langle \mathbf{u}_1\cdot\nabla\overline{\psi}, \Delta\overline{\psi}\right\rangle| \\
&\leqslant |\mathbf{u}_1|_4|\nabla\overline{\psi}|_4|\Delta\overline{\psi}|_2 \\
&\leqslant C|\mathbf{u}_1|_2^{1/2}|\nabla\mathbf{u}_1|_2^{1/2}|\nabla\overline{\psi}|_2^{1/2}|\Delta\overline{\psi}|_2^{3/2} \\
&\leqslant C|\Delta\overline{\psi}|_2^2+C|\mathbf{u}_1|_2^2|\nabla\mathbf{u}_1|_2^2|\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{VI}| &= |\left\langle \mathbf{u}\cdot\nabla\overline{\psi}_2, \Delta\overline{\psi}\right\rangle| \\
&\leqslant |\mathbf{u}|_4|\nabla\overline{\psi}_2|_4|\Delta\overline{\psi}|_2 \\
&\leqslant C|\nabla\mathbf{u}|_2|\nabla\overline{\psi}_2|_2^{1/2}|\Delta\overline{\psi}_2|_2^{1/2}|\Delta\overline{\psi}|_2 \\
&\leqslant C|\nabla\mathbf{u}|_2^2+C|\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2|\Delta\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{VII}| &= |\left\langle (f'(\psi_1)-f'(\psi_2))\nabla\overline{\psi}_1, \nabla\Delta\overline{\psi}\right\rangle| \\
&\leqslant |f''(\xi)|_\infty|\psi|_2|\nabla\overline{\psi}_1|_\infty|\nabla\Delta\overline{\psi}|_2 \\
&\leqslant C|f''(\xi)|_\infty|\nabla\overline{\psi}_1|_2^{1/2}|\nabla\Delta\overline{\psi}_1|_2^{1/2}|\psi|_2|\nabla\Delta\overline{\psi}|_2 \\
&\leqslant \frac{1}{8}|\nabla\Delta\overline{\psi}|_2+C|f''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2\langle\psi\rangle^2+C|f''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2|\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{VIII}| &= |\left\langle f'(\psi_2)\nabla\overline{\psi}, \nabla\Delta\overline{\psi}\right\rangle| \\
&\leqslant |f'(\psi_2)|_\infty|\nabla\overline{\psi}|_2|\nabla\Delta\overline{\psi}|_2 \\
&\leqslant \frac{1}{8}|\nabla\Delta\overline{\psi}|_2^2+C|f'(\psi_2)|_\infty^2|\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{IX}| &= |\left\langle \mathbf{u}_1 \cdot \nabla\overline{\psi}, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |\mathbf{u}_1|_4 |\nabla\overline{\psi}|_4 |\partial_t\overline{\psi}|_2 \\
&\leqslant C|\mathbf{u}_1|_2^{1/2} |\nabla\mathbf{u}_1|_2^{1/2} |\nabla\overline{\psi}|_2^{1/2} |\Delta\overline{\psi}|_2^{1/2} |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|\Delta\overline{\psi}|_2^2 + C|\mathbf{u}_1|_2^2 |\nabla\mathbf{u}_1|_2^2 |\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{X}| &= |\left\langle \mathbf{u} \cdot \nabla\overline{\psi}_2, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |\mathbf{u}|_4 |\nabla\overline{\psi}_2|_4 |\partial_t\overline{\psi}|_2 \\
&\leqslant C|\nabla\mathbf{u}|_2 |\nabla\overline{\psi}_2|_2^{1/2} |\Delta\overline{\psi}|_2^{1/2} |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|\nabla\overline{\psi}_2|_2 |\Delta\overline{\psi}_2|_2 |\nabla\mathbf{u}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{XI}| &= |\left\langle (f''(\psi_1) - f''(\psi_2))|\nabla\overline{\psi}_1|^2, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |f'''(\xi)|_\infty |\nabla\overline{\psi}_1|_\infty^2 |\psi|_2 |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|f'''(\xi)|_\infty^2 |\nabla\overline{\psi}_1|_\infty^4 \langle\psi\rangle^2 + C|f'''(\xi)|_\infty^2 |\nabla\overline{\psi}_1|_\infty^4 |\nabla\overline{\psi}|_2^2.
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{XII}| &= |\left\langle f''(\psi_2)\nabla\overline{\psi}_1 \cdot \nabla\overline{\psi}, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |f''(\psi_2)|_\infty |\nabla\overline{\psi}_1|_\infty |\nabla\overline{\psi}|_2 |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|f''(\psi_2)|_\infty^2 |\nabla\overline{\psi}_1|_\infty^2 |\nabla\overline{\psi}|_2^2.
\end{aligned}
$$

The remaining terms can be bounded exactly in the same way giving

$$
\begin{aligned}
|\mathrm{XIII}| &= |\left\langle f''(\psi_2)\nabla\overline{\psi} \cdot \nabla\overline{\psi}_2, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|f''(\psi_2)|_\infty^2 |\nabla\overline{\psi}_2|_\infty^2 |\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{XIV}| &= |\left\langle (f'(\psi_1) - f'(\psi_2))\Delta\overline{\psi}_1, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |f''(\xi)|_\infty |\psi|_4 |\Delta\overline{\psi}_1|_4 |\partial_t\overline{\psi}|_2 \\
&\leqslant C|f''(\xi)|_\infty |\psi|_2^{1/2} \|\psi\|_{H^1}^{1/2} |\Delta\overline{\psi}_1|_2^{1/2} |\nabla\Delta\overline{\psi}_1|_2^{1/2} |\partial_t\overline{\psi}|_2 \\
&\leqslant C|f''(\xi)|_\infty \left(\langle\psi\rangle + |\nabla\overline{\psi}|_2\right) |\Delta\overline{\psi}_1|_2^{1/2} |\nabla\Delta\overline{\psi}_1|_2^{1/2} |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|f''(\xi)|_\infty^2 |\Delta\overline{\psi}_1|_2 |\nabla\Delta\overline{\psi}_1|_2 \langle\psi\rangle^2 + C|f''(\xi)|_\infty^2 |\Delta\overline{\psi}_1|_2 |\nabla\Delta\overline{\psi}_1|_2 |\nabla\overline{\psi}|_2^2,
\end{aligned}
$$

$$
\begin{aligned}
|\mathrm{XV}| &= |\left\langle f'(\psi_2)\Delta\overline{\psi}, \partial_t\overline{\psi}\right\rangle| \\
&\leqslant |f'(\psi_2)|_\infty |\Delta\overline{\psi}|_2 |\partial_t\overline{\psi}|_2 \\
&\leqslant \frac{1}{14}|\partial_t\overline{\psi}|_2^2 + C|f'(\psi_2)|_\infty^2 |\Delta\overline{\psi}|_2^2.
\end{aligned}
$$

Having successfully bounded all the terms on the right hand side of (4.5.4), we can use the above estimates to deduce the following inequality

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left(|\nabla\mathbf{u}|_2^2 + |\nabla\overline{\psi}|_2^2 + |\Delta\overline{\psi}|_2^2 + \epsilon|\overline{\psi}|_2^2\right) + |\Delta\mathbf{u}|_2^2 + |\nabla\Delta\overline{\psi}|_2^2 + |\partial_t\overline{\psi}|_2^2 + \epsilon|\nabla\overline{\psi}|_2^2 \\
\leqslant & C\left(1 + |\nabla\mathbf{u}_1|_2^4 + |\mathbf{u}_2|_2^2|\nabla\mathbf{u}_2|_2^2 + |\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2\right)|\nabla\mathbf{u}|_2^2 \\
&+ C\Big(|\mu_1|_2^{4/3}\|\mu_1\|_{H^1}^{4/3} + |f(\xi)|_\infty^2|\nabla\overline{\psi}_2|_2|\nabla\Delta\overline{\psi}_2|_2 + |\nabla\overline{\psi}_2|_2^2|\nabla\Delta\overline{\psi}_2|_2^2 + |\Delta\overline{\psi}|_2^2 \\
&\quad + |\mathbf{u}_1|_2^2|\nabla\mathbf{u}_1|_2^2 + |f''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2 + |f'(\psi_2)|_\infty^2 + |f'''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_\infty^4 \\
&\quad + |f''(\psi_2)|_\infty^2|\nabla\overline{\psi}_1|_\infty^2 + |f''(\psi_2)|_\infty^2|\nabla\overline{\psi}_2|_\infty^2 + |f''(\xi)|_\infty^2|\Delta\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2\Big)|\nabla\overline{\psi}|_2^2 \\
&+ C\left(1 + |\nabla\overline{\psi}_2|_2|\Delta\overline{\psi}_2|_2 + |f'(\psi_2)|_\infty^2\right)|\Delta\overline{\psi}|_2^2 \\
&+ C\Big(|f(\xi)|_\infty^2|\nabla\overline{\psi}_2|_2|\nabla\Delta\overline{\psi}_2|_2 + |f''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2 \\
&\quad + |f'''(\xi)|_\infty^2|\nabla\overline{\psi}_1|_\infty^4 + |f''(\xi)|_\infty^2|\Delta\overline{\psi}_1|_2|\nabla\Delta\overline{\psi}_1|_2\Big)\left\langle\psi\right\rangle^2.
\end{aligned}
$$

It is easy to see that all the coefficients multiplying the quantities $|\nabla\mathbf{u}|_2^2$, $|\nabla\overline{\psi}|_2^2$, $|\Delta\overline{\psi}|_2^2$ and $\left\langle\psi\right\rangle^2$ on the right hand side of this last estimate are (uniformly w.r.t. ϵ) integrable as soon as the solution to system (4.0.1) belongs to the compact invariant set B introduced above. Recalling that from (4.3.2) we have $\left\langle\psi\right\rangle(t) = e^{-\epsilon t}\left\langle\psi_0\right\rangle$, we can apply the uniform Gronwall inequality (see (Temam, 1997, Lemma III.1.1)) obtaining

$$
\begin{aligned}
&|\nabla\mathbf{u}(t)|_2^2 + |\nabla\overline{\psi}(t)|_2^2 + |\Delta\overline{\psi}(t)|_2^2 + \epsilon|\overline{\psi}(t)|_2^2 \\
&\qquad\leqslant \left(\frac{1}{t}\int_0^t \left(|\nabla\mathbf{u}(s)|_2^2 + |\nabla\overline{\psi}(s)|_2^2 + |\Delta\overline{\psi}(s)|_2^2 + \epsilon|\overline{\psi}|_2^2\right)\mathrm{d}s + \frac{1}{2\epsilon}\left\langle\psi_0\right\rangle^2\right)e^{C(t)}.
\end{aligned}
$$

for any positive time t. However, by the continuous dependence estimate (4.3.5) we also know that

$$
\int_0^t \left(|\nabla\mathbf{u}(s)|_2^2 + |\nabla\overline{\psi}(s)|_2^2 + |\Delta\overline{\psi}(s)|_2^2 + \epsilon|\overline{\psi}|_2^2\right)\mathrm{d}s \leqslant C\left(|\mathbf{u}_0|_2^2 + \|\overline{\psi}_0\|_{H^1}^2\right),
$$

which gives the sought smoothing property. □

Proof of Lemma 4.1.8. We prove here the uniform (w.r.t. ϵ) Hölder time-continuity for solutions of equation (4.0.1). In particular, we are interested in showing that this holds on B_1. We just recall that

$$
\|g(t) - g(\tau)\|_X \leqslant (t-\tau)^{1/2}\|\partial_t g\|_{L^2(\tau,t;X)}
$$

where X is a Banach space and $t \geqslant \tau$. For our purpose, it will be sufficient to estimate the $L^2((\mathbf{H}^1_{0,\mathrm{div}})^*)$-norm of $\partial_t \mathbf{u}$ and the $L^2(L^2)$-norm of $\partial_t \overline{\psi}$. In particular, from the first equation in (4.1.3) we have

$$\begin{aligned}
&\|\partial_t \mathbf{u}\|_{(\mathbf{H}^1_{0,\mathrm{div}})^*} \\
\leqslant &\|(\mathbf{u}\cdot\nabla)\mathbf{u}\|_{(\mathbf{H}^1_{0,\mathrm{div}})^*} + \|\Delta \mathbf{u}\|_{(\mathbf{H}^1_{0,\mathrm{div}})^*} + \|\mu\nabla\overline{\psi}\|_{(\mathbf{H}^1_{0,\mathrm{div}})^*} \\
\leqslant &|\mathbf{u}|_4^2 + C|\nabla\mathbf{u}|_2 + C|\mu|_4|\nabla\overline{\psi}|_2 \\
\leqslant &C\left(|\mathbf{u}|_2|\nabla\mathbf{u}|_2 + |\nabla\mathbf{u}|_2 + |\mu|_2^{1/2}|\nabla\mu|_2^{1/2}|\nabla\overline{\psi}|_2\right)
\end{aligned}$$

where the right hand side is easily seen to be square integrable. Analogously, starting from the third and fourth equation in (4.1.3) we obtain

$$\begin{aligned}
&|\partial_t\overline{\psi}|_2 \\
\leqslant &|\mathbf{u}\cdot\nabla\overline{\psi}|_2 + \epsilon|\overline{\psi}|_2 + |\Delta^2\overline{\psi}|_2 + |\nabla f(\psi)|_2 \\
\leqslant &|\mathbf{u}|_4|\nabla\overline{\psi}|_4 + \epsilon|\overline{\psi}|_2 + |\Delta^2\overline{\psi}|_2 + |f''(\psi)|_2|\nabla\overline{\psi}|_\infty^2 + |f'(\psi)|_4|\Delta\overline{\psi}|_4 \\
\leqslant &\Big(|\mathbf{u}|_2^{1/2}|\nabla\overline{\psi}|_2^{1/2}|\nabla\mathbf{u}|_2^{1/2}|\Delta\overline{\psi}|_2^{1/2} + \epsilon|\overline{\psi}|_2 + |\Delta^2\overline{\psi}|_2 \\
&\quad + |f''(\psi)|_2|\nabla\overline{\psi}|_2|\Delta^2\overline{\psi}|_2 + |f'(\psi)|_4|\nabla\overline{\psi}|_2^{1/2}|\Delta^2\overline{\psi}|_2^{1/2}\Big).
\end{aligned}$$

From the above estimates we deduce that $(\mathbf{u},\overline{\psi})$ is Hölder continuous with respect to time with values in $(\mathbf{H}^1_{0,\mathrm{div}}(\Omega))^* \times L^2(\Omega)$. On the other hand, we also know that $(\mathbf{u},\overline{\psi})$ is uniformly bounded in $\mathbf{H}^1_{0,\mathrm{div}} \times H^2(\Omega)$. Thus, by interpolation, we deduce that the solution is Hölder continuous with values in $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$. □

Proof of Theorem 4.1.9. In order to prove our result we only need to verify that all the assumptions of Proposition 4.1.6 are satisfied by our system. This will give us a robust family of discrete-time exponential attractors. In order to complete the proof deducing the existence of a family of continuous-tie exponential attractors, as in (Miranville, 2011, Theorem 5.1), we will only need the uniform Hölder time-continuity for the solution semigroup of system (4.0.1), which has been proved in Lemma 4.1.8.

We start our argument by noticing that by the results of the previous section (in particular by Lemma 4.1.5) system (4.0.1) possesses a positively invariant absorbing set, which is given by

$$B = \bigcup_{\epsilon\geqslant 0}\left(\bigcup_{\substack{t=nT_0\\ n\in\mathbb{N}}} S_\epsilon(t)B_1\right)$$

where $S_\epsilon(t)$ is the solution semigroup associated with system (4.0.1) with the reaction parameter equal to ϵ. In this expression T_0 is the absorbing time of the set B_1 into itself and may depend

on ϵ. However, inspecting the dissipative estimates obtained so far, it is easy to see that this absorbing time T_0 can be increased so to be uniform (with respect to ϵ in a bounded interval).

We already obtained the continuous dependence estimate w.r.t. initial data and ϵ in Section 4.3. Therefore, we are only left with verifying that the solution semigroup $\{S_\epsilon\}_{t\geqslant 0}$ satisfies the required uniform smoothing property and the above mentioned time regularity. However, in the case $\epsilon \geqslant \epsilon_0 > 0$ on the phase space $\mathbf{L}^2_{0,\mathrm{div}}(\Omega) \times H^1(\Omega)$ the required smoothing property is showed by Lemma 4.1.7. From this we deduce the existence of a robust (w.r.t. $\epsilon > 0$) discrete-time exponential attractor. Moreover, arguing as in (Miranville, 2011, Theorem 5.1), the Hölder time continuity proved in Lemma 4.1.8 gives the existence of a robust family of continuous-time exponential attractors. Finally, the other case addressed in Theorem 4.1.9 (namely robustness up to $\epsilon = 0$) easily follows by the same computations. □

Bibliography

Abels, H. (2009). On a diffuse interface model for two-phase flows of viscous, incompressible fluids with matched densities. *Arch. Ration. Mech. Anal.*, 194(2):463–506.

Anderson, D. M., McFadden, G. B., & Wheeler, A. A. (1998). Diffuse-interface methods in fluid mechanics. volume 30 of *Annu. Rev. Fluid Mech.*, pages 139–165. Annual Reviews.

Boyer, F. (1999). Mathematical study of multi-phase flow under shear through order parameter formulation. *Asymptot. Anal.*, 20(2):175–212.

Choksi, R., Maras, M., & Williams, J. F. (2011). 2D phase diagram for minimizers of a Cahn-Hilliard functional with long-range interactions. *SIAM J. Appl. Dyn. Syst.*, 10(4):1344–1362.

Gal, C. G. & Grasselli, M. (2010a). Asymptotic behavior of a Cahn-Hilliard-Navier-Stokes system in 2D. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(1):401–436.

Gal, C. G. & Grasselli, M. (2010b). Trajectory attractors for binary fluid mixtures in 3D. *Chin. Ann. Math. Ser. B*, 31(5):655–678.

Huo, Y., Jiang, X., Zhang, H., & Yang, Y. (2003). Hydrodynamic effects on phase separation of binary mixtures with reversible chemical reaction. *J. Chem. Phys.*, 118:9830–9837.

Huo, Y., Zhang, H., & Yang, Y. (2004). Effects of reversible chemical reaction on morphology and domain growth of phase separating binary mixtures with viscosity difference. *Macromol. Theory Simul.*, 13(3):280–289.

Miranville, A. (2011). Asymptotic behavior of the Cahn-Hilliard-Oono equation. *J. Appl. Anal. Comput.*, 1(4):523–536.

Miranville, A. & Zelik, S. (2008). Attractors for dissipative partial differential equations in bounded and unbounded domains. In: *Handbook of differential equations: evolutionary equations. Vol. IV*, Handb. Differ. Equ., pages 103–200. Elsevier/North-Holland, Amsterdam.

Temam, R. (1984). *Navier-Stokes equations*, (third ed.), volume 2 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co. Theory and numerical analysis, With an appendix by F. Thomasset.

Temam, R. (1997). *Infinite-dimensional dynamical systems in mechanics and physics*, (second ed.), volume 68 of *Applied Mathematical Sciences*. Springer-Verlag.

Teramoto, T. & Nishiura, Y. (2002). Double gyroid morphology in a gradient system with nonlocal effects. *J. Phys. Soc. Jpn.*, 71(7):1611–1614.

Villain-Guillot, S. (2010). 1D Cahn–Hilliard equation for modulated phase systems. *Journal of Physics A: Mathematical and Theoretical*, 43:205102.

Zhao, L., Wu, H., & Huang, H. (2009). Convergence to equilibrium for a phase-field model for the mixture of two viscous incompressible fluids. *Commun. Math. Sci.*, 7(4):939–962.

CHAPTER 5

Cahn-Hilliard Equation with Nonlocal Singular Free Energies

Outline

A Cahn-Hilliard equation, which is the conserved gradient flow of a nonlocal total free energy functional, is considered on a bounded domain. This functional is characterised by a Helmholtz free energy density, which can be of logarithmic type. As a consequence, the equation for the chemical potential contains an integral operator with singular kernel acting on the order parameter, instead of the usual Laplace operator. First the existence and uniqueness of a weak solution and some regularity properties are established. Then the existence of a (connected) global attractor for the system considered is proved. Due to the lack of information concerning the regularity of solutions up to the boundary, the differential formulation of the weak problem considered is not fully known. However, a Neumann-like boundary condition can be recovered for the order parameter field provided that it is supposed to be regular enough.

In this chapter we conclude the presentation of our results concerning the model H and some of its generalisation by reporting some preliminary results about a nonlocal version of the Cahn-Hilliard equation. In particular, this can be seen to arise as a conserved gradient flow of the first variation of the following nonlocal total free energy functional E

$$E(\psi) = \frac{1}{2}\int_\Omega\int_\Omega (\psi(x)-\psi(y))^2 k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y + \int_\Omega f(\psi(x))\mathrm{d}x$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with $\mathbf{C}^2$-boundary $\partial\Omega$ ($n \in \{1,2,3\}$ in applications), k is the interaction kernel and f is the (singular) Helmholtz free energy density.

The chemical potential μ is the first variation of E and the Cahn-Hilliard equation can be then written as follows

$$\partial_t \psi = \nabla \cdot (M \nabla \mu),$$

where M is the so-called mobility. Therefore we consider the following problem

$$\partial_t \psi = \Delta \mu \qquad \text{in } \Omega \times (0, \infty) \tag{5.0.1}$$

$$\mu = \mathcal{L} c + f'(\psi) \qquad \text{in } \Omega \times (0, \infty) \tag{5.0.2}$$

$$\partial_{\mathbf{n}} \mu = 0 \qquad \text{on } \partial\Omega \times (0, \infty) \tag{5.0.3}$$

$$\psi|_{t=0} = \psi_0 \qquad \text{in } \Omega. \tag{5.0.4}$$

where $\mathcal{L}$ is a non-local linear operator defined as follows

$$\begin{aligned} \mathcal{L}u(x) &= \text{p. v.} \int_\Omega (u(x) - u(y)) k(x, y, x - y) \, \mathrm{d}y \\ &= \lim_{\epsilon \to 0} \int_{\Omega \setminus B_{\epsilon(x)}} (u(x) - u(y)) k(x, y, x - y) \, \mathrm{d}y, \end{aligned} \tag{5.0.5}$$

and $k \colon \mathbb{R}^n \times \mathbb{R}^n \times (\mathbb{R}^n \backslash \{0\}) \to \mathbb{R}$ is assumed to be $(n+2)$-times continuously differentiable and satisfies the following conditions (see Abels and Kassmann (2007)):

$$k(x, y, z) = k(y, x, -z), \tag{5.0.6}$$

$$|\partial_x^\beta \partial_y^\gamma \partial_z^\delta k(x, y, z)| \leqslant C_{\beta,\gamma,\delta} |z|^{-n-\alpha-|\delta|}, \tag{5.0.7}$$

$$c_0 |z|^{-n-\alpha} \leqslant k(x, y, z) \leqslant C_0 |z|^{-n-\alpha}. \tag{5.0.8}$$

for all $x, y, z \in \mathbb{R}^n$, $z \neq 0$ and $\beta, \gamma, \delta \in \mathbb{N}_0^n$ with $|\beta| + |\gamma| + |\delta| \leqslant n + 2$ where α is the order of the operator. Unless specified otherwise, throughout this chapter we will always consider the case $\alpha \in (1, 2)$. An example of a kernel $k(\,\cdot\,, \cdot\,, \cdot\,)$ satisfying the above assumptions is given by $k(x, y, z) = \omega(x, y)|z|^{-n-\alpha}$ with $\omega \in \mathbf{C}_b^{n+2}(\mathbb{R}^n)$. Note that the definition of the operator $\mathcal{L}$ depends on Ω. Formally, in the case $\Omega = \mathbb{R}^n$ and $k(x, y, z) = |z|^{-n-\alpha}$ one has $\mathcal{L} = C \times (-\Delta)^{\frac{\alpha}{2}}$ where $(-\Delta)^{\frac{\alpha}{2}}$ is a fractional power of the Laplace operator. If Ω is a bounded domain, the operator $\mathcal{L}$ has the same form as the generator of a censored stable process, cf., e.g., Bogdan et al. (2003) and is also known as reginal fractional Laplacian.

The well-posedness of the weak formulation of problem (5.0.1)–(5.0.4) together with a natural boundary condition for ψ, which will be part of the weak formulation itself, is the main result of this chapter. In the above (strong) formulation (5.0.1)–(5.0.4), a boundary condition for the variable ψ is missing. A further result is concerned with the characterisation of such a condition, provided that the weak solution is smooth enough (say, $\psi \in \mathbf{C}^{1,\beta}(\overline{\Omega})$) and k fulfills suitable assumptions. More precisely, we prove that

$$\nabla \psi(x_0) \cdot \mathbf{n}_{x_0} = 0,$$

where $\mathbf{n}_{x_0}$ depends on the interaction kernel k (see (5.5.2) below).

This condition reduces to the usual homogeneous Neumann boundary condition for ψ for symmetric kernels (cf. Theorem 5.5.1 and Remarks 5.5.2 and 5.5.3 below). Unfortunately, we are unable to prove that a weak solution is indeed as regular as it is required for this characterisation. Nonetheless, the weaker regularity results presenter here is sufficient to prove that the dissipative dynamical system generated by (5.0.1)–(5.0.4) has a (connected) global attractor.

This chapter is organised as follows. In Section 5.1 we introduce some basic notation and function spaces as well as we account for some preliminary results. Section 5.2 is essentially devoted to the computation of the subgradient of the (convex) functional

$$F(\psi) = \frac{1}{2}\int_\Omega\int_\Omega (\psi(x)-\psi(y))^2 k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y + \int_\Omega \phi(\psi(x))\,\mathrm{d}x$$

and to the characterisation of its domain (see Theorem 5.2.3 below). Here ϕ is the convex part of f (see Assumption 1). Combining the results of Sections 5.1 and 5.2 we give the proof of the well-posedness theorem (Theorem 5.1.1) in Section 5.3. The existence of the global attractor is established in Section 5.4. Finally, in Section 5.5 we show that a regular weak solution ψ does satisfy the above boundary condition.

5.1 Basic tools and well-posedness

Given a set M, its power set will be denoted by $2^(M)$. Moreover, we denote $\mathbb{R}^n_+ = \{x \in \mathbb{R}^n \mid x_n > 0\}$ and $\mathbb{R}_+ = \mathbb{R}^1_+$. If X is a (real) Banach space and X^* is its dual, then

$$\langle f, g\rangle \equiv {}_{X^*}\langle f, g\rangle_X = f(g), \qquad f \in X^*, g \in X,$$

denotes the duality product. Moreover, if H is a (real) Hilbert space, $(\,\cdot\,,\,\cdot\,)_H$ will indicate its inner product. In the following, all Hilbert spaces will be separable.

5.1.1 Function spaces

Throughout this chapter $\Omega \subseteq \mathbb{R}^n$ will be a bounded domain with $\mathbf{C}^2$-boundary. Let $L^p(\Omega)$, $1 \leqslant p \leqslant \infty$, be the set of p-integrable (or essentially bounded) functions $f\colon \Omega \to \mathbb{R}$ and set $|\cdot|_p \equiv \|\cdot\|_{L^p(\Omega)}$. In the case of the $L^2(\Omega)$ Hilbert space, we will use the simplified notation

$$(f,g) \doteq (f,g)_{L^2(\Omega)} \qquad \forall f, g \in L^2(\Omega)$$

to indicate the inner product when no ambiguity from the context may arise. Moreover, $H^m(\Omega)$, $m \in \mathbb{N}$, indicates the usual L^2-Sobolev space of order m and $H^m_0(\Omega)$ is the closure of $\mathbf{C}^\infty_0(\Omega)$ in $H^m(\Omega)$.

Given $f \in L^1(\Omega)$, we set

$$\langle f \rangle \doteq \frac{1}{|\Omega|} \int_\Omega f(x)\,\mathrm{d}x$$

and, for $m \in \mathbb{R}$ we define

$$L^2_{(m)}(\Omega) \doteq \{f \in L^2(\Omega) \mid \langle f \rangle = m\},$$

so that $P_0 f \doteq f - m(f)$ denotes the orthogonal projection onto $L^2_{(0)}(\Omega)$.

We then introduce

$$H^1_{(0)} = H^1_{(0)}(\Omega) = \left\{\psi \in H^1(\Omega) \mid \langle \psi \rangle = 0\right\}$$

equipped with the inner product

$$(c,d)_{H^1_{(0)}(\Omega)} = (\nabla c, \nabla d)_{L^2(\Omega)}, \qquad c,d \in H^1_{(0)}(\Omega).$$

Observe that $H^1_{(0)}(\Omega)$ is a Hilbert space due to Poincaré's inequality. Moreover, let $H^{-1}_{(0)} \equiv H^{-1}_{(0)}(\Omega) = H^1_{(0)}(\Omega)^*$ and consider the Riesz isomorphism $\mathcal{R}\colon H^1_{(0)}(\Omega) \to H^{-1}_{(0)}(\Omega)$ given by

$${}_{H^{-1}_{(0)}}\langle \mathcal{R}c, d\rangle_{H^1_{(0)}} = (c,d)_{H^1_{(0)}} = (\nabla c, \nabla d)_{L^2}, \qquad c,d \in H^1_{(0)}(\Omega),$$

i.e., $\mathcal{R} = -\Delta_N$ is the Laplacian with Neumann boundary conditions in the variational sense. Therefore we equip $H^{-1}_{(0)}(\Omega)$ with the inner product

$$(f,g)_{H^{-1}_{(0)}} = (\nabla \Delta_N^{-1} f, \nabla \Delta_N^{-1} g)_{L^2} = (\Delta_N^{-1} f, \Delta_N^{-1} g)_{H^1_{(0)}}.$$

Moreover, we embed $H^1_{(0)}(\Omega)$ and $L^2_{(0)}(\Omega)$ into $H^{-1}_{(0)}(\Omega)$ in the canonical way, that is,

$${}_{H^{-1}_{(0)}}\langle c, \varphi\rangle_{H^1_{(0)}} = \int_\Omega c(x)\varphi(x)\,\mathrm{d}x, \qquad \forall\, \varphi \in H^1_{(0)}(\Omega), c \in L^2_{(0)}(\Omega).$$

Finally, we need to introduce the so-called fractional L^2-Sobolev-Slobodeckii spaces as follows. Let $s \in (0,1)$. Then, for any $u \in L^2(\Omega)$, set

$$\|u\|^2_{H^s(\Omega)} \doteq |u|_2^2 + \int_\Omega \int_\Omega \frac{|u(x)-u(y)|^2}{|x-y|^{n+2s}}\,\mathrm{d}x\mathrm{d}y$$

and

$$H^s(\Omega) \doteq \{f \in L^2(\Omega) \mid \|f\|_{H^s(\Omega)} < \infty\}.$$

Let us denote by $H^s_0(\Omega)$ the closure of $\mathbf{C}^\infty_0(\Omega)$ in $H^s(\Omega)$, while $H^{-s}(\Omega)$ and $H^{-s}_{(0)}(\Omega)$ will be the dual spaces of $H^s(\Omega)$ and $H^s_{(0)}(\Omega)$, respectively. We refer the reader to Adams (1975) for the interpolation results for such spaces which will be used hereafter.

5.1.2 Weak formulation and main result

Before introducing a weak formulation of our problem we state our assumptions on f. As already mentioned, these assumptions are motivated by the so called regular solution model free energy suggested by Cahn and Hilliard Cahn and Hilliard (1958):

$$f(\psi) = \frac{\theta}{2}\left((1+\psi)\ln(1+\psi) + (1-\psi)\ln(1-\psi)\right) - \frac{\theta_c}{2}\psi^2, \quad \psi \in [-1,1] \tag{5.1.1}$$

where $\theta, \theta_c > 0$, $a = -1$, $b = 1$. Here the logarithmic terms are related to the entropy of the system. This free energy can be justified rigourously within the framework of statistical mechanics (see Giacomin and Lebowitz (1997, 1998)). Moreover, we note that f is convex if and only if $\theta \geqslant \theta_c$. In this case the mixed phase is stable. On the other hand, if $0 < \theta < \theta_c$, the mixed phase is unstable and phase separation occurs.

Namely, we suppose

Assumption 1. $f\colon [a,b] \to \mathbb{R}$, $a < 0 < b$, is a continuous function, which is twice continuously differentiable in (a,b), such that

$$\lim_{s\to a} f'(s) = -\infty, \qquad \lim_{s\to b} f'(s) = \infty,$$

and $f''(s) \geqslant -d$ for some $d \geqslant 0$.

Since f is defined on an interval $[a,b]$, we also extend $f(x)$ by $+\infty$ if $x \notin [a,b]$. Hence $E(c) < \infty$ implies $c(x) \in [a,b]$ for almost every $x \in \Omega$. Note that, although f is in general non-convex, it can be considered as a perturbation of a convex potential. Indeed, thanks to Assumption 1, we have that there exists a positive number $d > 0$ and a continuous, convex and twice continuously differentiable in (a,b) function $\phi\colon [a,b] \to \mathbb{R}$ such that the potential f can be decomposed as $f(s) = \phi(s) - \frac{d}{2}s^2$. This will be the key point in the following analysis, which is based on a decomposition of the associated operators in a monotone operator plus a Lipschitz perturbation. The condition $\lim_{c\to a}\phi'(c) = -\infty$, $\lim_{c\to b}\phi'(c) = \infty$ will force c to take values in the interval $[a,b]$ and ensures that the subgradient of the associated functional is single-valued with a suitable domain.

Let us introduce the symmetric bilinear form associated to $\mathcal{L}$

$$\mathcal{E}(u,v) = \frac{1}{2}\int_\Omega\int_\Omega (u(x)-u(y))(v(x)-v(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y$$

for all $u, v \in H^{\alpha/2}(\Omega)$.

The notion of weak solution to problem (5.0.1)-(5.0.2) is given by

Definition 5.1.1. Let $\psi_0 \in H^{\alpha/2}(\Omega)$ such that $E(\psi_0) < \infty$ be given. A pair (ψ,μ) is a global (weak) solution to (5.0.1)-(5.0.4) if $\mu \in L^2(0,T;H^1(\Omega))$ for all $T > 0$, $\psi \in L^\infty(\mathbb{R}_+; H^{\alpha/2}_{(0)}(\Omega))$ and

$\partial_t\psi \in L^2(\mathbb{R}_+; H^{-1}_{(0)}(\Omega))$ hold, if (ψ, μ) satisfies

$$ {}_{H^{-1}_{(0)}}\langle \partial_t\psi(t), \eta\rangle_{H^1_{(0)}} = -(\nabla\mu(t), \nabla\eta) \tag{5.1.2} $$

$$ (\mu(t), \varphi)_{L^2} = \mathcal{E}(\psi(t), \varphi) + (f'(\psi(t)), \varphi)_{L^2} \tag{5.1.3} $$

for all $\eta \in H^1_{(0)}(\Omega)$, all $\varphi \in H^{\alpha/2}(\Omega)$ and a.e. $t > 0$, and if

$$ \lim_{t\to 0} \psi(t) = \psi_0 \qquad \text{in } H^{\alpha/2}(\Omega). $$

The main result of this chapter is the following.

Theorem 5.1.1. *Let Assumption 1 hold. For every $\psi_0 \in H^{\alpha/2}(\Omega)$ with $E(\psi_0) < \infty$, there is a unique (global) solution $\psi \in BC([0,\infty); H^{\alpha/2}(\Omega))$ to (5.0.1)-(5.0.4) in the sense of Definition 5.1.1 which satisfies the energy identity*

$$ E(\psi(T)) + \int_0^T \|\nabla\mu(t)\|^2_{L^2(\Omega)}\,\mathrm{d}t = E(\psi_0) \tag{5.1.4} $$

for all $T > 0$. Furthermore, the following regularity properties hold

$$ \kappa\phi'(c) \in L^\infty(\mathbb{R}_+; L^2(\Omega)), $$
$$ \kappa\mu \in L^\infty(\mathbb{R}_+; H^1(\Omega)), \quad \text{and} $$
$$ \kappa\partial_t c \in L^\infty(\mathbb{R}_+; H^{-1}_{(0)}(\Omega)) \cap L^2(\mathbb{R}_+; H^{\alpha/2}_{(0)}(\Omega)), $$

where $\kappa(t) = \left(\frac{t}{1+t}\right)^{\frac{1}{2}}$. In addition, if $n \leqslant 3$, then there is some $\beta > 0$ depending only on n, such that

$$ \kappa\psi \in L^\infty(\mathbb{R}_+; \mathbf{C}^\beta(\overline{\Omega})). $$

Finally, setting $Z_m \doteq \left\{\widetilde{\psi} \in H^{\alpha/2}(\Omega) \mid E(\widetilde{\psi}) < \infty, \left\langle \widetilde{\psi} \right\rangle = m\right\}$, where $m \in (a,b)$ is given, the mapping $Z_m \ni \psi_0 \mapsto \psi(t) \in H^\gamma_{(m)}(\Omega)$, $\gamma < \frac{\alpha}{2}$ is strongly continuous.

5.1.3 Evolution equations with monotone operators

We refer, e.g., to Brézis Brézis (1973) and Showalter Showalter (1997) for results in the theory of monotone operators. In the following we just summarise some basic facts and definitions. Let H be a real-valued and separable Hilbert space. Recall that $\mathcal{A}\colon H \to \mathcal{P}(H)$ is a monotone operator if

$$ (w - z, x - y)_H \geqslant 0 \qquad \text{for all } w \in \mathcal{A}(x), z \in \mathcal{A}(y). $$

Moreover, $\mathcal{D}(A) = \{x \in H \mid \mathcal{A}(x) \neq \varnothing\}$. Now let $\varphi\colon H \to \mathbb{R} \cup \{+\infty\}$ be a convex function. Then $\mathrm{dom}(\varphi) = \{x \in H : \varphi(x) < \infty\}$ and φ is called proper if $\mathrm{dom}(\varphi) \neq \varnothing$. Moreover, the subgradient $\partial\varphi\colon H \to \mathcal{P}(H)$ is defined by $w \in \partial\varphi(x)$ if and only if

$$ \varphi(\xi) \geqslant \varphi(x) + (w, \xi - x)_H \qquad \text{for all } \xi \in H. $$

Then $\partial\varphi$ is a monotone operator and, if additionally φ is lower semicontinuous, then $\partial\varphi$ is maximal monotone, cf. (Brézis, 1973, Exemple 2.3.4).

The proof of Theorem 5.1.1 is based on the following result for the evolution problem associated to Lipschitz perturbations of monotone operators (see, e.g., (Abels and Wilke, 2007, Theorem 3.1))

Theorem 5.1.2. *Let H_0, H_1 be real, separable Hilbert spaces such that H_1 is densely embedded into H_0. Moreover, let $\varphi\colon H_0 \to \mathbb{R}\cup\{+\infty\}$ be a proper, convex and lower semicontinuous functional such that $\varphi = \varphi_1+\varphi_2$, where $\varphi_2 \geqslant 0$ is convex and lower semicontinuous,* $\operatorname{dom}\varphi_1 = H_1$, *and $\varphi_1|_{H_1}$ is a bounded, coercive, quadratic form on H_1 and set $\mathcal{A} = \partial\varphi$. Furthermore, assume that $\mathcal{B}\colon H_1 \to H_0$ is a globally Lipschitz continuous function. Then for every $u_0 \in \mathcal{D}(\mathcal{A})$ and $f \in L^2(0,T;H_0)$ there is a unique $u \in H^1(0,T;H_0)\cap L^\infty(0,T;H_1)$ with $u(t)\in\mathcal{D}(\mathcal{A})$ for a.e. $t>0$ solving*

$$\frac{d}{dt}u(t) + \mathcal{A}(u(t)) \quad \ni \quad \mathcal{B}(u(t)) + f(t) \quad \text{for a.e. } t\in(0,T) \tag{5.1.5}$$

$$u(0) \quad = \quad u_0 \tag{5.1.6}$$

Moreover, $\varphi(u)\in L^\infty(0,T)$.

5.1.4 Results on the nonlocal operator $\mathcal{L}$

Assumptions (5.0.6)–(5.0.8) allow us to deduce the following norm equivalence results.

Lemma 5.1.3. *Let $u\in H^{\alpha/2}(\Omega)$. Then there exist two positive constants c and C such that*

$$c\|u\|^2_{H^{\alpha/2}(\Omega)} \leqslant |\langle u\rangle|^2 + \mathcal{E}(u,u) \leqslant C\|u\|^2_{H^{\alpha/2}(\Omega)} \qquad \forall\, u\in H^{\alpha/2}(\Omega).$$

Corollary 5.1.4. *The following norm equivalences hold:*

$$\mathcal{E}(u,u) \sim \|u\|^2_{H^{\alpha/2}_{(0)}(\Omega)} \qquad \forall\, H^{\alpha/2}_{(0)}(\Omega), \tag{5.1.7}$$

$$\mathcal{E}(u,u) + |\langle u\rangle|^2 \sim \|u\|^2_{H^{\alpha/2}(\Omega)} \qquad \forall\, H^{\alpha/2}(\Omega). \tag{5.1.8}$$

We now consider the variational extension of the nonlocal linear operator $\mathcal{L}$ (see (5.0.5)). More precisely, abusing the notation, we define $\mathcal{L}\colon H^{\alpha/2}(\Omega)\to H^{-\alpha/2}(\Omega)$ by setting

$${}_{H^{-\alpha/2}}\langle \mathcal{L}u,\varphi\rangle_{H^{\alpha/2}} = \mathcal{E}(u,\varphi) \quad \text{for all } \varphi\in H^{\alpha/2}(\Omega).$$

In particular we have

$$\langle \mathcal{L}u, 1\rangle = \mathcal{E}(u,1) = 0$$

by definition.

Remark 5.1.1. This definition of $\mathcal{L}$ agrees with (5.0.5) as soon as $u\in H^\alpha_{\mathrm{loc}}(\Omega)\cap H^{\alpha/2}(\Omega)$ and $\varphi\in C^\infty_0(\Omega)$, cf. (Abels and Kassmann, 2007, Lemma 4.2).

We will also need the following regularity result, which essentially states that the operator $\mathcal{L}$ is of lower order with respect to the usual Laplace operator.

Lemma 5.1.5. *Let $g \in L^2_{(0)}(\Omega)$ and $\theta > 0$. Then the unique solution u the problem*

$$-\theta \int_\Omega \nabla u \cdot \nabla \varphi + \mathcal{E}(u, \varphi) = (g, \varphi) \qquad \text{in } \Omega, \tag{5.1.9}$$

for all $\varphi \in H^1_{(0)}(\Omega)$, belongs to $H^2_{\mathrm{loc}}(\Omega) \cap H^1_{(0)}(\Omega)$ and satisfies the estimate

$$\theta \|\nabla u\|^2_{L^2} + \|u\|^2_{H^{\alpha/2}} \leqslant C \|g\|^2_{L^2},$$

where C is independent of $\theta > 0$.

Proof. Existence and uniqueness of a solution $u \in H^1_{(0)}(\Omega)$to (5.1.9) easily follow from the continuity and coercivity of the bilinear form $\mathcal{E}(\,\cdot\,,\,\cdot\,)$ through the Lax-Milgram theorem. Also, the estimate can be obtained by choosing $\varphi = u$. The claimed inner regularity $u \in H^2_{\mathrm{loc}}(\Omega)$ can be shown by arguing as in (Abels and Kassmann, 2007, Lemma 4.3). □

The following regularity result is more involved. Its proof is obtained by using ideas of the proof of (Abels and Kassmann, 2007, Lemma 5.4).

Lemma 5.1.6. *Let $\partial\Omega$ of class $\mathbf{C}^2$ and let $u \in H^{\alpha/2}(\Omega)$ such that $\phi'(u) \in L^2(\Omega)$ and*

$$\mathcal{E}(u, \varphi) + \int_\Omega \phi'(u)\varphi \, dx = \int_\Omega g\varphi \, dx \qquad \forall\, \varphi \in H^{\alpha/2}(\Omega) \tag{5.1.10}$$

for some given $g \in H^1(\Omega)$. Then $u \in \mathbf{C}^\beta(\overline{\Omega})$ for some $\beta \in (0, 1)$ depending only on n and there is a constant $C > 0$ independent of u and g such that

$$\|u\|_{\mathbf{C}^\beta(\overline{\Omega})} \leqslant C \left(\|g\|_{H^1(\Omega)} + \|u\|_{H^{\alpha/2}(\Omega)} + \|\phi'(u)\|_{L^2(\Omega)} \right). \tag{5.1.11}$$

Proof. First, let us consider first the case of the half-space $\Omega = \mathbb{R}^n_+$. By approximating the tangential derivatives by difference quotients, we will prove that $u \in H^{\alpha/2}(\mathbb{R}_+; H^1(\mathbb{R}^{n-1})) \cap L^2(\mathbb{R}_+; H^{1+\alpha/2}(\mathbb{R}^{n-1}))$. Then, using the interpolation inequality

$$\|f\|_{H^{1+s}(\mathbb{R}^{n-1})} \leqslant C \|f\|^{\frac{2s}{\alpha}}_{H^{1+\alpha/2}(\mathbb{R}^{n-1})} \|f\|^{1-\frac{2s}{\alpha}}_{H^1(\mathbb{R}^{n-1})}$$

and direct estimates, one obtains

$$\begin{aligned} &u \in H^{\alpha/2}(\mathbb{R}_+; H^1(\mathbb{R}^{n-1})) \cap L^2(\mathbb{R}_+; H^{1+\alpha/2}(\mathbb{R}^{n-1})) \\ &\quad \hookrightarrow H^{\alpha/2-s}(\mathbb{R}_+; H^{1+s'}(\mathbb{R}^{n-1})) \hookrightarrow \mathbf{C}^\beta(\mathbb{R}_+, H^{1+s'}(\mathbb{R}^{n-1})) \hookrightarrow \mathbf{C}^\beta(\overline{\mathbb{R}^n_+}), \end{aligned}$$

for any $0 < s' < s < \frac{\alpha}{2} - \frac{1}{2}$, where we have used (Simon, 1990, Corollary 26).

We denote

$$\tau_{j,s}f(x)=f(x+se_j),\quad \Delta^+_{j,h}f(x)=\tau_{j,h}f(x)-f(x),\quad \Delta^-_{j,h}f(x)=f(x)-\tau_{j,-h}f(x),$$

for $h>0$, where e_j is the jth canonical unit vector, $j=1,\dots,n-1$. Replacing φ by $-h^{-s}\Delta^-_{j,h}\varphi$ with $s\in[0,1]$, $j\in\{1,\dots,n-1\}$ in (5.1.10), we obtain that $v_h=h^{-s}\Delta^+_{j,h}u$ solves

$$\mathcal{E}(v_h,\varphi)+h^{-s}\int_\Omega \Delta^+_{j,h}(\phi'(u))\varphi\,dx \quad=\quad -\mathcal{E}_{j,h}(\tau_{j,h}u,\varphi)-\int_\Omega gh^{-s}\Delta^-_{j,h}\varphi\,dx$$

for all $\varphi\in\mathbf{C}^\infty_0(\Omega)$, where $\mathcal{E}_{j,h}$ is the bilinear form with kernel $h^{-s}(k(x+he_j,y+he_j,z)-k(x,y,z))$. Note that by (5.0.7) the latter kernel is bounded by $C|z|^{-d-\alpha}$ uniformly in $h>0$.

First we discuss an auxiliary estimate, which will be needed to deal with some terms in the localisation procedure. To this end let $s\in(\frac12,\frac\alpha2)$. Then choosing $\varphi=v_h$, using (5.1.8) and

$$\int_\Omega \Delta^+_{j,h}(\phi'(u))\Delta^+_{j,h}u\,dx=\\ \int_\Omega \big(\phi'(u(x+he_j))-\phi'(u(x))\big)\,(u(x+he_j)-u(x))\,dx\geqslant 0$$

we conclude

$$\|v_h\|^2_{H^{\alpha/2}(\mathbb{R}^n_+)}\leqslant C\left(\|g\|_{L^2(\mathbb{R}^n_+)}\|h^{-s}\Delta^-_{j,h}v_h\|_{L^2(\mathbb{R}^n_+)}+\|v_h\|^2_{L^2(\mathbb{R}^n_+)}+\|u\|^2_{H^{\alpha/2}(\mathbb{R}^n_+)}\right)$$

We now use the inequality

$$\|h^{-s}\Delta^\pm_{j,h}w\|_{L^2(\mathbb{R}^n_+)}\leqslant C\|w\|_{H^s(\mathbb{R}^n_+)}\leqslant C\|w\|_{H^{\alpha/2}(\mathbb{R}^n_+)},$$

which follows from interpolation of $\|h^{-1}\Delta_{j,h}w\|_{L^2(\mathbb{R}^n_+)}\leqslant C\|w\|_{H^1(\mathbb{R}^n_+)}$ and the simple estimate $\|\Delta_{j,h}w\|_{L^2(\mathbb{R}^n_+)}\leqslant 2\|w\|_{L^2(\mathbb{R}^n_+)}$. Hence, we have

$$\sup_{j=1,\dots,n-1}\left\|h^{-2s}(\Delta^+_{j,h})^2u\right\|_{L^2(\mathbb{R}^n_+)}\leqslant\|v_h\|_{H^{\alpha/2}(\mathbb{R}^n_+)}\leqslant C\left(\|g\|_{L^2(\mathbb{R}^n_+)}+\|u\|_{H^{\alpha/2}(\mathbb{R}^n_+)}\right),$$

which implies that $u\in L^2(\mathbb{R}_+;B^{2s}_{2,\infty}(\mathbb{R}^{n-1}))\hookrightarrow L^2(\mathbb{R}_+;H^1(\mathbb{R}^{n-1}))$ (cf. (Bergh and Löfström, 1976, Theorem 6.2.5)). Also, we get

$$\sup_{j=1,\dots,n-1}\left\|\partial_{x_j}u\right\|_{L^2(\mathbb{R}^n_+)}\leqslant C\left(\|g\|_{L^2(\mathbb{R}^n_+)}+\|u\|_{H^{\alpha/2}(\mathbb{R}^n_+)}\right)$$

Next we choose $s=1$ in the definition of v_h and we obtain similarly

$$\begin{aligned}\|v_h\|_{H^{\alpha/2}(\mathbb{R}^n_+)}&\leqslant C\left(\sup_{j=1,\dots,n-1}\left\|\partial_{x_j}g\right\|_{L^2(\mathbb{R}^n_+)}+\|v_h\|_{L^2(\mathbb{R}^n_+)}+\|u\|_{H^{\alpha/2}(\mathbb{R}^n_+)}\right)\\&\leqslant C\left(\sup_{j=1,\dots,n-1}\left\|(\partial_{x_j}g,\partial_{x_j}u)\right\|_{L^2(\mathbb{R}^n_+)}+\|u\|_{H^{\alpha/2}(\mathbb{R}^n_+)}\right).\end{aligned}$$

Hence $v_h=h^{-1}\Delta^+_{j,h}u$, $h>0$, is uniformly bounded in $H^{\alpha/2}(\mathbb{R}^n_+)$ and therefore $\partial_{x_j}u\in H^{\alpha/2}(\mathbb{R}^n_+)$.

In order to prove the statement for a bounded domain Ω, it is sufficient to show that for every $x \in \overline{\Omega}$ and for some open neighbourhood U of x we have that $u \in \mathbf{C}^\beta(\overline{\Omega} \cap U)$. Let U_0 be an open neighbourhood of x and $F\colon \mathbb{R}^n \to \mathbb{R}^n$ be a $\mathbf{C}^2$-diffeomorphism which maps $U_0 \cap \overline{\Omega}$ onto $\overline{\mathbb{R}^n_+} \cap V_0$ for some open set V_0. Moreover, let $\chi \in \mathbf{C}^\infty_0(U_0)$ with $\chi \equiv 1$ on some neighbourhood $U_1 \Subset U_0$ of x, let V_1 be an open set such that $V_1 \cap \overline{\mathbb{R}^n_+} = F(U_1 \cap \overline{\Omega})$ and let $F^* l(x) = l(F(x))$ denote the pull-back of l by F. For $\varphi \in \mathbf{C}^\infty_0(\mathbb{R}^n_+)$ we obtain that $v \doteq F^{*,-1}(\chi u) \in H^{\alpha/2}_0(\mathbb{R}^n_+)$ solves

$$\begin{aligned}
&\widetilde{\mathcal{E}}(v,\varphi) + \int_{\mathbb{R}^n_+} \phi'(v)\varphi\omega\,dx \\
&\quad = \quad \mathcal{E}(\chi u, F^*(\varphi)) = \mathcal{E}(u, \chi F^*(\varphi)) + ([\mathcal{L},\chi]u, F^*(\varphi))_{L^2(\Omega)} \\
&\quad = \quad (g, \chi F^*(\varphi))_{L^2(\Omega)} + ([\mathcal{L},\chi]u, F^*(\varphi))_{L^2(\Omega)} \\
&\quad = \quad (\tilde{g},\varphi)_{L^2(\mathbb{R}^n_+)} + ([\mathcal{L},\chi]u, F^*(\varphi))_{L^2(\Omega)}
\end{aligned}$$

where

$$\widetilde{\mathcal{E}}(\varphi,\chi) = \int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+} (\varphi(x)-\varphi(y))(\chi(x)-\chi(y))\tilde{k}(x,y,x-y)dxdy \tag{5.1.12}$$

$$\tilde{k}(x,y,z) = k(F^{-1}(x), F^{-1}(y), A(x,y)z)\omega(x)\omega(y), \tag{5.1.13}$$

and

$$\begin{aligned}
A(x,y) &= \int_0^1 DF^{-1}((1-s)y + sx)ds, \\
\tilde{g}(x) &= g(F^{-1}(x))\omega(x), \qquad \omega(x) = \det DF^{-1}(x).
\end{aligned}$$

Moreover, $\widetilde{\mathcal{L}}$ denotes the integral operator associated to $\widetilde{\mathcal{E}}$. It is not difficult to prove that $\tilde{k} \in \mathcal{K}^\alpha(R')$ for some $R' = R'(R,F)$. Now all terms on the right-hand side of the equation above define a functional on $L^2(\mathbb{R}^n_+)$ (see (Abels and Kassmann, 2007, Lemma 3.6)). Hence $v \in L^2(\mathbb{R}_+; H^1(\mathbb{R}^{n-1}))$ by the first arguments in the case $\mathbb{R}^n_+$. Choosing now another $\chi \in \mathbf{C}^\infty_0(U_1)$ such that $\chi \equiv 1$ on an open neighbourhood $U_2 \Subset U_1$ of x, one obtains that $v \doteq F^{*,-1}(\chi u)$ solves

$$\begin{aligned}
&\widetilde{\mathcal{E}}(v,\varphi) = (\tilde{g},\varphi)_{L^2(\mathbb{R}^n_+))} - (\eta u, [\mathcal{L},\chi]F^*(\varphi))_{L^2(\Omega)} + ([\mathcal{L},\chi](1-\eta)u, F^*(\varphi))_{L^2(\Omega)} \\
&= (\tilde{g},\varphi)_{L^2(\mathbb{R}^n_+)} - (\tilde{\eta}v, [\widetilde{\mathcal{L}},\tilde{\chi}]\varphi)_{L^2(\mathbb{R}^n_+)} + ([\mathcal{L},\chi](1-\eta)u, F^*(\varphi))_{L^2(\Omega)}
\end{aligned}$$

for all $\varphi \in \mathbf{C}^\infty_0(\mathbb{R}^n_+)$, where $\eta \in \mathbf{C}^\infty_0(U_1)$ with $\eta \equiv 1$ on $\operatorname{supp}\chi$, and $\tilde{\chi} = F^{*,-1}(\chi), \tilde{\eta} = F^{*,-1}(\eta)$. Let us replace φ by $-h^{-1}\Delta^-_{j,h}\varphi$. We obtain

$$\begin{aligned}
&\widetilde{\mathcal{E}}(v, -h^{-1}\Delta^-_{j,h}\varphi) + h^{-1}\int_\Omega \Delta^+_{j,h}(\phi'(u))\varphi\omega\,dx \\
&\quad = \quad (h^{-1}\Delta^+_{j,h}\tilde{g} - \tau_h(\phi'(v))h^{-1}\Delta^+_{j,h}\omega, \varphi)_{L^2(\mathbb{R}^n_+)} - (h^{-1}\Delta^+_{j,h}(\tilde{\eta}v), [\widetilde{\mathcal{L}},\tilde{\chi}]\varphi)_{L^2(\mathbb{R}^n_+)} \\
&\qquad + (\tilde{\eta}v, h^{-1}[\Delta^-_{j,h}, [\widetilde{\mathcal{L}},\tilde{\chi}]]\varphi)_{L^2(\mathbb{R}^n_+)} + (h^{-1}\Delta^+_{j,h}F^{*,-1}([\mathcal{L},\chi](1-\eta)u), \varphi)_{L^2(\mathbb{R}^n_+)}.
\end{aligned}$$

Observe now that

$$\begin{aligned}\|h^{-1}\Delta^+_{j,h}\tilde g - \tau_h(\phi'(v))h^{-1}\Delta^+_{j,h}\omega\|_{L^2(\mathbb{R}^n_+)} &\leqslant C\left(\|\partial_{x_j}\tilde g\|_{L^2(\mathbb{R}^n_+)} + \|\phi'(v)\|_{L^2(\mathbb{R}^n_+)}\right)\\ &\leqslant C\left(\|g\|_{H^1(\Omega)} + \|\phi'(u)\|_{L^2(\Omega)}\right).\end{aligned}$$

On the other hand, since $\partial_{x_j}(\tilde\eta v), \partial_{x_j}\tilde g \in L^2(\mathbb{R}^n_+)$, then $h^{-1}\Delta^+_{j,h}(\tilde\eta v)$ and $h^{-1}\Delta^+_{j,h}\tilde g$ are bounded in $L^2(\mathbb{R}^n_+)$. Moreover, we have

$$\begin{aligned}([\mathcal{L},\chi](1-\eta)u)(x) &= -\chi(x)(\mathcal{L}(1-\eta)u)(x)\\ &= \int_\Omega \chi(x)(1-\eta(y))u(y)k(x,y,x-y)\,dy\end{aligned}$$

because of $\chi(1-\eta)\equiv 0$, where $\chi(1-\eta)k \in \mathbf{C}^1(\overline\Omega\times\overline\Omega)$ since $\operatorname{supp}\chi\cap\operatorname{supp}(1-\eta)=\varnothing$ and $k(x,y,x-y)$ is continuously differentiable for $x\neq y$. Therefore $([\mathcal{L},\chi](1-\eta)u)\in\mathbf{C}^1(\overline\Omega)$ and

$$h^{-1}\Delta^+_{j,h}F^{*,-1}([\mathcal{L},\chi](1-\eta)u)\in L^2(\mathbb{R}^n_+)$$

is uniformly bounded. Finally,

$$\begin{aligned}[h^{-1}\Delta^-_{j,h},[\widetilde{\mathcal{L}},\tilde\chi]]\varphi &= [\widetilde{\mathcal{L}},h^{-1}[\Delta^-_{j,h},\tilde\chi]]\varphi + [\tilde\chi,[\widetilde{\mathcal{L}},h^{-1}\Delta^-_{j,h}]]\varphi\\ &= [\widetilde{\mathcal{L}},h^{-1}(\Delta^-_{j,h}\tilde\chi)\tau_{j,-h}]\varphi + [\tilde\chi,\widetilde{\mathcal{L}}^-_{j,h}]\varphi,\end{aligned}$$

where $\widetilde{\mathcal{L}}^-_{j,h}$ is the integral operator with kernel $h^{-1}(\tilde k(x+he_j,y+he_j,z)-\tilde k(x,y,z))$ and by (5.0.7) the latter kernel is bounded by $C|z|^{-d-\alpha}$ uniformly in $h>0$. This implies that

$$\|[h^{-1}\Delta^-_{j,h},[\widetilde{\mathcal{L}},\tilde\chi]]\varphi\|_{L^2(\mathbb{R}^n_+)} \leqslant C\|\varphi\|_{H^{\alpha/2}(\Omega)}$$

uniformly in $h>0$. Hence choosing $\varphi = h^{-1}\Delta^+_{j,h}v$ one obtains arguing as in the half-space case that $\partial_{x_j}v\in H^{\alpha/2}(\mathbb{R}^n_+)$, $j=1,\dots,n-1$. This entails Hölder continuity of u in a neighbourhood of x. Estimate (5.1.11) thus follows from the estimates obtained in this proof. □

5.2 Subgradients

Let $\phi\colon[a,b]\to\mathbb{R}$ be a continuous function and set $\phi(x)=+\infty$ for $x\notin[a,b]$. Then fix $\theta\geqslant 0$ and consider the functional

$$F_\theta(\psi) = \frac{\theta}{2}\int_\Omega |\nabla\psi|^2\,\mathrm{d}x + \mathcal{E}(\psi,\psi) + \int_\Omega \phi(\psi(x))\,\mathrm{d}x \tag{5.2.1}$$

where

$$\begin{aligned}\operatorname{dom} F_0 &= \left\{\psi\in H^{\alpha/2}(\Omega)\cap L^2_{(m)}(\Omega) : \phi(\psi)\in L^1(\Omega)\right\},\\ \operatorname{dom} F_\theta &= H^1(\Omega)\cap\operatorname{dom} F_0 \qquad \text{if } \theta>0.\end{aligned}$$

for a fixed $m \in (a,b)$. Moreover, let

$$\mathcal{E}_\theta(u,v) = \theta \int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x + \mathcal{E}(u,v)$$

for all $u, v \in H^1(\Omega)$ if $\theta > 0$ and $u, v \in H^{\alpha/2}(\Omega)$ if $\theta = 0$.

We denote by $\partial F_\theta(\psi)\colon L^2_{(m)}(\Omega) \to \mathcal{P}(L^2_{(0)}(\Omega))$ the subgradient of F_θ at $\psi \in \operatorname{dom} F$ in the sense that $w \in \partial F_\theta(\psi)$ if and only if

$$(w, c' - c)_{L^2} \leqslant F_\theta(c') - F_\theta(\psi) \qquad \forall\, c' \in L^2_{(m)}(\Omega).$$

Note that $L^2_{(m)}(\Omega)$ is an *affine* subspace of $L^2(\Omega)$ with tangent space $L^2_{(0)}(\Omega)$. Therefore the standard definition of ∂F for functionals on Hilbert spaces does not apply. But the definition above is the obvious generalisation to affine subspaces of Hilbert spaces.

First of all let us prove the following

Lemma 5.2.1. *Let $\phi\colon [a,b] \to \mathbb{R}$ be a continuous and convex function. Then, for any $\theta \geqslant 0$, F_θ defined as in (5.2.1) is a proper, lower semicontinuous, convex functional.*

Proof. We only need to prove the lower semicontinuity. The case $\theta > 0$ may be handled as in (Abels and Wilke, 2007, Lemma 4.1). On the other hand, if $\theta = 0$, let $\psi_k \in L^2_{(m)}(\Omega)$ be such that $\lim_{k\to\infty} \psi_k = \psi$ in $L^2(\Omega)$ and $\liminf_{k\to\infty} F_\theta(\psi_k) < \infty$. By adding a suitable constant to ϕ, we can reduce to the case $\phi \geqslant 0$. Up to a subsequence, we can assume that $\psi_k \in \operatorname{dom} F_\theta$ and $\psi_k \rightharpoonup \psi^*$ in $H^{\alpha/2}(\Omega)$. Hence $\psi_k \to \psi^*$ in $L^2(\Omega)$ and almost everywhere in Ω. Thus we get $\psi = \psi^*$. Moreover, Fatou's lemma and the (weak) continuity of $\mathcal{E}$ imply $\psi \in \operatorname{dom} F_\theta$ and $F_\theta(\psi) \leqslant \liminf_{k\to\infty} F_\theta(\psi_k)$. □

Corollary 5.2.2. *Let ϕ and F_θ be as in Lemma 5.2.1 and let $m = 0$. Then, for any $\theta \geqslant 0$, ∂F_θ is a maximal monotone operator on $H = L^2_{(0)}(\Omega)$.*

Proof. In view of Lemma 5.2.1, this fact follows from Corollary 1.2 and Lemma 1.3 in (Showalter, 1997, Chapter IV). □

We now state our main result on the following characterisation of $\partial F(\psi)$:

Theorem 5.2.3. *Let $\phi\colon [a,b] \to \mathbb{R}$ be a convex function that is twice continuously differentiable in (a,b) and satisfies $\lim_{x\to a} \phi'(x) = -\infty$, $\lim_{x\to b} \phi'(x) = +\infty$. Moreover, we set $\phi'(x) = +\infty$ for $x \notin (a,b)$ and let F_θ be defined as in (5.2.1). Then*

$$\begin{aligned}\mathcal{D}(\partial F_0) \quad = \quad & \Big\{\psi \in H^\alpha_{\mathrm{loc}}(\Omega) \cap H^{\alpha/2}(\Omega) \cap L^2_{(m)}(\Omega) : \phi'(\psi) \in L^2(\Omega), \exists f \in L^2(\Omega) : \\ & \mathcal{E}(\psi,\varphi) + \int_\Omega \phi'(\psi)\varphi \,dx = \int_\Omega f\varphi \,\mathrm{d}x \quad \forall\, \varphi \in H^{\alpha/2}(\Omega)\Big\}\end{aligned}$$

if $\theta = 0$ *and*

$$\begin{aligned}\mathcal{D}(\partial F_\theta) \quad = \quad & \Big\{\psi \in H^2_{\mathrm{loc}}(\Omega) \cap H^1(\Omega) \cap L^2_{(m)}(\Omega) : \phi'(\psi) \in L^2(\Omega), \exists f \in L^2(\Omega) : \\ & \mathcal{E}_\theta(\psi, \varphi) + \int_\Omega \phi'(\psi)\varphi \, dx = \int_\Omega f\varphi \, \mathrm{d}x \quad \forall\, \varphi \in H^1(\Omega)\Big\}\end{aligned}$$

if $\theta > 0$ *as well as*

$$\partial F_\theta(\psi) = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) \quad \textit{in } \mathcal{D}'(\Omega) \qquad \textit{for } \theta \geqslant 0.$$

Moreover, the following estimates hold

$$\begin{aligned}\theta\|c\|^2_{H^1} + \|c\|^2_{H^{\alpha/2}} + \|\phi'(\psi)\|_2^2 &\leqslant C\left(\|\partial F_\theta(\psi)\|_2^2 + \|c\|_2^2 + 1\right) \\ \int_\Omega\int_\Omega (\phi'(\psi(x)) - \phi'(c(y)))(\psi(x) - c(y))k(x, y, x-y)\,\mathrm{d}x\mathrm{d}y & \\ &\leqslant C\left(\|\partial F_\theta(\psi)\|_2^2 + \|c\|_2^2 + 1\right) \\ \theta\int_\Omega \phi''(\psi)|\nabla\psi|^2\,\mathrm{d}x &\leqslant C\left(\|\partial F_\theta(\psi)\|_2^2 + \|c\|_2^2 + 1\right)\end{aligned} \tag{5.2.2}$$

for some constant $C > 0$ *independent of* $\psi \in \mathcal{D}(\partial F_\theta)$ *and* $\theta \geqslant 0$.

Proof. We will follow the same strategy as in (Abels and Wilke, 2007, Theorem 4.3). Let us introduce first some technical tools and simplifications. If we replace $\psi(x)$ by $\bar\psi(x) = \psi(x) - m$ and ϕ by $\bar\phi(\psi) = \phi(\psi + m)$, we can assume w.l.o.g. that $m = 0 \in (\bar a, \bar b)$. Moreover, replacing $\phi(\psi)$ by $\bar\phi(\psi) = \phi(\psi) + b_1\psi(x) + b_2$, $b_j \in \mathbb{R}$ means changing F only by an affine linear functional, for which the subgradient is trivial. In this way, we may also assume that $\phi'(0) = \phi(0) = 0$. Furthermore, we define $\phi_+(\psi) = \phi(\psi)$ if $\psi > 0$, $\phi_+(\psi) = 0$ if $\psi \leqslant 0$ and $\phi_-(\psi) = \phi(\psi) - \phi_+(\psi)$. Then $\phi_\pm \colon \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ are convex functions, which are continuously differentiable in (a, b).

In the following, we would like to evaluate the directional derivative of $F_\theta(\psi)$ along $\phi'(\psi)$. Formally, this requires the estimate of $\|\phi'(\psi)\|_2$, but we cannot do this directly due to the singular behaviour of ϕ. Therefore we approximate ϕ'_+ (and analogously ϕ'_-) from below by a sequence f_n^+ of smooth potentials as follows. Since ϕ' is continuous and monotone, $\phi'(0) = 0$, and $\lim_{\psi\to b}\phi'(\psi) = +\infty$, for every $n \in \mathbb{N}$ sufficiently large there is some $\psi_n \in (\frac{b}{2}, b)$ such that $\phi'(\psi_n) = n$. Therefore we can define

$$f_n^+(\psi) = \begin{cases} \phi'(\psi) & \text{for } \psi \in [\frac{b}{2}, \psi_n) \\ n + \phi''(\psi_n)(\psi - \psi_n) & \text{for } \psi \geqslant \psi_n \\ 0 & \text{for } \psi \leqslant 0 \end{cases}$$

for $\psi \notin (0, \frac{b}{2})$. Moreover, we can extend f_n^+ to $\mathbb{R}$ such that $f_n^+ \colon \mathbb{R} \to \mathbb{R}$ are C^1-functions with $0 \leqslant f_n^+ \leqslant \phi'_+$ and with first derivative bounded by $M_n \doteq \sup_{0\leqslant x\leqslant\psi_n}\phi''(x)$.

We have to work in the subspace $L^2_{(0)}(\Omega)$. Then we will use "bump functions" supported in suitable sets to correct the mean value of functions. For this let $\psi \in H^1_{(0)}(\Omega)$ be fixed and let $I \subset [a,b]$ be an interval such that $|\{\psi(x) \in I\}| > 0$. We say that φ is a *bump function supported in* $\{\psi \in I\}$ if $\varphi \in H^1(\Omega) \cap L^\infty(\Omega)$, $\varphi \geqslant 0$, $\varphi(x) = 0$ if $\psi(x) \notin I$ and if $m(\varphi) = 1$. Such a function can be constructed as follows. Choose a smooth function $\zeta\colon \mathbb{R} \to [0,1]$ with bounded first derivative such that $\zeta(s) = 0$ if $s \notin I$ and $\zeta(s) > 0$ otherwise. Then $\varphi = \frac{\zeta(\psi)}{m(\zeta(\psi))}$ has the stated properties. Furthermore, we note that, if $I = [a, a']$ with $a' \in (a,b)$, then we can choose ζ such that $\zeta'(s) \leqslant 0$. This implies that the constructed function φ has the property

$$(\nabla\psi, \nabla\varphi)_{L^2(\Omega)} = \frac{1}{m(\zeta(\psi))} \int_\Omega \zeta'(\psi)|\nabla\psi|^2 \,\mathrm{d}x \leqslant 0 \tag{5.2.3}$$

as well as

$$\begin{aligned}\mathcal{E}(\psi,\varphi) &= \frac{1}{2\langle\zeta(\psi)\rangle} \int_\Omega\int_\Omega (\psi(x)-\psi(y))(\zeta(\psi(x))-\zeta(\psi(y)))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ &= \frac{1}{2\langle\zeta(\psi)\rangle} \int_\Omega\int_\Omega \zeta'(\xi)(\psi(x)-\psi(y))^2 k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \leqslant 0\end{aligned} \tag{5.2.4}$$

where $\xi(x,y)$ is a measurable function which is bounded above and below by $\max\{\psi(x),\psi(y)\}$ and $\min\{\psi(x),\psi(y)\}$ respectively. Given such a bump function φ, we define $M_\varphi\colon L^2(\Omega) \to H^1(\Omega)\cap L^\infty(\Omega)$ by

$$(M_\varphi f)(x) = m(f)\varphi, \qquad f \in L^2(\Omega).$$

Then $f - M_\varphi f \in L^2_{(0)}(\Omega)$ and

$$\|M_\varphi f\|_{H^1} \leqslant C\left|\int_\Omega f(x)\,\mathrm{d}x\right| \qquad \forall\ f \in L^2(\Omega). \tag{5.2.5}$$

Observe now that

$$|\{\psi(x) - a \geqslant t\}| \leqslant \frac{1}{t}\int_\Omega (\psi(x)-a)\,\mathrm{d}x = \frac{|a||\Omega|}{t}$$

for $t > 0$ since $\psi \in L^2_{(0)}(\Omega)$. This implies that $|\{\psi < \frac{b}{2}\}| \geqslant \frac{b}{b+2|a|}|\Omega| > 0$. Hence the interval $I = [a, \frac{b}{2})$ is admissible for the construction of bump functions supported in $\{\psi \in (a, \frac{b}{2})\}$.

After these preliminary considerations, let $\psi \in \mathcal{D}(\partial F_\theta)$. We define $\widetilde{\psi}_t(x)$, $0 < t \leqslant \frac{2}{M_n}$, $x \in \Omega$, as solution of

$$\widetilde{\psi}_t(x) = \psi(x) - t f_n^+(\widetilde{\psi}_t(x)), \tag{5.2.6}$$

which exists by the contraction mapping principle. Then $\widetilde{\psi}_t(x) = \psi(x)$ if $\psi(x) < 0$ since $f_n^+(\widetilde{\psi}_t(x)) = 0$ in this case. Moreover, we have that $0 \leqslant \widetilde{\psi}_t(x) = \psi(x) - t f_n^+(\widetilde{\psi}_t(x)) \leqslant \psi(x)$ if $\psi(x) \geqslant 0$. More formally, $\widetilde{\psi}_t$ can be expressed in the form $\widetilde{\psi}_t(x) = F_t^n(\psi(x))$, where $F_t^n\colon [a,b] \to [a,b]$ is a continuous differentiable mapping with $F_t^n(x) \to x$, $(F_t^n)'(x) \to 1$ as $t \to 0+$ uniformly

in $[a,b]$. Hence, if $\theta>0$, $\widetilde{\psi}_t\in H^1(\Omega)$ and $\widetilde{\psi}_t\to_{t\to 0}\psi$ in $H^1(\Omega)$ and almost everywhere. If else $\theta=0$, we deduce $\widetilde{\psi}_t\in H^{\alpha/2}(\Omega)$ and $\widetilde{\psi}_t\to_{t\to 0}\psi$ in $H^{\alpha/2}(\Omega)$ and almost everywhere.

Since, in general, $\widetilde{\psi}_t(x)\notin L^2_{(0)}(\Omega)$, we set $\psi_t=\widetilde{\psi}_t+tM_\varphi(f_n^+(\widetilde{\psi}_t))$, where φ is a bump function supported in $\{\psi(x)<\frac{b}{2}\}$ satisfying (5.2.3) and (5.2.4). Then $\psi_t\in L^2_{(0)}(\Omega)$. Furthermore, $\psi_t(x)=\widetilde{\psi}_t(x)$ and $f_n^+(\psi_t(x))=f_n^+(\widetilde{\psi}_t(x))$ if $\psi(x)>\frac{b}{2}$ and $\psi_t(x)=\widetilde{\psi}_t(x)+tM_\varphi(f_n^+(\psi_t))\in[a,\frac{3}{4}b]$ if $\psi(x)\leqslant\frac{b}{2}$ and if $0<t<\frac{b}{4M_n'}$ where $M_n'=\sup_{0\leqslant t\leqslant b}f_n^+(t)\|\varphi\|_\infty$. We denote $d_t=M_\varphi(f_n^+(\widetilde{\psi}_t))$.

We now assume that $w\in\partial F_\theta(\psi)$. Thus we have

$$F_\theta(\psi)-F_\theta(\psi_t)\leqslant t(w,f_n^+(\widetilde{\psi}_t)-d_t)_{L^2(\Omega)}.$$

Moreover, if $t>0$ is sufficiently small, a direct computation involving the definition of F and the above construction gives

$$\begin{aligned}
&F_\theta(\psi)-F_\theta(\psi_t)\\
=&\int_\Omega(\phi(\psi(x))-\phi(\psi_t(x)))\,\mathrm{d}x+\theta t(\nabla\psi,\nabla f_n^+(\widetilde{\psi}_t))_{L^2}-\theta tm(f_n^+(\widetilde{\psi}_t))(\nabla\psi,\nabla\varphi)_{L^2}\\
&-\theta\frac{t^2}{2}\|\nabla(f_n^+(\widetilde{\psi}_t)-d_t)\|_{L^2}^2-\mathcal{E}(\psi-\psi_t,\psi-\psi_t)\\
&+t\int_\Omega\int_\Omega(f_n^+(\widetilde{\psi}_t(x))-f_n^+(\widetilde{\psi}_t(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&-t\left\langle f_n^+(\widetilde{\psi}_t)\right\rangle\int_\Omega\int_\Omega(\varphi(x)-\varphi(y))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y
\end{aligned}$$

Therefore, we deduce

$$\begin{aligned}
&F_\theta(\psi)-F_\theta(\psi_t)\\
\geqslant&t\int_{\{\psi(x)>\frac{b}{2}\}}\phi'(\psi_t(x))f_n^+(\psi_t(x))\,\mathrm{d}x+t\int_{\{\psi(x)\leqslant\frac{a}{2}\}}(\phi(\psi(x))-\phi(\psi(x)+td_t))\,\mathrm{d}x\\
&+\int_{\{\frac{a}{2}\leqslant\psi(x)\leqslant\frac{b}{2}\}}\Big(\phi(\psi(x))-\phi(\widetilde{\psi}_t(x)+td_t)\Big)\,\mathrm{d}x+\theta t(\nabla\psi,\nabla f_n^+(\widetilde{\psi}_t))\\
&+t\int_\Omega\int_\Omega(f_n^+(\widetilde{\psi}_t(x))-f_n^+(\widetilde{\psi}_t(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&-\mathcal{E}(\psi-\psi_t,\psi-\psi_t)-\theta\frac{t^2}{2}\|\nabla(f_n^+(\widetilde{\psi}_t)-d_t)\|_{L^2}^2.
\end{aligned}$$

Hence

$$\begin{aligned}
&F_\theta(\psi)-F_\theta(\psi_t)\\
\geqslant&t\int_{\{\psi(x)>\frac{b}{2}\}}f_n^+(\psi_t(x))^2\,\mathrm{d}x+\theta t(\nabla\psi,\nabla f_n^+(\widetilde{\psi}_t))-\theta\frac{t^2}{2}\|\nabla(f_n^+(\widetilde{\psi}_t)-d_t)\|_{L^2}^2\\
&+\int_{\{\frac{a}{2}\leqslant\psi(x)\leqslant\frac{b}{2}\}}(\phi(\psi(x))-\phi(\psi(x)+td_t))\,\mathrm{d}x-\mathcal{E}(\psi-\psi_t,\psi-\psi_t)\\
&+t\int_\Omega\int_\Omega(f_n^+(\widetilde{\psi}_t(x))-f_n^+(\widetilde{\psi}_t(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y,
\end{aligned}$$

where we have used that $\phi(\psi)-\phi(\psi_t)\geqslant\phi'(\psi_t)(\psi-\psi_t)$ and $\psi_t<\psi$ if $\psi>\frac{b}{2}$, $\phi'(\psi_t)\geqslant f_n^+(\psi_t)$ as well as (5.2.3), (5.2.4) and $\phi(\psi)-\phi(\psi+td_t)\geqslant 0$ if $\psi\leqslant\frac{a}{2}$ and $t\leqslant\frac{a}{2M_n'}$. Hence we deduce

$$\begin{aligned}
&(w,f_n^+(\widetilde{\psi}_t)-d_t)_{L^2(\Omega)}\\
\geqslant&\int_{\{\psi(x)>\frac{b}{2}\}} f_n^+(\psi_t(x))^2\,\mathrm{d}x+\theta(\nabla\psi,\nabla f_n^+(\widetilde{\psi}_t))-\theta\frac{t}{2}\|\nabla(f_n^+(\psi_t)-d_t)\|_{L^2}^2\\
&+\int_\Omega\int_\Omega(f_n^+(\widetilde{\psi}_t(x))-f_n^+(\widetilde{\psi}_t(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&-\frac{t}{2}\mathcal{E}(f_n^+(\widetilde{\psi}_t)-d_t,f_n^+(\widetilde{\psi}_t)-d_t)\\
&+\int_{\{\frac{a}{2}\leqslant\psi(x)\leqslant\frac{b}{2}\}}\frac{1}{t}\left(\phi(\psi(x))-\phi(\widetilde{\psi}_t(x)+td_t)\right)\,\mathrm{d}x,
\end{aligned}$$

which yields for $t\to 0$

$$\begin{aligned}
&(w,f_n^+(\psi)-M_\varphi(f_n^+(\psi)))_{L^2(\Omega)}\\
\geqslant&\int_{\{\psi(x)\geqslant\frac{b}{2}\}} f_n^+(\psi(x))^2\,\mathrm{d}x\\
&+\int_{\{\frac{a}{2}\leqslant\psi(x)\leqslant\frac{b}{2}\}}\phi'(\psi(x))(f_n^+(\psi(x))-M_\varphi(f_n^+(\psi)))\,\mathrm{d}x\\
&+\theta\left(\nabla\psi,\nabla f_n^+(\psi)\right)\\
&+\int_\Omega\int_\Omega(f_n^+(\psi(x))-f_n^+(\psi(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y
\end{aligned}$$

since $\lim_{t\to0}\widetilde{\psi}_t=\psi$ in $H^1(\Omega)$ for $\theta>0$ (in $H^{\alpha/2}(\Omega)$ for $\theta=0$) and almost everywhere and since $\phi(\psi)$ is continuously differentiable in $[\frac{a}{2},\frac{3}{4}b]$. Observe now that

$$\begin{aligned}
\theta\left(\nabla\psi,\nabla f_n^+(\psi)\right)&=\theta\int_\Omega(f_n^+)'(\psi(x))|\nabla\psi(x)|^2\,\mathrm{d}x\geqslant 0,\\
&\int_\Omega\int_\Omega(f_n^+(\psi(x))-f_n^+(\psi(y)))(\psi(x)-\psi(y))k(x,y,x-y))\,\mathrm{d}x\mathrm{d}y\\
&=\int_\Omega\int_\Omega(f_n^+)'(\xi)(\psi(x)-\psi(y))^2k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\geqslant 0,
\end{aligned}$$

where $\xi(x,y)$ is a measurable function which is bounded above and below by $\max\{\psi(x),\psi(y)\}$ and $\min\{\psi(x),\psi(y)\}$, respectively, and use the fact that $\|M_\varphi(f_n^+(\psi))\|_2\leqslant C\|f_n^+(\psi)\|_2$ on account of (5.2.5). Therefore, we get

$$\begin{aligned}
&\|f_n^+(\psi)\|_{L^2(\Omega)}^2+\theta\int_\Omega(f_n^+)'(\psi(x))|\nabla\psi(x)|^2\,\mathrm{d}x\\
&\quad+\int_\Omega\int_\Omega(f_n^+(\psi(x))-f_n^+(\psi(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
\leqslant&C\left(\|w\|_{L^2(\Omega)}^2+\int_{\{\frac{a}{2}\leqslant\psi(x)\leqslant\frac{b}{2}\}}|\phi'(\psi(x))|^2\,\mathrm{d}x+1\right)\\
\leqslant&C'\left(\|w\|_{L^2(\Omega)}^2+\int_\Omega|\psi(x)|^2\,\mathrm{d}x+1\right)
\end{aligned}$$

by Young's inequality and letting $n \to \infty$ we infer

$$\|\phi'_+(\psi)\|^2_{L^2(\Omega)} + \theta \int_\Omega \phi''_+(\psi(x))|\nabla\psi(x)|^2 \,\mathrm{d}x + \int_\Omega\int_\Omega (\phi'_+(\psi(x)) - \phi'_+(\psi(y)))(\psi(x)-\psi(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \leqslant C\left(\|w\|^2_{L^2(\Omega)} + |c|_2^2 + 1\right) \quad (5.2.7)$$

by Fatou's lemma. By symmetry the same is true for ϕ_- instead of ϕ_+ and therefore also for ϕ.

In particular, $\phi'(\psi) \in L^2(\Omega)$ implies $\psi(x) \in (a,b)$ almost everywhere in Ω. Thus $|\{\psi(x) \in (a+\delta, b-\delta)\}| > 0$ for sufficiently small $\delta > 0$. Because of this, we can use a bump function φ supported in $\{\psi(x) \in (a+\delta, b-\delta)\}$ for some fixed $\delta > 0$. Moreover, let $\zeta_M \colon \mathbb{R} \to [0,1]$, $M \in \mathbb{N}$, be smooth functions such that $\zeta_M(s) = 0$ if $|s| \geqslant M+1$, $\zeta_M(s) = 1$ if $|s| \leqslant M$, and $|\zeta'_M(s)| \leqslant 2$. Set $\chi_M(x) = \zeta_M(\phi'(\psi(x)))$. Then $\chi_M \in H^1(\Omega)$ and $\chi_M(x) = 0$ if $\phi'(\psi(x)) \geqslant M+1$. Moreover, $\chi_M \to_{M\to\infty} 1$ almost everywhere and in $L^p(\Omega)$, $1 \leqslant p < \infty$. On the other hand, we have

$$(\nabla\psi, \nabla(\chi_M\zeta))_{L^2(\Omega)} = (\nabla\psi, \chi_M\nabla\zeta)_{L^2(\Omega)} + \int_\Omega \phi''(\psi(x))|\nabla\psi(x)|^2\zeta(x)\zeta'_M(\phi'(\psi(x)))\,\mathrm{d}x$$

for all $\zeta \in C^\infty(\overline{\Omega})$ if $\theta > 0$. Since $\phi''(\psi)|\nabla\psi|^2 \in L^1(\Omega)$ due to (5.2.7) and $\zeta'_M(\phi'(\psi(x))) \to_{M\to\infty} 0$ almost everywhere, we conclude

$$\lim_{M\to\infty} (\nabla\psi, \nabla(\chi_M\zeta))_{L^2(\Omega)} = (\nabla\psi, \nabla\zeta)_{L^2(\Omega)} \qquad \forall\,\zeta \in C^\infty(\overline{\Omega}) \quad (5.2.8)$$

as soon as $\theta > 0$. Analogously, for all $\zeta \in \mathbf{C}^\infty(\overline{\Omega})$, we also have

$$\begin{aligned}
&\mathcal{E}(\psi, \chi_M\zeta)\\
=&\frac{1}{2}\int_\Omega\int_\Omega (\psi(x)-\psi(y))(\chi_M(x)\zeta(x) - \chi_M(y)\zeta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
=&\frac{1}{2}\int_\Omega\int_\Omega (\psi(x)-\psi(y))\chi_M(x)(\zeta(x)-\zeta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&+\frac{1}{2}\int_\Omega\int_\Omega (\psi(x)-\psi(y))(\chi_M(x)-\chi_M(y))\zeta(y)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y.
\end{aligned}$$

Recalling that ϕ' is monotone and $|\zeta'_M(s)| \leqslant 2$, for any positive and bounded ζ we have

$$|(\psi(x)-\psi(y))(\chi_M(x)-\chi_M(y))\zeta(y)k(x,y,x-y)| \leqslant 2(\psi(x)-\psi(y))(\phi'(\psi(x)) - \phi'(\psi(y)))\zeta(y)k(x,y,x-y)$$

and therefore we deduce

$$(\psi(x)-\psi(y))(\chi_M(x)-\chi_M(y))\zeta(y)k(x,y,x-y) \in L^1(\Omega\times\Omega).$$

Moreover, $\chi_M(x) - \chi_M(y) \to 0$ almost everywhere in $\Omega \times \Omega$ and $\chi_M(x) \to 1$ almost everywhere in Ω, so that by the dominated convergence theorem we obtain, for all $\theta \geqslant 0$,

$$\lim_{M\to\infty} \mathcal{E}(\psi, \chi_M\zeta) = \mathcal{E}(\psi, \zeta) \qquad \forall\, \zeta \in \mathbf{C}^\infty(\overline{\Omega}). \tag{5.2.9}$$

We now set $\psi_t^M = \psi - t\chi_M\zeta + tM_\varphi(\chi_M\zeta)$, $\zeta \in \mathbf{C}^\infty(\overline{\Omega})$, $t > 0$, $M \in \mathbb{N}$. Then $\psi_t^M \in \operatorname{dom} F_\theta$ for sufficiently small $t > 0$ (depending on M) and

$$\begin{aligned}
&t\,(w, \chi_M\zeta - M_\varphi(\chi_M\zeta))\\
\geqslant& F_\theta(\psi) - F_\theta(\psi_t^M)\\
=& \int_{\{\phi'(\psi(x))\leqslant M+1\}} \big(\phi(\psi(x)) - \phi(\psi_t^M(x))\big)\,\mathrm{d}x + \theta t(\nabla\psi, \nabla(\chi_M\zeta - M_\varphi(\chi_M\zeta)))_{L^2}\\
&- \frac{\theta t^2}{2}|\nabla(\chi_M\zeta - M_\varphi(\chi_M\zeta))|_2^2\\
&- t^2\mathcal{E}(\chi_M\zeta - M_\varphi(\chi_M\zeta), \chi_M\zeta - M_\varphi(\chi_M\zeta))\\
&+ t\int_\Omega\int_\Omega (\chi_M(x)\zeta(x) - \chi_M(y)\zeta(y))(\psi(x) - \psi(y))k(x, y, x-y)\,\mathrm{d}x\mathrm{d}y\\
&- t\,\langle\chi_M\zeta\rangle\int_\Omega\int_\Omega (\varphi(x) - \varphi(y))(\psi(x) - \psi(y))k(x, y, x-y)\,\mathrm{d}x\mathrm{d}y.
\end{aligned}$$

Dividing by t and passing to the limit $t \to 0$, we conclude

$$\begin{aligned}
&(w, \chi_M\zeta - M_\varphi(\chi_M\zeta))\\
\geqslant& \int_\Omega \phi'(\psi(x))(\chi_M\zeta - M_\varphi(\chi_M\zeta))\,\mathrm{d}x + \theta(\nabla\psi, \nabla(\chi_M\zeta - M_\varphi(\chi_M\zeta)))_{L^2}\\
&+ \int_\Omega\int_\Omega (\chi_M(x)\zeta(x) - \chi_M(y)\zeta(y))(\psi(x) - \psi(y))k(x, y, x-y)\,\mathrm{d}x\mathrm{d}y\\
&- \langle\chi_M\zeta\rangle\int_\Omega\int_\Omega (\varphi(x) - \varphi(y))(\psi(x) - \psi(y))k(x, y, x-y)\,\mathrm{d}x\mathrm{d}y
\end{aligned}$$

for all $\zeta \in C^\infty(\overline{\Omega})$. Replacing ζ by $-\zeta$, we obtain equality in the above inequality. Finally, letting $M \to \infty$, we get

$$(w, \zeta)_{L^2(\Omega)} = (\phi'(\psi), \zeta)_{L^2(\Omega)} + \theta(\nabla\psi, \nabla\zeta)_{L^2(\Omega)} + \mathcal{E}(\psi, \zeta)$$

for all $\zeta \in \mathbf{C}^\infty(\overline{\Omega})$, $\langle\zeta\rangle = 0$, where we have used (5.2.5), (5.2.8), (5.2.9), and

$$\lim_{M\to\infty}\int_\Omega \chi_M\zeta\,\mathrm{d}x = \lim_{M\to\infty}\int_\Omega (\chi_M - 1)\zeta\,\mathrm{d}x = 0 \qquad \text{if } m(\zeta) = 0.$$

Hence $-\theta\Delta_N\psi + \mathcal{L}\psi = w - P_0\phi'(\psi) \in L^2_{(0)}(\Omega)$. Using Lemma 5.1.5 we deduce $\theta^{1/2}\psi \in H^2_{\mathrm{loc}}(\Omega)$, $\psi \in H^\alpha_{\mathrm{loc}}(\Omega) \cap H^{\alpha/2}(\Omega)$ and

$$\theta^{\frac{1}{2}}\|\psi\|_{H^1} + \|\psi\|_{H^{\alpha/2}} \leqslant C|\phi'|_2 + C|w|_2.$$

Using this last estimate and (5.2.7), we obtain (5.2.2). Moreover, the previous observations imply that $\partial F_\theta(\psi) = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi)$ is single-valued and $\mathcal{D}(\partial F_\theta)$ is contained in the set on the right-hand side of the identities for $\mathcal{D}(\partial F_\theta)$ (see statement of this theorem).

Conversely, recalling the definition of subdifferential, the properties of coercive bilinear forms $(\nabla u, \nabla v)$ and $\mathcal{E}(u, v)$ as well as the convexity of ϕ, it can be easily checked that $-\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) \in \partial F_\theta(\psi)$ for any ψ in the set on the right-hand side of the identities for $\mathcal{D}(\partial F_\theta)$. This finishes the proof. □

Corollary 5.2.4. *Let $\theta > 0$ and let the functional F_θ be defined as above. Extend F_θ to a functional $\widetilde{F_\theta}\colon H^{-1}_{(0)}(\Omega) \to \mathbb{R} \cup \{+\infty\}$ by setting $\widetilde{F_\theta}(\psi) = F_\theta(\psi)$ if $\psi \in \operatorname{dom} F_\theta$ and $\widetilde{F_\theta}(\psi) = +\infty$ else. Then $\widetilde{F_\theta}$ is a proper, convex, and lower semicontinuous functional, $\partial\widetilde{F_\theta}$ is a maximal monotone operator with $\partial\widetilde{F_\theta}(\psi) = -\Delta_N \partial F_\theta(\psi)$ and*

$$\mathcal{D}(\partial\widetilde{F_\theta}) = \{\psi \in \mathcal{D}(\partial F_\theta) \mid \partial F_\theta(\psi) = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) \in H^1_{(0)}(\Omega)\}. \tag{5.2.10}$$

Proof. The lower semicontinuity is proved in the same way as in Lemma 5.2.1. Then the fact that $\partial\widetilde{F_\theta}$ is a maximal monotone operator follows from Corollary 1.2 and Lemma 1.3 in (Showalter, 1997, Chapter IV).

First, let $\psi \in \mathcal{D}(\partial\widetilde{F_\theta})$ and $w \in \partial\widetilde{F_\theta}(\psi)$, i.e.,

$$(w, \psi' - \psi)_{H^{-1}_{(0)}} \leqslant \widetilde{F_\theta}(\psi') - \widetilde{F_\theta}(\psi) \qquad \text{for all } \psi' \in H^{-1}_{(0)}(\Omega). \tag{5.2.11}$$

Then let $\mu_0 = -\Delta_N^{-1} w$ and choose $\psi' \in L^2(\Omega)$. Thus we have

$$\begin{aligned} &(\mu_0, \psi' - \psi)_{L^2} \\ =& -(\nabla\mu_0, \nabla\Delta_N^{-1}(\psi' - \psi))_{L^2} = (\nabla\Delta_N^{-1} w, \nabla\Delta_N^{-1}(\psi' - \psi))_{L^2} \\ =& (w, \psi' - \psi)_{H^{-1}_{(0)}} \leqslant \widetilde{F_\theta}(\psi') - \widetilde{F_\theta}(\psi) = F_\theta(\psi') - F_\theta(\psi) \end{aligned}$$

for all $\psi' \in L^2(\Omega)$. Hence $\mu_0 = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) \in \mathcal{D}(\partial F_\theta)$. On the other hand, $\mu_0 = -\Delta_N^{-1} w \in H^1_{(0)}(\Omega)$. This implies that $\partial\widetilde{F_\theta}(\psi) = -\Delta_N \partial F_\theta(\psi)$ and

$$\mathcal{D}(\partial\widetilde{F_\theta}) \subseteq \left\{\psi \in \mathcal{D}(\partial F_\theta) \mid \mu_0 = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) \in H^1_{(0)}(\Omega)\right\}.$$

Conversely, let $\psi \in \mathcal{D}(\partial F_\theta)$ such that $\mu_0 = -\theta\Delta\psi + \mathcal{L}\psi + P_0\phi'(\psi) = \partial F_\theta(\psi) \in H^1_{(0)}(\Omega)$. Then one easily verifies that $w = -\Delta_N\mu_0$ satisfies (5.2.11) arguing as above. Hence $\psi \in \mathcal{D}(\partial F_\theta)$ and (5.2.10) follows. □

5.3 Existence of unique solutions

We first prove the existence of a weak solution. Let us consider the regularized (formal) problem

$$\begin{cases} \partial_t \psi_\theta = \Delta \mu_\theta & \text{in } \Omega \times (0,\infty) \\ \mu_\theta = -\theta \Delta \psi_\theta + \mathcal{L}\psi_\theta + f'(\psi_\theta) & \text{in } \Omega \times (0,\infty) \\ \partial_\nu \mu_\theta = \partial_\nu \psi_\theta = 0 & \text{on } \partial\Omega \times (0,\infty) \\ \psi_\theta|_{t=0} = \psi_{0\theta} & \text{in } \Omega \end{cases} \tag{5.3.1}$$

where $\theta > 0$ is a (small) positive real number.

Without loss of generality we suppose

$$\langle \psi_{0\theta} \rangle = \frac{1}{|\Omega|} \int_\Omega \psi_{0\theta} \, \mathrm{d}x = 0. \tag{5.3.2}$$

As in the previous section we can reduce to this case by a simple shift. Since (5.3.2) and the definition of $\mathcal{L}$ imply that any solution of (5.3.1) as in Theorem 5.1.1 satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \psi_\theta(x,t) \, \mathrm{d}x = \int_\Omega \Delta \mu_\theta \, \mathrm{d}x = 0,$$

we conclude $\langle \psi_\theta(t) \rangle = 0$ for almost all $t > 0$.

Problem (5.3.1) can be formulated as follows (see (Abels and Wilke, 2007, Theorem 1.2))

$$\partial_t \psi_\theta + \mathcal{A}_\theta(\psi_\theta) + \mathcal{B}\psi_\theta = 0, \qquad t > 0, \tag{5.3.3}$$

$$\psi_\theta|_{t=0} = \psi_{0\theta} \tag{5.3.4}$$

where

$$\begin{aligned} {}_{H^{-1}_{(0)}}\langle \mathcal{A}_\theta(\psi_\theta), \varphi \rangle_{H^1_{(0)}} &= (\nabla \mu_\theta, \nabla \varphi)_{L^2} \qquad \text{with } \mu_\theta = -\theta \Delta \psi_\theta + \mathcal{L}\psi_\theta + \phi'(\psi) \\ {}_{H^{-1}_{(0)}}\langle \mathcal{B}\psi_\theta, \varphi \rangle_{H^1_{(0)}} &= d(\nabla \psi_\theta, \nabla \varphi)_{L^2} \end{aligned}$$

for all $\varphi \in H^1_{(0)}(\Omega)$ and

$$\begin{aligned} \mathcal{D}(\mathcal{A}_\theta) = \big\{ & \psi \in H^2_{\mathrm{loc}}(\Omega) \cap H^1(\Omega) \mid \psi(x) \in [a,b] \ \forall\, x \in \Omega, \phi'(\psi) \in L^2(\Omega), \\ & \int_\Omega \int_\Omega (\phi'(\psi(x)) - \phi'(\psi(y)))(\psi(x) - \psi(y)) k(x,y,x-y) \, \mathrm{d}x\mathrm{d}y < \infty, \\ & \phi''(\psi)|\nabla \psi|^2 \in L^1(\Omega),\ \partial F_\theta(\psi) \in H^1(\Omega),\ \partial_\nu \psi|_{\partial\Omega} = 0 \big\} \\ \mathcal{D}(\mathcal{B}) = {} & H^1_{(0)}(\Omega) \subset H^{-1}_{(0)}(\Omega). \end{aligned}$$

In other words

$$\mathcal{A}_\theta(\psi) = -\Delta_N(-\theta \Delta \psi - \mathcal{L}\psi + P_0 \phi'(\psi)), \qquad \mathcal{B}\psi = -d\Delta_N \psi,$$

where $\Delta_N\colon H^1_{(0)}(\Omega) \subset H^{-1}_{(0)}(\Omega) \to H^{-1}_{(0)}(\Omega)$ is the Laplace operator with Neumann boundary conditions as above, which is considered as an unbounded operator on $H^{-1}_{(0)}(\Omega)$. Moreover, the initial datum $\psi_{0\theta}$ appearing in (5.3.1) is a regularisation of the given original datum for problem (5.0.1)–(5.0.4). In particular, we need $\psi_{0\theta}$ to satisfy

$$\langle \psi_{0\theta} \rangle = \langle \psi_0 \rangle, \quad \lim_{\theta\to 0} \theta \|\psi_{0\theta}\|_{H^1} = 0 \quad \text{and} \quad \lim_{\theta\to 0} \psi_{0\theta} = \psi_0 \text{ in } H^{\alpha/2}(\Omega).$$

This can be obtained by considering $\psi_{0\theta} = \Psi_{\epsilon(\theta)} * \psi_0$ where Ψ_ϵ is a suitable mollifier (e.g., a gaussian kernel) and $\epsilon(\theta)$ is chosen to be sufficiently slowly convergent to 0 if $\theta \to 0$. Finally, we also introduce a suitable regularized energy for system (5.3.1), namely,

$$E_\theta(\psi) \doteq \mathcal{E}_\theta(\psi,\psi) + \int_\Omega f(\psi(x))\,\mathrm{d}x.$$

In order to apply Theorem 5.1.2 for θ strictly positive we recall that, on account of Corollary 5.2.4, $\mathcal{A} = \partial\widetilde{F_\theta}$ is a maximal monotone operator with $\widetilde{F_\theta} = \varphi_1 + \varphi_2$,

$$\begin{aligned}
\varphi_1(\psi) &= \frac{\theta}{2}\int_\Omega |\nabla\psi(x)|^2\,\mathrm{d}x + \mathcal{E}(\psi,\psi), \qquad \operatorname{dom}\varphi_1 = H^1_{(0)}(\Omega),\\
\varphi_2(\psi) &= \int_\Omega \phi(\psi(x))\,\mathrm{d}x,\\
\operatorname{dom}\varphi_2 &= \operatorname{dom}\varphi = \{\psi \in H^1_{(0)}(\Omega) \mid \psi \in [a,b] \text{ a.e. in } \Omega\}
\end{aligned}$$

Obviously, $\varphi_1|_{H^1_{(0)}(\Omega)}$ is a bounded, coercive quadratic form on $H^1_{(0)}(\Omega)$.

We apply Theorem 5.1.2 with $H_1 = H^1_{(0)}(\Omega)$, $H_0 = H^{-1}_{(0)}(\Omega)$, $f = 0$, and φ_1, φ_2 as above, where we assume that $\phi(\psi) \geqslant 0$ without loss of generality. As a consequence there exists a unique solution $\psi\colon [0,\infty) \to H_0$ to (5.3.3)-(5.3.4) such that $\psi \in H^1(0,T;H_0) \cap L^\infty(0,T;H_1)$, $\varphi(\psi) \in L^\infty(0,T)$ for every $T > 0$ and $\psi(t) \in \mathcal{D}(\mathcal{A}_\theta)$ for almost all $t > 0$.

In order to prove the equivalence of (5.1.4), namely

$$E_\theta(\psi_\theta(t)) + \int_0^t |\nabla\mu_\theta(s)|_2^2\,\mathrm{d}s = E_\theta(\psi_{0\theta}) \quad \text{for all } t > 0, \tag{5.3.5}$$

we take advantage of the identity

$$E_\theta(\psi_\theta(t)) = \widetilde{F_\theta}(\psi_\theta(t)) - \frac{d}{2}|\psi_\theta(t)|_2^2.$$

Because of Lemma 4.3 in (Showalter, 1997, Chapter IV), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{F_\theta}(\psi_\theta(t)) = (\partial\widetilde{F_\theta}(\psi_\theta(t)), \partial_t\psi_\theta(t))_{H^{-1}_{(0)}} = -\|\partial_t\psi_\theta(t)\|^2_{H^{-1}_{(0)}} - (\mathcal{B}\psi_\theta(t), \partial_t\psi_\theta(t))_{H^{-1}_{(0)}}.$$

Moreover, we have

$$\begin{aligned}
(\mathcal{B}\psi_\theta(t), \partial_t\psi_\theta(t))_{H^{-1}_{(0)}} &= -d(\Delta_N\psi_\theta(t), \partial_t\psi_\theta(t))_{H^{-1}_{(0)}} = d(\nabla\psi_\theta(t), \nabla\Delta_N^{-1}\partial_t\psi_\theta(t))_{L^2}\\
&= -d\,{}_{H^{-1}_{(0)}}\langle \partial_t\psi_\theta(t), \psi_\theta(t)\rangle_{H^1_{(0)}} = -\frac{d}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\psi_\theta(t)|_2^2
\end{aligned}$$

due to (Zeidler, 1990, Proposition 23.23) and $\|\partial_t\psi_\theta(t)\|_{H^{-1}_{(0)}} = \|\Delta_N\mu_\theta(t)\|_{H^{-1}_{(0)}} = \|\mu_\theta(t)\|_{H^1_{(0)}}$. Hence an integration over $[0,t]$ yields

$$\mathcal{E}(\psi_\theta(t),\psi_\theta(t)) + \frac{\theta}{2}|\nabla\psi_\theta(t)|_2^2 + \int_\Omega f(\psi_\theta(x,t))\,\mathrm{d}x + \int_0^t |\nabla\mu_\theta(s)|_2\,\mathrm{d}s \\ = \mathcal{E}(\psi_{0\theta},\psi_{0\theta}) + \frac{\theta}{2}|\nabla\psi_{0\theta}|_2^2 + \int_\Omega f(\psi_{0\theta}(x))\,\mathrm{d}x.$$

In particular, this implies

$$\partial_t\psi_\theta = \Delta_N\mu_\theta \in L^2(\mathbb{R}_+;H^{-1}_{(0)}(\Omega)), \qquad \theta^{1/2}\psi_\theta \in L^\infty(\mathbb{R}_+;H^1_{(0)}(\Omega)).$$

In order to derive higher regularity, we apply ∂_t^h to (5.3.3) and take the inner product with $\partial_t^h\psi_\theta$ in $H^{-1}_{(0)}(\Omega)$, where $\partial_t^h f(t) = \frac{1}{h}(f(t+h)-f(t))$, $t,h>0$. For any $0<s<t$, this gives

$$\begin{aligned}&\frac{1}{2}\|\partial_t^h\psi_\theta(t)\|^2_{H^{-1}_{(0)}} + \theta\int_s^t(\nabla\partial_t^h\psi_\theta(\tau),\nabla\partial_t^h\psi_\theta(\tau))_{L^2}\,\mathrm{d}\tau + \int_s^t\mathcal{E}(\partial_t^h\psi_\theta(\tau),\partial_t^h\psi_\theta(\tau))\mathrm{d}\tau\\ \leqslant& d\int_s^t\|\partial_t^h\psi_\theta(\tau)\|^2_{L^2}\,\mathrm{d}\tau + \frac{1}{2}\|\partial_t^h\psi_\theta(s)\|^2_{H^{-1}_{(0)}}\\ \leqslant&\frac{\psi_0}{2}\int_s^t\|\partial_t^h\psi_\theta(\tau)\|^2_{H^{\alpha/2}_{(0)}}\,\mathrm{d}\tau + C\int_s^t\|\partial_t^h\psi_\theta(\tau)\|^2_{H^{-1}_{(0)}}\,\mathrm{d}\tau + \frac{1}{2}\|\partial_t^h\psi_\theta(s)\|^2_{H^{-1}_{(0)}},\end{aligned}$$

where we have used Ehrling's Lemma applied to $H^{\alpha/2}_{(0)}(\Omega)\hookrightarrow\hookrightarrow L^2_{(0)}(\Omega)\hookrightarrow H^{-1}_{(0)}(\Omega)$ and

$$(\partial_t^h\mathcal{A}_\theta(\psi_\theta(\tau)),\partial_t^h\psi_\theta(\tau))_{H^{-1}_{(0)}} \geqslant \theta(\partial_t^h\psi_\theta(\tau),\partial_t^h\psi_\theta(\tau))_{H^1} + \mathcal{E}(\partial_t^h\psi_\theta(\tau),\partial_t^h\psi_\theta(\tau)).$$

Here $\psi_0>0$ is such that $\mathcal{E}(u,u)\geqslant\psi_0\|u\|^2_{H^{\alpha/2}_{(0)}}$. Furthermore, since $\partial_t\psi_\theta\in L^2(\mathbb{R}_+;H^{-1}_{(0)}(\Omega))$, there holds

$$\|\partial_t^h\psi_\theta(s)\|_{H^{-1}_{(0)}} \leqslant \frac{1}{h}\int_s^{s+h}\|\partial_t\psi_\theta(\tau)\|_{H^{-1}_{(0)}}\,\mathrm{d}\tau \to_{h\to0}\|\partial_t\psi_\theta(s)\|_{H^{-1}_{(0)}}$$

for almost every $s>0$ and $\|\partial_t^h\psi_\theta\|_{L^2(\mathbb{R}_+;H^{-1}_{(0)})}\leqslant\|\partial_t\psi_\theta\|_{L^2(\mathbb{R}_+;H^{-1}_{(0)})}$. Hence $\theta\|\partial_t^h\psi_\theta\|^2_{L^2(s,t;H^1_{(0)})}$, $\|\partial_t^h\psi_\theta\|_{L^2(s,t;H^{\alpha/2}_{(0)}(\Omega))}$ and $\|\partial_t^h\psi_\theta(t)\|_{H^{-1}_{(0)}}$ are uniformly bounded in $h>0$, for all $0<s<t$. On the other hand, we have

$$\partial_t^h\psi_\theta \to_{h\to0}\partial_t\psi_\theta$$

in $L^2(\mathbb{R}_+;H^{-1}_{(0)}(\Omega))$. Therefore, the uniform (w.r.t. $h>0$) bounds on $\partial_t^h\psi_\theta$ yield that $\partial_t\psi_\theta\in L^2(s,t;H^{\alpha/2}_{(0)}(\Omega))\cap L^\infty(s,t;H^{-1}_{(0)}(\Omega))$ for every $0<s<t$.

In order to derive the estimate near $t=0$, we again apply ∂_t^h to (5.3.3) and take the inner product with $t\partial_t^h\psi_\theta$. This gives

$$\frac{t}{2}\|\partial_t^h\psi_\theta(t)\|^2_{H^{-1}_{(0)}} + \theta\int_0^t\tau|\nabla\partial_t^h\psi_\theta(\tau)|_2^2\,\mathrm{d}\tau + \int_0^t\tau\mathcal{E}(\partial_t^h\psi_\theta(\tau),\partial_t^h\psi_\theta(\tau))\,\mathrm{d}\tau \\ \leqslant C\int_0^t(1+\tau)|\partial_t^h\psi_\theta(\tau)|_2^2\,\mathrm{d}\tau.$$

Proceeding as above, we get

$$t^{1/2}\partial_t\psi_\theta \in L^2(0,1;H^{\alpha/2}_{(0)}(\Omega)) \cap L^\infty(0,1;H^{-1}_{(0)}(\Omega)).$$

This implies $\kappa\mu_\theta = \kappa\Delta_N^{-1}\partial_t\psi_\theta \in L^\infty(\mathbb{R}_+;H^1_{(0)}(\Omega))$. Thus (5.2.2) yields $\kappa\phi'(\psi_\theta) \in L^\infty(\mathbb{R}_+;L^2(\Omega))$ since $\kappa\partial F_\theta(\psi) = \kappa\mu_\theta + \kappa d\psi_\theta \in L^\infty(\mathbb{R}_+;L^2(\Omega))$. All these norms are uniformly bounded in $\theta \in (0,1]$.

We are now ready to pass to the limit for $\theta \to 0$ in (5.3.3). Indeed, for any $\theta > 0$ we have proven that there exist (unique) functions $\psi_\theta(t)$ and $\mu_\theta(t)$ satisfying

$$\begin{cases} \partial_t\psi_\theta = \Delta_N\mu_\theta \\ (\mu_\theta,\zeta)_{L^2} + \theta(\nabla\psi_\theta,\nabla\zeta)_{L^2} + \mathcal{E}(\psi_\theta,\zeta) + (\phi'(\psi_\theta),\zeta)_{L^2} = d(\psi_\theta,\zeta)_{L^2} \end{cases} \tag{5.3.6}$$

for all $\zeta \in H^1_{(0)}(\Omega)$ and for almost every $t > 0$. Moreover, from the previous estimates, for all $\theta \in (0,1]$, we have

$$\begin{aligned} \psi_\theta &\in L^\infty(\mathbb{R}_+;H^{\alpha/2}_{(0)}(\Omega)) \\ \theta^{1/2}\psi_\theta &\in L^\infty(\mathbb{R}_+;H^1(\Omega)) \\ \kappa\partial_t\psi_\theta &\in L^\infty(\mathbb{R}_+;H^{-1}_{(0)}(\Omega)) \cap L^2(\mathbb{R}_+;H^{\alpha/2}_{(0)}(\Omega)) \\ \mu_\theta &\in L^2(0,T;H^1(\Omega)) \qquad \text{for all } T > 0 \\ \kappa\mu_\theta &\in L^\infty(\mathbb{R}_+;H^1(\Omega)) \\ \kappa\phi'(\psi_\theta) &\in L^\infty(\mathbb{R}_+;L^2(\Omega)) \end{aligned}$$

where all the bounds deduced are uniform with respect to θ. Therefore, there exists a sequence $\{\theta_n\}_{n\in\mathbb{N}}$, $\theta_n \to_{n\to\infty} 0$ such that ψ_{θ_n}, μ_{θ_n} and $\phi'(\psi_{\theta_n})$ converge weakly (or weakly*) in the above spaces to ψ, μ and χ respectively as θ vanishes. More precisely, by a suitable diagonal argument on intervals of the form $[0,m]$, we can assume that also $\mu_{\theta_n} \to \mu$ in $L^2(0,m;H^1(\Omega))$ for any $m \in \mathbb{N}$. We can easily pass to the limit in the first equation of (5.3.6) deducing

$$\partial_t\psi(t) = \Delta\mu(t) \qquad \text{in } H^{-1}_{(0)}(\Omega), \text{ for a.e. } t > 0$$

Let $\zeta \in \mathbf{C}^\infty(\overline{\Omega})$ and let $s > 0$. Thanks to the convergences listed above, for almost any $t > s$ we can pass to the limit for $\theta \to 0$ in the second equation in (5.3.6) to find

$$(\mu(t),\zeta)_{L^2(\Omega)} + \mathcal{E}(\psi(t),\zeta) + (\chi(t),\zeta)_{L^2(\Omega)} = d(\psi(t),\zeta)_{L^2(\Omega)}$$

for almost all $t > 0$ since s can be taken arbitrarily small.

In order to prove the existence of a weak solution for (5.0.1)–(5.0.4) on $\mathbb{R}^+$, we only have to identify the (weak) limit $\chi = \lim_{n\to\infty}\phi'(\psi_{\theta_n})$. Let $0 < s < t$ and $m \in \mathbb{N}$ be fixed. Thanks to

Aubin-Lions Lemma, $\partial_t \psi_{\theta_n} \in L^2(0,T;H^{-1}_{(0)}(\Omega))$ and $\psi_{\theta_n} \in L^\infty(0,T;H^{\alpha/2}_{(0)}(\Omega))$ uniformly in n for all $T>0$ imply the convergence $\psi_{\theta_n} \to \psi_{\theta_n}$ (up to a subsequence) in $\mathbf{C}([0,T);L^2_{(0)}(\Omega))$ for any $T>0$. Therefore, we deduce $\psi_{\theta_n}(t) \to \psi(t)$ almost everywhere in Ω. On the other hand, thanks to Egorov's theorem, there exists a set $\Omega_m \subset \Omega$ such that $|\Omega_m| \geqslant |\Omega| - \frac{1}{2m}$ and on which $\psi_{\theta_n} \to \psi$ uniformly. We now use the (uniform with respect to $\theta>0$) estimate on $\phi'(\psi_{\theta_n}(t))$ in $L^2(\Omega)$. By definition, the quantity

$$M_{\delta,n} \doteq |\{x \in \Omega \mid |\psi_{\theta_n}(x)| > 1-\delta\}|$$

is decreasing in δ for all $n \in \mathbb{N}$. Since $\phi'(y)$ is unbounded for $y \to \pm 1$, we set

$$\psi_\delta \doteq \inf_{|\psi| \geqslant 1-\delta} |\phi'(\psi)| \to_{\delta \to 0} \infty,$$

and we have the uniform Tchebychev inequality

$$\int_\Omega |\phi'(\psi_{\theta_n})|^2 \,\mathrm{d}x \geqslant \psi_\delta^2 |M_{\delta,n}|.$$

From the uniform (with respect to θ) estimate on the norm of $\phi'(\psi_{\theta_n})$ in $L^2(\Omega)$ we obtain

$$|M_{\delta,n}| \to 0 \qquad \text{for } \delta \to 0, \text{ uniformly in } n \in \mathbb{N}.$$

Therefore, we deduce

$$\lim_{\delta \to 0} |\{x \in \Omega \mid |\psi_{\theta_n}(x)| > 1-\delta\}| = 0 \qquad \text{uniformly in } n \in \mathbb{N}.$$

Thus there exists $\delta = \delta(m)$, independent of n, such that

$$|\{x \in \Omega \mid |\psi_{\theta_n}(x)| > 1-\delta\}| \leqslant \frac{1}{2m} \qquad \forall n \in \mathbb{N}.$$

Consider now $N \in \mathbb{N}$ so large that by uniform convergence we have $|\psi_{\theta_n} - \psi| < \frac{\delta}{2}$, $\forall n > N$ on Ω_m and let $\Omega'_m \subset \Omega_m$ be defined by

$$\Omega'_m \doteq \Omega_m \cap \{x \in \Omega \mid |\psi_{\theta_N}(x)| < 1-\delta\}.$$

By the above construction we immediately deduce that $|\Omega'_m| > |\Omega| - \frac{1}{m}$ and that $|\psi_{\theta_n}(x)| < 1 - \frac{\delta}{2}$ for all $n \geqslant N$ and for all $x \in \Omega'_m$. Therefore, by the regularity assumptions on the potential ϕ' we deduce that $\phi'(\psi_{\theta_n}) \to \phi'(\psi)$ uniformly on Ω'_m. Since m and s are arbitrary we have $\phi'(\psi_{\theta_n}) \to \phi'(\psi)$ almost everywhere in $\Omega \times \mathbb{R}^+$. Finally, the uniqueness of weak and pointwise limits gives $\chi = \phi'(\psi)$ as claimed[1].

[1] Let $\{f_n\}_{n\in\mathbb{N}}$ be a sequence of functions such that $f_n \rightharpoonup f$ in $L^p(\Omega)$ and that $f_n(x) \to g(x)$ for a.e. $x \in \Omega$. Assume that $f \neq g$ on a set of finite positive measure $\Omega_0 \subset \Omega$ on which g is bounded. By Egorov's theorem there exists a set of positive measure $\Omega_1 \subset \Omega_0$ such that $f_n \to g$ uniformly in Ω_1. Therefore, $f_n \to g$ in $L^p(\Omega_1)$ and hence $f_n \rightharpoonup g$ in $L^p(\Omega_1)$. This contradicts the uniqueness of weak limits and therefore implies $f = g$ throughout Ω.

We now prove uniqueness of weak solutions. To this end let $\psi_0^j \in Z_0$, $j = 1, 2$, and let $\psi_j(t)$ be weak solutions to (5.3.3) with initial values $\psi_j(0) = \psi_0^j$. Set $\psi \doteq \psi_1 - \psi_2$ and $\mu \doteq \mu_1 - \mu_2$. Then multiplying the equation

$$\partial_t \psi = \Delta_N \mu$$

by $\psi(t)$ in $H^{-1}_{(0)}(\Omega)$ we deduce

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\psi(t)\|^2_{H^{-1}_{(0)}} + \mathcal{E}(\psi(t), \psi(t)) + \big(\phi'(\psi(t)), \psi(t)\big) = d|\psi(t)|_2^2.$$

Using the inequality

$$|w|_2^2 \leqslant \|w\|^{4/(2+\alpha)}_{H^{\alpha/2}_{(0)}} \|w\|^{2\alpha/(2+\alpha)}_{H^{-1}_{(0)}} \leqslant C_\epsilon \|w\|^2_{H^{-1}_{(0)}} + \epsilon \|w\|^2_{H^{\alpha/2}_{(0)}}$$

and the coercivity of $\mathcal{E}$, that is,

$$\frac{1}{C}\|\psi(t)\|^2_{H^{\alpha/2}_{(0)}} \leqslant \mathcal{E}(\psi(t), \psi(t)) + \big(\phi'(\psi(t)), \psi(t)\big)\,,$$

we infer

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\psi(t)\|^2_{H^{-1}_{(0)}} + \frac{1}{C}\|\psi(t)\|^2_{H^{\alpha/2}} \leqslant C\|\psi(t)\|^2_{H^{-1}_{(0)}}.$$

Hence Gronwall's lemma implies

$$\|\psi(t)\|^2_{H^{-1}_{(0)}} \leqslant e^{2Ct}\|\psi_0\|^2_{H^{-1}_{(0)}}, \tag{5.3.7}$$

which entails uniqueness whenever $\psi_0^1 = \psi_0^2$.

Let us now prove the energy identity (5.1.4). First we observe that by taking $\eta = (-\Delta_N)^{-1}\psi$ and $\varphi = \psi$ in (5.1.2) and (5.1.3) respectively we deduce (5.1.4) for almost any $t > 0$ in the same way as in (Abels and Wilke, 2007, Proof of Theorem 1.2). In order to obtain the energy identity for all times, we observe that any weak solution can be approximated by a family of functions $\{\psi_\theta\}_{\theta>0}$ defined by (5.3.1). From the regularity of the solution ψ, we know that $\psi \in \mathbf{C}([0,T]; H^\beta(\Omega))$ for all $\beta < \frac{\alpha}{2}$, Moreover, for all positive times t, we have $\psi_\theta \in \mathbf{C}([0,T]; H^{\alpha/2}(\Omega))$ and therefore $\psi_\theta(t) \in H^{\alpha/2}(\Omega)$ with uniform bound in θ. Passing to the limit for $\theta \to 0$ and arguing by contradiction, we deduce $\psi(t) \in H^{\alpha/2}(\Omega)$ for all positive times. Finally, since solution departing from $\psi(t) \in H^{\alpha/2}(\Omega)$ are unique and since we already know that the energy identity holds for almost all times, for any $t > 0$ we can find $\overline{t} > t$ such that the two following identities hold

$$E(\psi(\overline{t})) + \int_0^{\overline{t}} |\nabla\mu(s)|_2^2 \,\mathrm{d}s = E(\psi_0)$$
$$E(\psi(\overline{t})) + \int_t^{\overline{t}} |\nabla\mu(s)|_2^2 \,\mathrm{d}s = E(\psi(t)).$$

Taking the difference we deduce for any time t

$$E(\psi(t)) + \int_0^t |\nabla\mu(s)|_2^2 \,\mathrm{d}s = E(\psi_0),$$

which is the desired energy identity for all $t > 0$.

We still have to prove the continuity of the map $\psi_0 \mapsto \psi(t)$. Observe that the strong continuity in $H^{-1}_{(0)}(\Omega)$ is an immediate consequence of the continuous dependence estimate (5.3.7). Moreover, since

$$Z_0 \ni \psi_0 \mapsto \psi(t) \in H^{\alpha}_{\mathrm{loc}}(\Omega) \cap H^{\alpha/2}_{(0)}(\Omega)$$

is a bounded mapping, interpolation yields the continuity $\psi_0 \mapsto \psi(t)$ with respect to the $H^{\gamma}_{(0)}(\Omega)$-norm with $\gamma < \frac{\alpha}{2}$. Because of the boundedness of $[0,\infty) \ni t \mapsto \psi(t) \in H^{\alpha}_{(0)}(\Omega)$, this mapping is also weakly continuous.

Finally, note that the energy equality holding for all $t > 0$ entails the continuity of solutions $\psi(t)$ with values in $H^{\alpha/2}_{(0)}(\Omega)$ so that $\psi(t) \to_{t\to 0} \psi_0$ in $H^{\alpha/2}_{(0)}(\Omega)$ using that weak convergence plus convergence of norms imply strong convergence. This finishes the proof.

5.4 Long-time behaviour

Here we describe the global asymptotic behaviour of the dynamical system associated with (5.1.2)–(5.1.3). As above we can reduce to the case that ψ_0 has mean value zero by adding a suitable constant. Let us define the (metric) phase-space

$$\mathcal{X} = \left\{ z \in H^{\alpha/2}_{(0)}(\Omega) \,:\, \int_\Omega f(z)\,\mathrm{d}x < \infty \right\}$$

endowed with the metric

$$d_{\mathcal{X}}(z_1, z_2) = \|z_1 - z_2\|_{H^{\alpha/2}_{(0)}(\Omega)} + \left| \int_\Omega f(z_1)\,\mathrm{d}x - \int_\Omega f(z_2)\,\mathrm{d}x \right|.$$

Thanks to Theorem 5.1.1 and inequality (5.3.7), we can define a closed semigroup (see Pata and Zelik (2007)) on $\mathcal{X}$ by setting $S(t)\psi_0 = \psi(t)$, where ψ is the unique weak solution to (5.1.2)–(5.1.3) with initial datum ψ_0.

Our result is the following

Theorem 5.4.1. *The dynamical system $(\mathcal{X}, S(t))$ has a (connected) global attractor.*

Proof. Let us show first that the dynamical system has a bounded absorbing set. Consider equation (5.1.3) defining the chemical potential and choose ψ as test function. From this we deduce that

$$\begin{aligned} \mathcal{E}(\psi(t),\psi(t)) + \big(f'(\psi(t)),\psi(t)\big) &= (\mu(t),\psi(t)) = (\mu(t) - \langle \mu(t) \rangle, \psi(t)) \\ &\leqslant C \int_\Omega |\nabla \mu(x,t)|\,\mathrm{d}x \leqslant \frac{1}{2}|\nabla \mu|_2^2 + C \end{aligned} \tag{5.4.1}$$

holds for almost every $t \geqslant 0$. Here we used the fact that $\psi(t)$ has zero mean and that it is pointwise bounded. Moreover, from the assumptions on the potential f we have

$$f(\psi) = \phi(\psi) - \frac{d}{2}\psi^2$$

where ϕ is convex. By the convexity of ϕ we deduce

$$\phi'(s)s \geqslant \phi(s) - \phi(0) \qquad \forall s$$

and therefore we can write

$$\begin{aligned}\big(f'(\psi(t)), \psi(t)\big) &= \big(\phi'(\psi), \psi\big) - d|\psi(t)|_2^2 \\ \geqslant \int_\Omega \phi(\psi(t))\,\mathrm{d}x - |\Omega|\phi(0) - d|\psi(t)|_2^2 &= \int_\Omega f(\psi(t))\,\mathrm{d}x - C.\end{aligned}$$

Substituting this estimate from below in the inequality (5.4.1) above we get

$$\mathcal{E}(\psi(t), \psi(t)) + \int_\Omega f(\psi(t))\,\mathrm{d}x \leqslant \frac{1}{2}|\nabla\mu(t)|_2^2 + C.$$

We now consider the energy identity (5.1.4) and differentiate it with respect to time. This gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{E}(\psi(t), \psi(t)) + \int_\Omega f(\psi(t))\,\mathrm{d}x\right) + |\nabla\mu(t)|_2^2 \leqslant 0.$$

Summing the last two inequalities together, we infer

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{E}(\psi(t), \psi(t)) + \int_\Omega f(\psi(t))\,\mathrm{d}x\right) + \mathcal{E}(\psi(t), \psi(t)) + \int_\Omega f(\psi(t))\,\mathrm{d}x \leqslant C$$

for almost every $t \geqslant 0$. Gronwall's Lemma thus gives

$$\mathcal{E}(\psi(t), \psi(t)) + \int_\Omega f(\psi(t))\,\mathrm{d}x \leqslant e^{-t}\left(\mathcal{E}(\psi_0, \psi_0) + \int_\Omega f(\psi_0)\,\mathrm{d}x\right) + C$$

where the constant C appearing on the right hand side is independent of the initial datum ψ_0. This proves that there is a bounded absorbing set $\mathcal{B}$ in $\mathcal{X}$.

On account of (Pata and Zelik, 2007, Theorem 2), we only need to prove that there exists a divergent sequence $\{t_n\}$ such that $\alpha(S(t_n)B) = 0$ as n goes to ∞. Here $\alpha(E)$ denotes the Kuratowski measure of noncompactness. Actually we prove more, that is, $\alpha(S(t)B) = 0$ for all $t > 0$.

Let $\{\psi_{0n}\} \subset \mathcal{X}$ be bounded and set $\psi_n(t) = S(t)\psi_{0n}$. From estimates analogous to those deduced in our proof of existence of solutions in Section 5.3 and thanks to the existence of the absorbing set deduced above, we have the following (uniform with respect to n) estimates:

$$\begin{aligned}\psi_n &\in L^\infty(0, T; H^{\alpha/2}_{(0)}(\Omega)) && \text{for all } T > 0 \\ \partial_t\psi_n &\in L^2(s, T+s; H^{\alpha/2}_{(0)}(\Omega)) && \text{uniformly in } s \geqslant \varepsilon > 0, \text{ for all } T > 0 \\ \mu_n &\in L^2(s, T+s; H^1(\Omega)) && \text{uniformly in } s \geqslant 0, \text{ for all } T > 0 \\ f'(\psi_n) &\in L^\infty(\epsilon, T; L^2(\Omega)) && \text{for all } T > \epsilon > 0.\end{aligned}$$

Arguing as in the proof of existence, up to a subsequence, we deduce that there exist functions ψ, μ satisfying for any fixed ϵ and T

$$\begin{aligned} \psi_n &\overset{*}{\rightharpoonup} c && \text{in } L^\infty(0,T;H^{\alpha/2}_{(0)}(\Omega)) \\ \partial_t\psi_n &\rightharpoonup \partial_t\psi && \text{in } L^2(s,T+s;H^{\alpha/2}_{(0)}(\Omega)) \\ \mu_n &\rightharpoonup \mu && \text{in } L^2(s,T+s;H^1(\Omega)) \\ f'(\psi_n) &\overset{*}{\rightharpoonup} f'(\psi) && \text{in } L^\infty(\epsilon,T;L^2(\Omega)) \end{aligned}$$

as $n \to \infty$. Here ψ and μ satisfy (5.1.2)–(5.1.3). On the other hand we also know that

$$\psi_n \in \mathbf{C}([0,T];H^{\alpha/2}_{(0)}(\Omega)) \qquad \text{for all } T>0$$

with a uniform bound in n. Moreover, the estimate on $\partial_t\psi_n$ implies that the family $\{\psi_n\}_{n\in\mathbb{N}}$ is also equicontinuous with values in $H^{\alpha/2}_{(0)}(\Omega)$. Indeed, this follows from the following simple computation

$$\begin{aligned} &\|\psi_n(t)-\psi_n(s)\|_{H^{\alpha/2}_{(0)}(\Omega)} \\ &\leqslant \int_s^t \|\partial_t\psi_n(\tau)\|_{H^{\alpha/2}_{(0)}(\Omega)}\,\mathrm{d}\tau \leqslant (t-s)^{1/2}\left(\int_s^t \|\partial_t\psi_n(\tau)\|^2_{H^{\alpha/2}_{(0)}}\,\mathrm{d}\tau\right)^{1/2}. \end{aligned}$$

Moreover, we know that

$$\mathcal{L}\psi(t) = \mu(t) - f'(\psi(t)) \in L^2_{(0)}(\Omega)$$

holds for almost any $t>0$. In particular, in the last expression, the right hand side is uniformly bounded for all $t \geqslant \epsilon > 0$. Since $L^2_{(0)}(\Omega) \subset\subset H^{-\alpha/2}_{(0)}(\Omega)$ and since $\mathcal{L}^{-1}$ is continuous as an operator from $H^{-\alpha/2}_{(0)}(\Omega)$ to $H^{\alpha/2}_{(0)}(\Omega)$ we deduce that

$$\psi(t) \in K_\epsilon \subset\subset H^{\alpha/2}_{(0)}(\Omega) \qquad \text{for a.e. } t \geqslant \epsilon > 0$$

holds with K_ϵ independent of t. Moreover, thanks to the continuity of the solutions ψ_n taking values in $H^{\alpha/2}_{(0)}(\Omega)$ this is true for all $t \geqslant \epsilon > 0$. Appealing to the Ascoli-Arzelà Theorem (see, for instance, (Folland, 1999, Theorem 4.43)), this implies that, up to a subsequence, $\psi_n \to \psi$ in $\mathbf{C}([\epsilon,T];H^{\alpha/2}_{(0)}(\Omega))$ uniformly on the interval $[\epsilon,T]$. Applying the above argument to intervals of the form $[m^{-1},m]$, $m\in\mathbb{N}$ and performing a diagonal selection procedure, we finally obtain

$$\psi_n(t) \to \psi(t) \qquad \text{in } H^{\alpha/2}_{(0)}(\Omega), \text{ for all } t>0.$$

We now consider the convergence

$$\int_\Omega f(\psi_n(t))\,\mathrm{d}x \to \int_\Omega f(\psi(t))\,\mathrm{d}x \qquad \text{for all } t>0.$$

This follows as a consequence of the dominated convergence on account of the boundedness of f and pointwise convergence almost everywhere in Ω of $\{f(\psi_n(\cdot,t))\}$. The latter is implied by the strong convergence of $\psi_n(t)$ in $H^{\alpha/2}_{(0)}(\Omega)$. Summing up we have that, up to a subsequence, $\psi_n(t)$ converges to $\psi(t)$ in $\mathcal{X}$ for any $t>0$. Therefore we are in a position to apply (Pata and Zelik, 2007, Theorem 2 and Proposition 4) to conclude the proof. □

Remark 5.4.1. In order to prove the connectedness of the attractor, in Pata and Zelik (2007) (see comments after Theorem 2) it is assumed that balls of the phase space $\mathcal{X}$ are connected. However, connectedness of the attractor can be obtained by assuming only that the whole phase space is connected as was shown in (Ball, 1997, Theorem 4.2 and Corollary. 4.3) (cf. also Ball (1998)). In our case, although connectedness of the balls of $\mathcal{X}$ does not seem evident, nonetheless the d-convexity of F implies that $\mathcal{X}$ is connected.

5.5 Boundary conditions for variational solutions

In this section we want to discuss the natural boundary condition satisfied by the weak solution u to the problem

$$\mathcal{E}(u,\zeta)=(g,\zeta)\qquad \forall \zeta\in H^{\alpha/2}_{(0)}(\Omega). \tag{5.5.1}$$

Here g is a given function with $m(g)=0$. Of course, we can confine ourselves to consider the linear nonlocal equation neglecting the derivative of the potential f. Note that (5.5.1) also holds true for all $\zeta\in H^{\alpha/2}(\Omega)$ since both sides vanish on constants. For simplicity we only consider the case $\Omega=\mathbb{R}^n_+$. But the case of a bounded sufficiently smooth domain can be reduced to this case by standard techniques.

The main theorem is a conditional result, namely,

Theorem 5.5.1. *Let $\Omega=\mathbb{R}^n_+$ and $1\leqslant p\leqslant\infty$ such that $\alpha-1>\frac{n}{p}$. Let $\alpha>\frac{3}{2}$ and let $u\in H^{\alpha/2}_{(0)}(\Omega)\cap H^{\alpha}_{\mathrm{loc}}(\Omega)$ be a solution to (5.5.1) with $g\in L^p_{(0)}(\Omega)$. Suppose that $u\in\mathbf{C}^{1,\beta}(\overline{\Omega})$. If $n\geqslant 2$, we assume that the following limit exists*

$$\mathbf{n}_{x_0}=\lim_{\delta\to 0}\delta^{-1-n+\alpha}\int_\Omega\int_\Omega (x-y)(\varphi_\delta(x)-\varphi_\delta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \tag{5.5.2}$$

and is non-zero, where

$$\varphi_\delta(x)=\begin{cases}1-\frac{|x-x_0|}{\delta} & \text{if } |x-x_0|<\delta\\ 0 & \text{otherwise.}\end{cases}$$

If $n=1$, let $\mathbf{n}_{x_0}=1$. Then we have

$$\nabla u(x_0)\cdot\mathbf{n}_{x_0}=0\qquad \forall\, x_0\in\partial\Omega. \tag{5.5.3}$$

Remark 5.5.1. Observe that (5.5.1) holds in particular for any $\zeta \in \mathbf{C}_0^\infty(\Omega)$. Arguing as in (Abels and Kassmann, 2007, Lemma 4.2) (see also (Abels and Kassmann, 2007, Lemma 3.5)), we have

$$\begin{aligned}
&\mathcal{E}(u,\zeta)\\
&= \lim_{\epsilon\to 0}\frac{1}{2}\int_{\{|x-y|>\epsilon\}\cap\Omega}(u(x)-u(y))(\zeta(x)-\zeta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&= \lim_{\epsilon\to 0}\frac{1}{2}\int_\Omega\int_{\Omega\setminus B_\epsilon(x)}(u(x)-u(y))\zeta(x)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&\quad+\lim_{\epsilon\to 0}\frac{1}{2}\int_\Omega\int_{\Omega\setminus B_\epsilon(x)}(u(x)-u(y))\zeta(x)k(y,x,y-x)\,\mathrm{d}x\mathrm{d}y\\
&= \lim_{\epsilon\to 0}\int_\Omega\int_{\Omega\setminus B_\epsilon(x)}(u(x)-u(y))k(x,y,x-y)\,\mathrm{d}y\,\zeta(x)\mathrm{d}x\\
&= \int_\Omega \mathcal{L}u(x)\zeta(x)\,\mathrm{d}x
\end{aligned}$$

provided that $u \in H^\alpha_{\mathrm{loc}}(\Omega)\cap H^{\alpha/2}(\Omega)$. Therefore,

$$(\mathcal{L}u,\zeta) = (g,\zeta)$$

holds for all $\zeta \in \mathbf{C}_0^\infty(\Omega)$. This implies that the weak solution u to (5.5.1) satisfies the equation

$$\mathcal{L}u(x) = g(x) \qquad \text{a.e. } x\in\Omega.$$

Hence $\mathcal{L}u \in L^p(\Omega)$ since $g \in L^p(\Omega)$. Unfortunately, we cannot say anything on the boundary condition due to the lack of information about the regularity of u. More precisely, we cannot answer to the question: Does u belong to $H^\alpha_{(0)}(\Omega)$ with $\alpha > \frac{3}{2}$. In addition, assuming that the limit (5.5.2) exists, we do not know if

$$\nabla u(x_0)\cdot\mathbf{n}_{x_0} = 0$$

holds on $\partial\Omega$ in the sense of traces under general assumptions.

We can thus just conjecture that u should satisfy (5.5.3).

Remark 5.5.2. The limit (5.5.2) exists in many examples of interaction kernel which are interesting for applications. Among them there are kernels given by a homogeneous principal part of order α perturbed by lower order terms. For instance

$$k(x,y,x-y) = \frac{C}{|x-y|^{n+\alpha}} + o(|x-y|^{-n-\alpha}) \tag{5.5.4}$$

or, more generally,

$$k(x,y,x-y) = \frac{g(x,y)}{|x-y|^{n+\alpha}} + o(|x-y|^{-n-\alpha})$$

with $g \in \mathbf{C}(\overline{\Omega}\times\overline{\Omega})$. In the latter cases a simple calculation using the homogeneity of $|x-y|^{-n-\alpha}$ and the continuity of g in (x_0,x_0) yields

$$\mathbf{n}_{x_0} = \int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+}(x-y)(\varphi_1(x)-\varphi_1(y))k(x_0,x_0,x-y)\,\mathrm{d}x\mathrm{d}y.$$

Remark 5.5.3. In the case (5.5.4), using the higher-order term symmetry, we have

$$\mathbf{n}_{x_0} = \int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+} (x-y)(\varphi_1(x)-\varphi_1(y))k(x_0,x_0,x-y)\,\mathrm{d}x\mathrm{d}y. = C\boldsymbol{\nu}$$

where $\boldsymbol{\nu}$ is the unit outward normal to the boundary and $C \neq 0$. Therefore, in this case we recover the usual Neumann boundary conditions.

5.5.1 Proof of Theorem 5.5.1: case $n = 1$

Before proving Theorem 5.5.1 in the case $n \geqslant 2$, we first discuss the simpler one-dimensional case. For $\mathbb{R}^n_+$ with $n \geqslant 2$ the same general strategy applies with the required changes (see Section 5.5.2). Throughout this section we assume that u is as in the assumption of Theorem 5.5.1 and $n = 1$.

Consider the cut-off function at $x = 0$ defined by

$$\varphi_\delta(x) = \begin{cases} 1 - \frac{x}{\delta} & \text{for } x \in [0,\delta), \\ 0 & \text{otherwise.} \end{cases}$$

Observe also that the function φ_δ is Lipschitz continuous and hence belongs to $H^\gamma(\Omega)$ for any $\gamma \in [0,1]$ and thus to $H^{\alpha/2}(\Omega)$.

Using (5.5.1), we obtain

$$\begin{aligned} |\mathcal{E}(u,\varphi_\delta)| &= \left|\int_0^\infty g(x)\varphi_\delta(x)\,\mathrm{d}x\right| \\ &\leqslant \|g\|_p\|\varphi_\delta\|_{p'} \leqslant C\|g\|_p\delta^{1/p'} = O(\delta^{1/p'}) \qquad \text{as } \delta \to 0. \end{aligned}$$

We now consider the quantity $\mathcal{E}(u,\varphi_\delta)$ in more detail. We have

$$\begin{aligned} &\mathcal{E}(u,\varphi_\delta) \\ =&\frac{1}{2}\int_0^\infty\int_0^\infty (u(x)-u(y))(\varphi_\delta(x)-\varphi_\delta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ =&\frac{1}{2}\int_0^\delta\int_0^\delta (u(x)-u(y))\left(\left(1-\frac{x}{\delta}\right)-\left(1-\frac{y}{\delta}\right)\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ &+\frac{1}{2}\int_\delta^\infty\int_0^\delta (u(x)-u(y))\left(1-\frac{x}{\delta}\right)k(x,y,x-y)\mathrm{d}x\mathrm{d}y \\ &-\frac{1}{2}\int_0^\delta\int_\delta^\infty (u(x)-u(y))\left(1-\frac{y}{\delta}\right)k(x,y,x-y)\mathrm{d}x\mathrm{d}y \\ =&I_1+I_2+I_3. \end{aligned} \tag{5.5.5}$$

The first integral reduces to

$$I_1 = \frac{1}{2\delta}\int_0^\delta\int_0^\delta (u(x)-u(y))(y-x)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y.$$

By using Taylor series expansion near 0 for u, this integral can be estimated by

$$\begin{aligned} I_1 \sim & \frac{1}{2\delta}\int_0^\delta\int_0^\delta u'(0)(x-y)(y-x)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ & + \frac{C}{\delta}\int_0^\delta\int_0^\delta (x-y)^{1+\beta}(y-x)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ = & -\frac{1}{2\delta}u'(0)\int_0^\delta\int_0^\delta (x-y)^2 k(x,y,x-y)\mathrm{d}x\mathrm{d}y + O(\delta^{2+\beta-\alpha}), \end{aligned}$$

Here the notation $A \sim B$ means that the quantities A and B are equivalent for $\delta \to 0$, i.e., that, for δ sufficiently small, there exist two positive constants c and C such that $cB \leqslant A \leqslant CB$. Indeed, notice that by assumption (5.0.8), $(x-y)^{1+\alpha}k(x,y,x-y)$ is uniformly bounded away from zero from below and from above.

In the sequel, $\omega(\delta^\gamma)$ indicates a quantity which is asymptotical to δ^γ in the following sense

$$g(\delta) \in \omega(\delta^\gamma) \qquad \text{if} \qquad c \leqslant \liminf_{\delta\to 0}\frac{g(\delta)}{\delta^\gamma} \leqslant \limsup_{\delta\to 0}\frac{g(\delta)}{\delta^\gamma} \leqslant C, \qquad c, C > 0.$$

From the above computations we deduce

$$I_1 = -u'(0)\omega(\delta^{2-\alpha}) + O(\delta^{2+\beta-\alpha}).$$

The remaining two terms I_2 and I_3 in (5.5.5) are equivalent. Thus it suffices to observe that

$$\begin{aligned} I_3 = & \int_0^\delta\int_\delta^\infty (u(y)-u(x)+u'(y)(x-y))\left(1-\frac{y}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ & + \int_0^\delta\left(\int_\delta^\infty (y-x)k(x,y,x-y)\,\mathrm{d}x\right)u'(y)\left(1-\frac{y}{\delta}\right)\mathrm{d}y. \end{aligned}$$

However, the first of these two terms are of order $O(\delta^{2+\beta-\alpha})$, while we can easily estimate the inner integral appearing in the second one as

$$\begin{aligned} & \int_\delta^\infty (y-x)k(x,y,x-y)\,\mathrm{d}x \sim \int_\delta^\infty (y-x)|x-y|^{-1-\alpha}\,\mathrm{d}x \\ & \sim -\int_\delta^\infty (x-y)^{-\alpha}\,\mathrm{d}x \sim -(\delta-y)^{1-\alpha}, \end{aligned}$$

where we used the fact that $x > y$ always when I_3 will be computed. Therefore we deduce

$$\begin{aligned} I_3 & \sim -\int_0^\delta (\delta-y)^{1-\alpha}u'(y)\left(1-\frac{y}{\delta}\right)\mathrm{d}y + O(\delta^{2+\beta-\alpha}) \\ & \sim -\frac{1}{\delta}\int_0^\delta (\delta-y)^{2-\alpha}u'(0)\,\mathrm{d}y + O(\delta^{2+\beta-\alpha}) \\ & \sim \frac{1}{\delta}u'(0)\left.\frac{(\delta-y)^{3-\alpha}}{3-\alpha}\right|_0^\delta + O(\delta^{2+\beta-\alpha}) \sim -u'(0)\delta^{2-\alpha} + O(\delta^{2+\beta-\alpha}). \end{aligned}$$

Combining all the above estimates we obtain, for some positive constants c and C,

$$-Cu'(0)\delta^{2-\alpha} - C\delta^{2+\beta-\alpha} \leqslant \mathcal{E}(u,\varphi_\delta) \leqslant -cu'(0)\delta^{2-\alpha} + C\delta^{2+\beta-\alpha}.$$

Because of (5.5.1), we have

$$\mathcal{E}(u,\varphi_\delta)=\int_0^\infty g(x)\varphi_\delta(x)\mathrm{d}x$$

so that

$$-u'(0)\delta^{2-\alpha}+O(\delta^{2+\beta-\alpha})=O(\delta^{1/p'})\qquad\text{as }\delta\to 0.$$

However, since $\alpha-1>\frac{1}{p}$, one readily sees that this is possible only if $u'(0)=0$.

5.5.2 Proof of Theorem 5.5.1: case $n\geqslant 2$

Here we consider the case $n\geqslant 2$ in the statement of Theorem 5.5.1. In this section, unless otherwise stated, we will denote by B_δ^+ the half ball of centre $x_0\in\partial\mathbb{R}^n_+$ contained in the half-space $\mathbb{R}^n_+$ and having radius δ. Before giving the details of the proof we prove a useful technical lemma.

Lemma 5.5.2. *Let r be a real number such that $r>-1-n$. Then the following relation holds*

$$I_r\doteq\int_{B_\delta^+}\int_{B_\delta^+}|x-y|^r\,||x-x_0|-|y-x_0||\,\mathrm{d}x\mathrm{d}y=\omega(\delta^{1+r+2n})\qquad\textit{for }\delta\to 0.$$

Proof. First of all by a simple translation we can reduce to the case $x_0=0$. Then using the change of variable $x=\delta\tilde{x}, y=\delta\tilde{y}$ we obtain

$$I_r=\delta^{1+r+2n}\int_{B_1^+}\int_{B_1^+}|x-y|^r\,||x|-|y||\,\mathrm{d}x\mathrm{d}y,$$

where the last integral can be estimate as

$$\int_{B_1^+}\int_{B_1^+}|x-y|^r\,||x|-|y||\,\mathrm{d}x\mathrm{d}y\leqslant\int_{B_1^+}\int_{B_1^+}|x-y|^{r+1}\,\mathrm{d}x\mathrm{d}y<\infty$$

since $r+1>-n$. Since the integral on the left-hand side is obviously positive, the statement follows. □

The main idea of our proof is to consider an appropriate family of test functions concentrating at one point of the boundary. Let us consider the bilinear form

$$\mathcal{E}(u,v)=\frac{1}{2}\int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+}(u(x)-u(y))(v(x)-v(y))k(x,y,x-y)\mathrm{d}x\mathrm{d}y.$$

Let x_0 be a point belonging to the boundary of $\mathbb{R}^n_+$ and consider the test function $\varphi_\delta\in\mathbf{C}(\mathbb{R}^n_+)\cap H^1(\mathbb{R}^n_+)\subset H^{\alpha/2}(\mathbb{R}^n_+)$ defined by

$$\varphi_\delta(x)=\begin{cases}1-\frac{x-x_0}{\delta} & \text{if } |x-x_0|<\delta \text{ and } x\in\mathbb{R}^n_+,\\ 0 & \text{otherwise.}\end{cases}$$

In particular, we have by (5.5.1)

$$|\mathcal{E}(u,\varphi_\delta)| = \left|\int_{\mathbb{R}^n_+} g(x)\varphi_\delta(x)\,\mathrm{d}x\right| \leqslant \|g\|_{L^p(\mathbb{R}^n_+)}\|\varphi_\delta\|_{L^{p'}(\mathbb{R}^n_+)}.$$

Moreover, there holds

$$\|\varphi_\delta\|_{L^p(\mathbb{R}^n_+)} = \left(\int_{B^+_\delta}\left(1-\frac{|x-x_0|}{\delta}\right)^{p'}\mathrm{d}x\right)^{1/p'} \sim \delta^{n/p'}.$$

Observe now that

$$\begin{aligned}
\mathcal{E}(u,\varphi_\delta) =& \frac{1}{2}\int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+}(u(x)-u(y))(\varphi_\delta(x)-\varphi_\delta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
=& \frac{1}{2\delta}\int_{B^+_\delta}\int_{B^+_\delta}(u(x)-u(y))\left(|x-x_0|-|y-x_0|\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&+\frac{1}{2}\int_{B^+_{>\delta}}\int_{B^+_\delta}(u(x)-u(y))\left(1-\frac{|x-x_0|}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&+\frac{1}{2}\int_{B^+_\delta}\int_{B^+_{>\delta}}(u(x)-u(y))\left(1-\frac{|y-x_0|}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
=& J_1+J_2+J_3. \qquad (5.5.6)
\end{aligned}$$

Here $B^+_{>\delta}$ denotes the set

$$B^+_{>\delta} \doteq \{x\in\mathbb{R}^n_+ \mid |x-x_0|>\delta\}.$$

We must evaluate the asymptotic behaviour of J_1, J_2 and J_3 as $\delta\to 0$. Concerning the first one, using Taylor expansion, up to the first order we can write

$$u(x)-u(y) = \nabla u(x_0)\cdot(x-y)+O(\delta^\beta)|x-y| \qquad \text{for } x,y\in B_\delta$$

where we have used

$$\begin{aligned}
&u(x)-u(y)-\nabla u(x_0)\cdot(x-y)\\
=&\int_0^1(\nabla u(x+s(y-x))-\nabla u(x_0))\cdot(x-y)\,\mathrm{d}s\\
=&O(\delta^\beta)|x-y|
\end{aligned}$$

for all $x,y\in B_\delta$. Therefore, we obtain

$$\begin{aligned}
J_1 =& \frac{1}{2\delta}\nabla u(x_0)\cdot\int_{B^+_\delta}\int_{B^+_\delta}(x-y)\left(|x-x_0|-|y-x_0|\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y\\
&+O(\delta^{1+\beta+n-\alpha}).
\end{aligned}$$

We are now left to analyse J_2 and J_3 (see (5.5.6)). This can be done similarly as in the case

$n = 1$. Indeed, we have

$$\begin{aligned} J_2 =& \frac{1}{2}\int_{B_\delta^+}\int_{B_{>\delta}^+}(u(x)-u(y))\left(1-\frac{|x-x_0|}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ =& \frac{1}{2}\nabla u(x_0)\cdot\int_{B_\delta^+}\left(\int_{B_{>\delta}^+}(x-y)\left(1-\frac{|x-x_0|}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\right)\mathrm{d}y \\ &+ O(\delta^\beta)\int_{B_\delta^+}\left(\int_{B_{>\delta}^+}|x-y|\left(1-\frac{|x-x_0|}{\delta}\right)k(x,y,x-y)\,\mathrm{d}x\right)\mathrm{d}y \\ \equiv& J_{2,1}+J_{2,2} \end{aligned}$$

Thus, in this case, we only have to bound integrals of the form

$$\begin{aligned} J_4 \doteq& \int_{B_\delta^+}\left(\int_{B_{>\delta}^+}|x-y|^{1-\alpha-n}\left(1-\frac{|x-x_0|}{\delta}\right)\mathrm{d}y\right)\mathrm{d}x \\ =& \int_{B_\delta^+}\left(1-\frac{|x-x_0|}{\delta}\right)\left(\int_{B_{>\delta}^+}|x-y|^{1-\alpha-n}\,\mathrm{d}y\right)\mathrm{d}x. \end{aligned}$$

Let us set

$$J_x \doteq \int_{B_{>\delta}^+}|x-y|^{1-\alpha-n}\,\mathrm{d}y$$

and observe that

$$J_x \leqslant \int_{B_{>(\delta-|x|)}}|y|^{1-\alpha-n}\,\mathrm{d}y = \int_{\delta-|x|}^{+\infty}\rho^{-\alpha}\,\mathrm{d}\rho \sim (\delta-|x|)^{1-\alpha}.$$

Then we have

$$J_4 \leqslant C\frac{1}{\delta}\int_{B_\delta^+}(\delta-|x|)^{2-\alpha}\,\mathrm{d}x = C\delta^{1+n-\alpha}\int_0^1(1-t)^{2-\alpha}t^{n-1}\,\mathrm{d}t \sim \delta^{1+n-\alpha}.$$

From such estimates we deduce

$$J_2 = J_{2,1} + O(\delta^{1+\beta+n-\alpha}).$$

The quantity J_3 is controlled in the same way, just interchanging the role of x and y.

Recalling that

$$\mathcal{E}(u,\varphi_\delta) = \int_{\mathbb{R}^n_+}\mathcal{L}u(x)\varphi_\delta(x)\,\mathrm{d}x$$

and using the above estimates for J_1, J_2 and J_3, we get

$$\begin{aligned} &\nabla u(x_0)\cdot\int_{\mathbb{R}^n_+}\int_{\mathbb{R}^n_+}(x-y)(\varphi_\delta(x)-\varphi_\delta(y))k(x,y,x-y)\,\mathrm{d}x\mathrm{d}y \\ &+ O(\delta^{1+\beta+n-\alpha}) = O(\delta^{n/p'}). \end{aligned}$$

Since the double integral belongs to $\omega(\delta^{1+n-\alpha})$ by Lemma 5.5.2, on account of (5.5.2), and $1+n-\alpha < \frac{n}{p'}$ (which is equivalent to $\alpha - 1 > \frac{n}{p'}$), we finally deduce

$$\nabla u(x_0)\cdot\mathbf{n}_{x_0} = 0.$$

Bibliography

Abels, H. & Kassmann, M. (2007). An analytic approach to purely nonlocal Bellman equations arising in models of stochastic control. *J. Differential Equations*, 236(1):29–56.

Abels, H. & Wilke, M. (2007). Convergence to equilibrium for the Cahn-Hilliard equation with a logarithmic free energy. *Nonlinear Anal.*, 67(11):3176–3193.

Adams, R. A. (1975). *Sobolev Spaces*. Academic Press, New York, San Francisco, London.

Ball, J. M. (1997). Continuity properties and global attractors of generalized semiflows and the Navier-Stokes equations. *J. Nonlinear Sci.*, 7(5):475–502.

Ball, J. M. (1998). Erratum: "Continuity properties and global attractors of generalized semiflows and the Navier-Stokes equations". *J. Nonlinear Sci.*, 8(2):233.

Bergh, J. & Löfström, J. (1976). *Interpolation Spaces*. Springer.

Bogdan, K., Burdzy, K., & Chen, Z.-Q. (2003). Censored stable processes. *Probab. Theory Related Fields*, 127(1):89–152.

Brézis, H. (1973). *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*. North-Holland Publishing Co. North-Holland Mathematics Studies, No. 5. Notas de Matemática (50).

Cahn, J. W. & Hilliard, J. E. (1958). Free energy of a nonuniform system. i. interfacial free energy. *The Journal of Chemical Physics*, 28(2):258–267.

Folland, G. B. (1999). *Real analysis*, (second ed.). Pure and Applied Mathematics (New York). John Wiley & Sons Inc. Modern techniques and their applications, A Wiley-Interscience Publication.

Giacomin, G. & Lebowitz, J. L. (1997). Phase segregation dynamics in particle systems with long range interactions. I. Macroscopic limits. *J. Statist. Phys.*, 87(1-2):37–61.

Giacomin, G. & Lebowitz, J. L. (1998). Phase segregation dynamics in particle systems with long range interactions. II. Interface motion. *SIAM J. Appl. Math.*, 58(6):1707–1729.

Pata, V. & Zelik, S. (2007). A result on the existence of global attractors for semigroups of closed operators. *Commun. Pure Appl. Anal.*, 6:481–486.

Showalter, R. E. (1997). *Monotone Operators in Banach Space and Nonlinear Partial Differential Equations*, volume 49 of *Mathematical Surveys and Monographs*. American Mathematical Society.

Simon, J. (1990). Sobolev, Besov and Nikolskiĭ fractional spaces: imbeddings and comparisons for vector valued spaces on an interval. *Ann. Mat. Pura Appl. (4)*, 157:117–148.

Zeidler, E. (1990). *Nonlinear functional analysis and its applications. II/A*. Springer-Verlag.

Part II

Strain deformation in p-n junctions

Summary

The second part of this thesis studies the coupling mechanisms between mechanical deformations and electronic properties in semiconductors. The description of these phenomena is of outmost importance for the development of thin film electronics such as sensors and solar cells. As it is the case of most semiconductor-based electronic devices, the concentration of charge carriers (i.e. electrons ad holes) shows sharp transitions and carriers separation at the boundaries between differently doped regions in the devices.

First of all, the classical drift-diffusion model is reviewed. The mobilities of the charge carriers, the band gap and the minority carriers equilibrium concentrations are then identified as the terms with the most relevant strain dependency and models for these quantities proposed. Finally, the Shockley relation for the p-n junction under deformations is deduced.

Notation used in Part II

$[\,\cdot\,]$	jump through a surface	p.189
$C(\mathbf{x})$	doping profile, specific number of dopants (kg^{-1})	p.191
D_n	electrons' diffusion constant (m^2/s)	p.191
$\mathbf{D}_n$	electrons' diffusion constant tensor (m^2/s)	p.192
D_p	holes' diffusion constant (m^2/s)	p.191
$\mathbf{D}_p$	holes' diffusion constant tensor (m^2/s)	p.192
$\mathbf{d}$	electric displacement field (C/m^2)	p.189
E	Young modulus (Pa)	p.219
E_C	energy of the conduction band (J or eV)	p.177
E_F	Fermi level (J or eV)	p.184
E_g	energy gap in the semiconductor (J or eV)	p.178
E_V	energy of the valence band (J or eV)	p.177
$\mathbf{e}$	electric field (V/m)	p.189
$\mathbf{J}$	total current density (A/m^2)	p.190
$\mathbf{J}_n$	electrons' current density (A/m^2)	p.189
$\mathbf{J}_p$	holes' current density (A/m^2)	p.190
J_s	saturation current density for a p-n junction (A/m^2)	p.217
k_B	Boltzmann constant (8.617×10^{-5} eV/K $= 1.380 \times 10^{-23}$ C V/K)	p.193
M_C	weighted number of valleys in the conduction band (number)	p.202
m_0	rest mass of a free electron (9.1×10^{-31} kg)	p.200
m^*	effective mass of charge carriers (kg)	p.180
N_A	specific number of acceptors (kg^{-1})	p.191

N_C effective specific number of states in the conduction band (kg^{-1}) p.201

N_D specific number of donors (kg^{-1}) p.191

N_V effective specific number of states in the valence band (kg^{-1}) p.201

n specific number of free electrons' (kg^{-1}) p.188

$\mathbf{n}$ normal versor to a given surface p.189

n_i thermal equilibrium specific number of carriers (m^{-3}) p.193

p specific number of free holes' (kg^{-1}) p.188

$\mathbf{p}$ electric polarization field ($\mathrm{C/m}^2$) p.190

q elementary charge (1.6×10^{-19} C) p.189

R volumetric recombination rate ($\mathrm{s}^{-1}\ \mathrm{m}^{-3}$) p.190

R_n volumetric electrons' recombination rate ($\mathrm{s}^{-1}\ \mathrm{m}^{-3}$) p.189

R_p volumetric holes' recombination rate ($\mathrm{s}^{-1}\ \mathrm{m}^{-3}$) p.190

$\mathbf{t}$ tangent versor to the boundary of a given closed surface p.189

ϵ_0 vacuum permittivity (8.85×10^{-12} C/V m) p.190

ϵ_r relative permittivity (number) p.190

$\boldsymbol{\epsilon}_r$ semiconductor's relative permittivity tensor (number) p.191

ϵ_s semiconductor's permittivity (C/V m) p.190

Θ total charge density ($\mathrm{C/m}^3$) p.189

θ absolute temperature (K) p.193

μ_n electrons' mobility (m^2/V s) p.191

$\boldsymbol{\mu}_n$ electrons' mobility tensor (m^2/V s) p.192

μ_p holes' mobility (m^2/V s) p.191

$\boldsymbol{\mu}_p$ holes' mobility tensor (m^2/V s) p.192

$\boldsymbol{\nu}$ exterior pointing normal versor to $\partial\Omega$ (number) p.189

ρ mass density ($\mathrm{kg/m}^{-3}$) p.189

Σ a surface in $\mathbb{R}^3$ p.189

τ_n electrons' mean recombination time (s^{-1}) p.193

τ_p holes' mean recombination time (s^{-1}) p.193

Φ electric potential (V) p.188

χ electric susceptibility (number) p.190

Ω domain in $\mathbb{R}^2$ or $\mathbb{R}^3$ p.188

CHAPTER 6

Statement of the problem with an overview of semiconductor physics

Outline

The main problem considered in the second part of this thesis is presented in this chapter and its relevance for application is discussed. Challenges and open questions in the modelling of strained semiconductors are outlined. Moreover, a brief review of semiconductor's solid state physics and band structure is also given. The band structure of silicon is discussed and its influence on macroscopic electric properties reviewed. These will be used in later chapters in order to understand the effects of deformations.

In the latest years commercial thin films electronic devices have lost their status of fancy science-fiction gadgets and have started to play an important role in the electronic market. Many promising technologies, both based on organic and inorganic materials, have been developed recently and show properties interesting for mass-market applications (we refer the interested reader to Rogers et al. (2010) and references therein for a recent overview of the state of the art).

Traditional semiconductors are very sensible to mechanical deformations and usually are not able to sustain deformations larger than 1% before breaking and loosing their electronic properties. Therefore, in the development of flexible electronic devices only two approaches seem possible: either using new semiconducting materials which have better mechanical properties (such as polymers) or devising special microstructured components, which can accomodate large strains. Particular film architectures can be designed such that the electronic material has to sustain

only a small fraction of the global strain (see Rogers et al. (2010) for an example). In thin films electronics, this can be achieved, e.g., by moving the active part of the device as near as possible to the neutral surface of the film, which is not stretched during bending (see Park et al. (2008)).

Possible applications of flexible electronic devices include wearable electronics, enhanced non planar sensors (like CCD sensors) or solar cells. In particular, the size of these lasts and the relevance of the bulk properties of the semiconducting material suggest a treatment of the coupling effects between electronic and mechanical properties within the framework of continuum mechanics. Furthermore, in the case of inorganic electronic materials, if the construction of the device is done with precaution, typical deformation of the active electronic components range at most to a fraction of 1%. However, experimental evidence suggests that many relevant electronic properties vary significantly within this range of deformations (see Sun et al. (2009) and references therein).

Therefore, a consistent, continuum-mechanics-based modelling of the strain effects on the electronic properties of semiconductors under small strains (i.e. $|\epsilon| \leqslant 1\%$) seems to be critical in the description and improvement of these new classes of electronic devices.

Among different silicon-based technologies, we recall three main options. Silicon displays interesting semiconducting properties both in its amorphous phase as well as in its polycrystalline and crystalline phase. Due to the simpler description one can give to crystalline silicon over amorphous one, we will consider, in this first attempt to model this problem, that all the device considered is made up by crystalline silicon. From the microscopical point of view, in a crystalline semiconductor the forbidden band (band gap, see below) is essentially empty of energy levels. This leads to a description of the conducting properties of the semiconductor in terms of charge carriers only (the so called drift-diffusion model, see, e.g., Markowich et al. (1990)). On the other hand, in the case of amorphous silicon, the number of energy levels populating the band-gap is much higher, so that a description of the continuum through the number of electrons and holes only is no longer satisfactory. Therefore, a more precise model taking into account the probability distribution of charges in the band-gap and the so called deep states is required (see Shur and Hack (1984); Shur et al. (1989) or Street (2005)). The case of polycrystalline In order to keep our arguments as simple as possible, we will consider here only the case of crystalline silicon.

Our strategy in tackling this problem will be as follows. First, in this chapter, we will review the standard modelling of solid state semiconductors focusing, in particular, on silicon. In Chapter 7, we will introduce the well-known drift-diffusion model, describing the electronic properties of a semiconductor. We will also discuss on which terms of this model the effects of strain are important. Finally in Chapter 8, we will study the p-n junction and will deduce A simple 1D model predicting the characteristic curve of this device.

Our preliminary results can be summarised as follows: by the end of Chapter 8 we will have

identified the most relevant coupling mechanisms and will be able to give a qualitative as well as quantitative evaluation of the strain effects on the I-V curve of a p-n junction.

6.1 On the physics of semiconductors

A semiconductor is a material, whose electric conductivity is between the one of a conductor (such as metals) and the one of an insulator (such has ceramics or glass). Typical examples of semiconductors include both pure substances (as silicon), compounds (such as gallium arsenide) as well as organic materials (such as polyacetylene). In this section we will follow a standard approach to the description of the electronic properties of semiconductors. The interested reader can find more detailed accounts in Casey (1999); Sapoval and Hermann (1990); Sze and Ng (2007) among other books on this subject.

Most of the electric properties of a semiconducting material can be understood from its electronic band structure. This band structure is the result of the interaction of the electronic energy levels of all the atoms constituting the solid (often a crystal) being studied. When one considers the interaction between a very large number of atoms, the initially sharply defined admissible electronic energy levels associated to each atom blur. As a result, instead of a discrete number of well spaced energy states admissible for the electrons of a given crystal, the energy diagram shows clustering of admissible electronic levels, which become undistinguishable one from the other as the number of atoms constituting the crystal becomes infinite. The typical situation is represented in Figure 6.1. In all these diagrams the absolute zero temperature state (i.e. the bands occupancy at 0 K) is depicted, with electrons always occupying the lowest possible energy levels. The occupied energy levels in this fundamental state make up the valence band(s) while the free energy levels constitute the conduction band.

In the case of conductors, the highest energy level occupied by electrons is in the middle of an energy band. Therefore, a small amount of energy is needed in order to promote one electron stuck in the full valence band to a free conduction energy level. Therefore, even at temperatures of a few Kelvin degrees, when the classical physics description of conductivity looses its validity, the number of electrons free to move through the crystal is very large and hence the solid is a conductor.

The case of insulators is drastically different. In this case, between the valence and the conduction bands there is a large band gap of prohibited energy levels, where no electron can stand. The size of the band gap can be evaluated more precisely by comparing it to the thermal energy of electrons, but usually its order of magnitude is of a few eVs. Referring to Figure 6.1 again, we will denote by E_V the highest energy among those of the energy levels in the valance band.

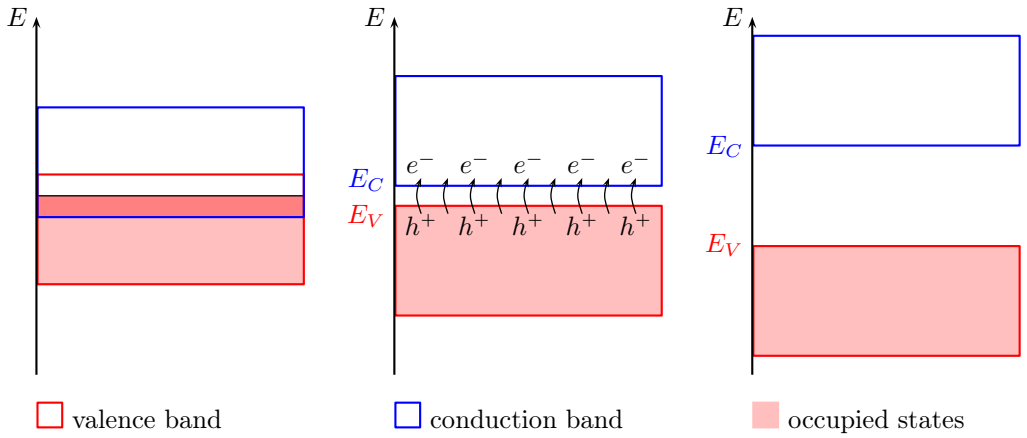


Figure 6.1: Simplified representation of the energy band structure of conductors, semiconductors and insulators. The difference in the macroscopic electric behaviour can be understood in terms of the energy required by electrons to be promoted to a free (conduction) level compared to the thermal agitation energy. Here E_C and E_V are the energies of the conduction and valence bands respectively (see text for more details).

Similarly, E_C will be the energy of the lowest energy level in the conduction band. Obviously, the band gap will be defined by

$$E_g = E_C - E_V$$

In the case of insulators, the energy gap has a width proportional to several times the mean energy of electrons of the crystal. Thus, although even in this case some electrons get promoted from the valence to the conduction band due to thermal agitation, the number of carriers in the conduction band is so small that it can be neglected when compared to the conductor case.

Semiconductors have intermediate properties between these two classes of materials. Although their energy band diagram resembles the one of insulators, the band gap is small when compared to the mean thermal energy of electrons. This results in a significant number of electrons being promoted to the conduction level. However, their number is not sufficient to guarantee properties comparable to the conductors' ones. Although only electrons are free to more in usual semiconductor crystals and although in principle a description of the electronic state of a semiconductor is possible in terms of the electrons' energy occupancy levels only, it is often a useful conceptual tool to think that every electron being promoted from the valance to the conduction band leaves behind him a "gap" in the electronic structure of lower energy levels, where an expected electron is missing. Therefore, a description of the charge carriers in the valence band is possible in terms of virtual positive charges called holes, which represent missing electrons in the sense just specified.

From the microscopic point of view, an hole moving in the valence band of a semiconductor can

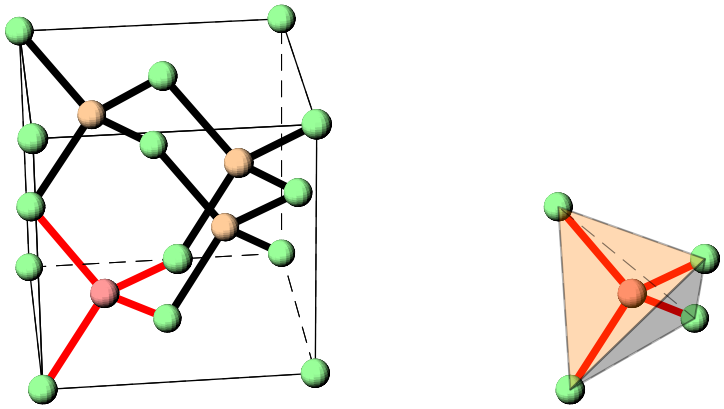


Figure 6.2: A representation of the crystalline structure of silicon. The diamond cubic crystalline structure is clearly visible on the left hand side of the picture, with the coordination number equal to four apparent on the right part of the picture.

be thought as an empty seat at the end of a otherwise full row of seats in a theatre, with people (electrons) sliding along the row one seat at a time to occupy it. However, from a macroscopic point of view a hole can be thought as a virtual particle on its own right having its equivalent mass and subject to laws of motion in all aspects analogous to those obeyed by electrons.

6.1.1 Energy bands

As a result of the previous discussion, a more detailed understanding of the electronic properties of semiconductors involves a finer description of the energy bands. In particular, this involves a brief discussion of the crystalline structure of semiconductors. Though this information is today known for most semiconductors used in applications, w e will focus here on the case of silicon. As represented in Figure 6.2, silicon (as well as gallium arsenide) exhibits a diamond cubic crystalline structure with coordination number equal to four. An eight of its Brillouin zone (i.e. its basic crystallographic element in the space of wave vectors) is represented in Figure 6.3. In this section, Γ will be the centre of the Brillouin zone, X will be its border in the Δ direction (this corresponds to the directions [100] and symmetric ones), while L will be its border in the Λ direction (i.e. in the [111] direction).

In order to better account for the band structure of a semiconductor, one has to give a description of the energy of electrons in the crystal as a function of their wave vector. In principle, the energy levels should be known for any point in the Brillouin zone introduced above. Due to symmetry reasons, for most practical considerations it is enough to know the behaviour of energy levels along the symmetry axis Δ and Λ only. The band structure of crystalline silicon and of

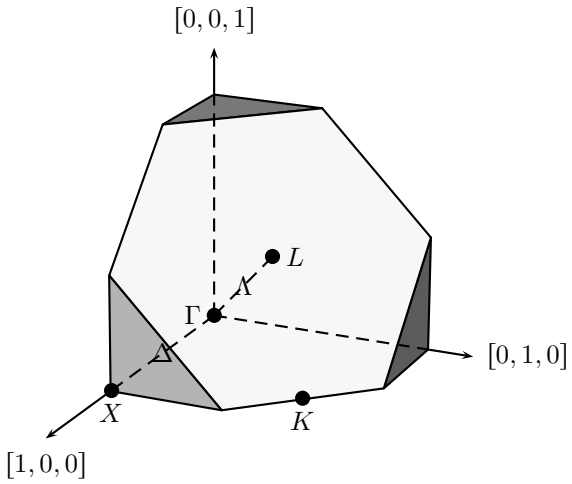


Figure 6.3: An eight of the Brillouin zone for a silicon crystal.

gallium arsenide is depicted in Figure 6.4.

A first major difference between the two diagrams in Figure 6.4 is evident: in the case of gallium arsenide, the maximum of the valence band and the minimum of the conduction band are located at the same point in the Brillouin zone (in particular both these extremal values are reached at Γ, i.e. for the wave vector $[0, 0, 0]$). On the other hand, in silicon, the maximum of the valence band is attained at Γ again, but this does not hold for the minimum of the conduction band. Indeed, due to symmetry, the conduction band has six minima, two along each of the three Δ directions. Semiconductors as gallium arsenide showing corresponding extrema in the conduction and valence are called direct band gap semiconductor, while those like silicon, having "mismatched" extrema are called indirect band gap semiconductors.

Not only the level of the energy bands at a certain wave vector is important, but also the curvature of the isoenergetic levels of the bands plays a crucial role in determining the macroscopic electrical properties of a semiconductor. Indeed, the curvature of these bands is associated to the electric resistance of the material through the effective mass (m^*) of the charge carriers. This last can be interpreted as a parameter summarising the interaction of a charge with a periodic (lattice) potential: charges moving in a periodic crystal essentially behave as free particles as soon as one considers a different value for their mass. In particular, the (density-of-states) effective mass tensor of the carriers is given by the formula (see (Sze and Ng, 2007, Section 1.3))

$$\frac{1}{(m^*)_{ij}} = \frac{1}{\hbar^2} \frac{\partial^2 E(\mathbf{k})}{\partial k_i \partial k_j}, \tag{6.1.1}$$

Together with the models introduced later in Chapter 7, which describe the relation between effective mass and mobility (see Section 7.3.5), this implies that the higher the curvature of the

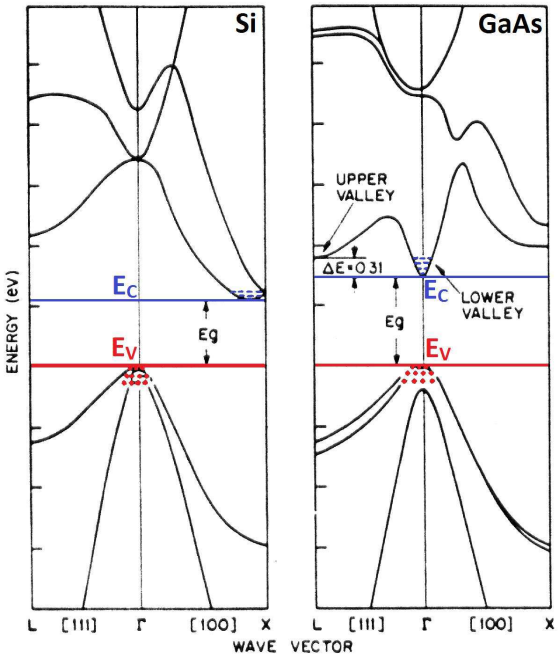


Figure 6.4: The energy band diagram for silicon and gallium arsenide. See text for a discussion.

bands, the higher the conductivity of the medium. In the case of the conduction band of silicon, the effective mass of electrons is given by $.92m_0$ in the longitudinal direction and by $.19m_0$ in the transversal one. Here m_0 is the rest mass of electrons (see Vv.Aa. for these and other material properties of silicon and common semiconductors).

As mentioned before, in this work we will focus on crystalline silicon electronics. Let us briefly describe in greater detail the band structure of this semiconductor. As it has already been stated, the conduction band in crystalline silicon shows six minima oriented in the three Δ directions. These can be described my means of the six-valley model (see Sze and Ng (2007) and references therein) in which the isoenergetic curves at all these minima have the same ellipsoidal shape (cf. Figure 6.5a). In particular, the isoenergetic curve at these minima can be approximated by revolution ellipsoids having the major axis directed towards the [000] wave vector and two minor axis orthogonal to the first one.

On the other hand, the structure of the valence band is more complex. Near the maximum energy point in the valence band, at least two different energy bands are seen to interact. As it is apparent from Figure 6.4, the two interacting bands have different curvature at the maximum point (Γ). Recalling the formula (6.1.1), these two bands are called the light holes band (LH—the more sharply peaked one) and heavy holes band (HH—the more shallow one). These bands strongly interact with each other. Therefore, a simple description of the resulting energy levels

by means of quadratic forms, as it was the case for the minima of the conduction band, is not possible (see Figure 6.5b for a representation of the isoenergetic levels at the maximum of the valence band). Moreover, at energies slightly beneath the edge of the valence band, a third band exists. This is known as split-off band and also has a maximum for $\mathbf{k} = [000]$, which is however slightly lower than the top of the valence band (44meV lower in silicon, see Vv.Aa.). The closedness of the split-off band to HH and LH bands causes strong interactions between the three, in particular a strong warping of the resulting valence band under small strains. This, in turn, implies a strong effect on the effective masses of holes and therefore on their mobility.

In order to model the shape of these degenerate energy band, a quantum mechanical description is required. The valence band can be calculated from a perturbation theory argument giving rise to the Luttinger Hamiltonian (see Luttinger and Kohn (1955); Luttinger (1956))

$$\begin{bmatrix} -P-Q & L & -M & 0 & \frac{1}{\sqrt{2}}L & -\sqrt{2}M \\ L^* & -P+Q & 0 & -M & \sqrt{2}Q & -\sqrt{\frac{3}{2}}L \\ -M^* & 0 & -P+Q & -L & -\sqrt{\frac{3}{2}}L^* & -\sqrt{2}Q \\ 0 & -M^* & -L^* & -P-Q & \sqrt{2}M^* & \frac{1}{\sqrt{2}}L^* \\ \frac{1}{\sqrt{2}}L^* & \sqrt{2}Q^* & -\sqrt{\frac{3}{2}}L & \sqrt{2}M & -P-\Delta & 0 \\ -\sqrt{2}M^* & -\sqrt{\frac{3}{2}}L^* & -\sqrt{2}Q^* & \frac{1}{\sqrt{2}}L & 0 & -P-\Delta \end{bmatrix} \tag{6.1.2}$$

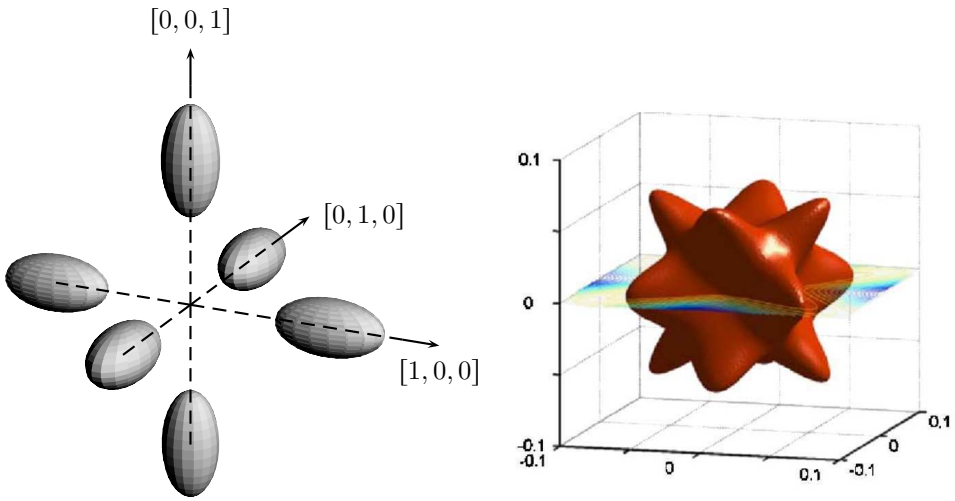
where

$$\begin{aligned} P &= \frac{\hbar^2}{2m_0}\gamma_1(k_x^2+k_y^2+k_z^2) \\ Q &= \frac{\hbar^2}{2m_0}\gamma_2(k_x^2+k_y^2-2k_z^2) \\ L &= \frac{\sqrt{3}\hbar^2}{m_0}\gamma_3(k_x-ik_y)k_z \\ M &= -\frac{\sqrt{3}\hbar^2}{2m_0}(\gamma_2(k_x^2-k_y^2)-2i\gamma_3 k_x k_y). \end{aligned}$$

Here, m_0 is the rest mass of the electron, the γ_is are the Luttinger parameters, while Δ is the split-off energy (see Sun et al. (2007) for a description of the parameters of this model). Significant values for the parameters appearing in these and in the above expressions defining the Luttinger Hamiltonian are (see (Sun et al., 2007, Table II))

$$\gamma_1 \approx 4.22, \qquad \gamma_2 \approx 0.39 \quad \text{and} \quad \gamma_3 \approx 1.44. \tag{6.1.3}$$

The eigenvalues of the above Hamiltonian, which depends on $\mathbf{k}$, represent the energy level of the three bands making up the valence band of Si. The values prescribed are relative to the top of the conduction band. Indeed, a straightforward computation shows that for $\mathbf{k} = [000]$, there are four coinciding 0 eigenvalues corresponding to the HH and LH bands and two eigenvalues equal to $-\Delta$ which describe the split-off band.



(a) Si conduction band

(b) Si valence band.

Figure 6.5: The shape of the isoenergetic surfaces in wave vector space for the energy bands of crystalline silicon. In the picture the conduction band can be modelled through a six-valleys model. On the right hand side, strong interaction between different bands belonging to the valence energy levels is observed, resulting in irregular isoenergetic surface. Image 6.5b credits (Sun et al., 2009, Figure 4.33).

Finally we recall that a possible, simpler model can be obtained from the Luttinger Hamiltonian above by considering only the interactions between HH and LH bands. This amounts to keeping only the 4x4 north-western extracted Hamiltonian from the previous expression. In particular, one can deduce the following expression for the edge of the valence band as a function of the wave vector

$$E(\mathbf{k}) = -P \pm \sqrt{Q^2 + L^2 + M^2}.$$

6.1.2 Doping

The relevance of semiconductor to technology is essentially due to another aspect beyond their particular band structure. Indeed, the number of the freely moving electrons in the conduction band and the number of holes in the valence band can easily be modified through the introduction in a pure silicon crystal of small fraction of suitably chosen chemical elements. This technique is called doping, and the resulting semiconductor is called doped.

The typical doping concentrations are very low (usually no more than a few atoms of dopant every million atoms of silicon). In doping silicon, usually elements from the IIIB (like boron) and VB groups (like phosphorus) are used. If a boron atom is added to a silicon crystal lattice, the resulting effect will be a missing electron in the valence band or, describing this situation from

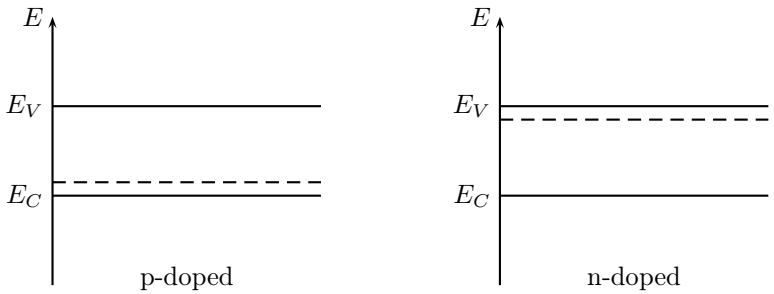


Figure 6.6: The effects of doping on the energy levels of a semiconductor. The dashes represent the additional energy states introduced through doping.

the reciprocal point of view, an additional hole. The situation can be depicted as on the left hand side of Figure 6.6. The introduction of boron atoms creates additional unoccupied energy levels in the band-gap near to the border of the valence band corresponding to electrons sequestrated from the valence band and newly introduced holes. The resulting doped semiconductor, showing a higher density of holes, is called p-doped semiconductor.

Similarly, an addition of phosphorus atoms to crystalline silicon supplies a larger number of electrons in the conduction band. Again this is explained in terms of additional energy levels in the band gap near the border of the conduction band, which, due to thermal agitation, free electrons directly to the adjacent conduction band. The resulting semiconductor is called n-doped.

We will always assume that the doping concentrations in the semiconductor are not too high. By this we mean that all doped atoms can be considered ionised. Therefore, in p-doped semiconductors a net negative charge will be considered attached to the lattice, while in n-doped semiconductors, ionised phosphorus atoms will give to the lattice a net positive charge. Obviously, the overall charge of the semiconductor will remain balanced: only a bias is the relative abundance of fixed and moving charge carriers is introduced through doping.

A further comment is important at this point. By changing the energy distribution of charge carriers, doping also affects the Fermi level (E_F) of the semiconductor. This is the theoretical energy level which would have 50% of probability of being occupied at any given time at thermodynamical equilibrium. In a pure semiconductor, considerations from statistical mechanics (see, e.g., Sapoval and Hermann (1990)) imply that the Fermi level is near the middle of the band gap. On the other hand, in doped semiconductors, the newly introduced energy levels push it towards the edge of the band gap: up towards the conduction band for n-doped semiconductors and down towards the valence band for p-doping.

The Fermi energy levels will be of crucial importance in understanding the functioning of semiconductor devices such as the p-n junction, which will be thoroughly studied in Chapter 8.

Bibliography

Casey, H. (1999). *Devices for integrated circuits: silicon and III-V compound semiconductors*. John Wiley.

Luttinger, J. M. (1956). Quantum theory of cyclotron resonance in semiconductors: General theory. *Phys. Rev.*, 102:1030–1041.

Luttinger, J. M. & Kohn, W. (1955). Motion of electrons and holes in perturbed periodic fields. *Phys. Rev.*, 97:869–883.

Markowich, P. A., Ringhofer, C. A., & Schmeiser, C. (1990). *Semiconductor equations*. Springer-Verlag.

Park, S.-I., Ahn, J.-H., Feng, X., Wang, S., Huang, Y., & Rogers, J. A. (2008). Theoretical and experimental studies of bending of inorganic electronic materials on plastic substrates. *Advanced Functional Materials*, 18(18):2673–2684.

Rogers, J. A., Someya, T., & Huang, Y. (2010). Materials and mechanics for stretchable electronics. *Science*, 327(5973):1603–1607.

Sapoval, B. & Hermann, C. (1990). *Physique des Semi-conducteurs*. Ellipses.

Shur, M. & Hack, M. (1984). Physics of amorphous silicon based alloy field-effect transistors. *Journal of Applied Physics*, 55(10):3831–3842.

Shur, M., Hack, M., & Shaw, J. (1989). A new analytic model for amorphous silicon thin-film transistors. *Journal of Applied Physics*, 66(7):3371–3380. cited By (since 1996)85.

Street, R. A. (2005). *Hydrogenated amorphous silicon*. Cambridge University Press.

Sun, Y., Thompson, S., & Nishida, T. (2007). Physics of strain effects in semiconductors and metal-oxide-semiconductor field-effect transistors. *Journal of applied physics*, 101(10):104503–104503.

Sun, Y., Thompson, S., & Nishida, T. (2009). *Strain effect in semiconductors: theory & device applications*. Springer.

Sze, S. & Ng, K. (2007). *Physics of semiconductor devices*. Wiley-Interscience publication. Wiley-Interscience.

Vv.Aa. Electronic archive, New Semiconductor Materials. Characteristics and Properties.

CHAPTER 7

The Drift-Diffusion model and strain

Outline

The drift-diffusion model for electronic effects in semiconductors in considered. The microscopic effects of strain on the electronic properties of solid state semiconductors are discussed and those relevant at a macroscopic level are identified. In particular, the case of crystalline silicon is studied. Among others, the changes in the band gap and in the shape of the valence and conduction bands are discussed and their effects on the main parameters of the drift-diffusion model estimated. Finally, simple macroscopic models for the strain-dependent mobilities and band gap are proposed.

The drift-diffusion (DD) model for semiconductors was first derived in Van Roosbroeck (1950) in 1950. Since then the DD model has enjoyed a wide popularity due to both its simplicity and its effectiveness in describing electronic properties under quite a large range of standard working conditions for electronic devices (see (Sze and Ng, 2007, Section 1.8) for an introduction overview of this model). In particular, only three quantities are used to describe the state of the semiconductor: the electric potential through the device and the concentrations of the two change carriers, electrons and holes. Moreover, the DD model offers a simple explanation of the working mechanism of some of the key electronic devices such has p-n junctions (see

Chapter 8 for a discussion of this kind of devices). The standard DD system reads as follows

$$\begin{cases} \nabla \cdot (\boldsymbol{\epsilon_s} \nabla \Phi) = q\rho\left((n - N_D) - (p - N_A)\right) \\ q\partial_t(\rho n) = \nabla \cdot \mathbf{J}_n - qR_n(n,p) \qquad \mathbf{J}_n = q\mathbf{D}_n \nabla(\rho n) - q\boldsymbol{\mu}_n \rho n \nabla\Phi \\ q\partial_t(\rho p) = -\nabla \cdot \mathbf{J}_p - qR_p(n,p) \qquad \mathbf{J}_p = q\mathbf{D}_p \nabla(\rho p) + q\boldsymbol{\mu}_p \rho p \nabla\Phi. \end{cases} \tag{7.0.1}$$

Here the unknown quantities are the electric potential (Φ), as well as the specific number of electrons and holes (i.e. the number of carriers per unit mass) denoted by n and p respectively. Moreover, ρ will be the density of the continuum considered. This slightly unusual choice for the meaning of the relevant quantities n and p can be justified keeping in mind the macroscopic, continuum-mechanical description of strained semiconductors, which is one of the main goal of our research and which will be addressed in great detail in a forthcoming paper (see Bosia et al.). We refer to Section 7.1 for a comprehensive description of all other physical constants appearing in (7.0.1).

From the point of view of applications, the DD model is particularly well-suited for the description of the behaviour of crystalline semiconductors where valence bands are well separated (see Chapter 6) and only a few energetic levels populate the band-gap. Moreover, this model can also be given firm theoretical grounds: it was rigourously derived in the context of statistical mechanics in Poupaud (1988) through a perturbation argument inspired by the works of Hilbert. We refer the interested reader to (Markowich et al., 1990, Section 2.2) for a brief discussion of this argument.

In order to clarify the phenomena described by the drift-diffusion system, we only discuss in Section 7.1 the original derivation of this model due to Van Roosbroek (see also Van Roosbroeck (1950)). After reviewing the standard DD model, we discuss in Section 7.3 the possibile influences of strain on the electronic properties of a semiconductor. We will focus on crystalline silicon and we will identify which parameters of the DD model require modelling in order to account for strain effects. Moreover, modelling of the relevant quantities as functions of strain will be given in the case of uniaxial traction and compression.

7.1 Derivation of the DD model

We will assume that our continuum occupies a region $\Omega \subset \mathbb{R}^n$ with $n = 2$ or $n = 3$. As it is the case for many phenomenological physical models, the drift-diffusion system is the composition of general physical laws with constitutive equations accounting for the particular phenomena observed in the considered system. In particular, for the DD model, the physical laws involved reduce to the Gauss law, to the Maxwell law and to the charge conservation laws. Together

with three constitutive equations for the polarisation of the semiconductor, for the charge density and the current flow through the device, these lead to the closed-form system (7.0.1). We start this section by briefly reviewing these fundamental relations; later we deduce from these the DD system stated above as well as we introduce some additional constitutive equations which are usually verified in practical situations.

The electrostatic equation Let $\mathbf{d}$ be the electric displacement field. Gauss law in finite form can be written as (see e.g. Griffiths (1998))

$$\int_{\partial\Omega} \mathbf{d}\cdot\boldsymbol{\nu}\,\mathrm{d}\sigma = \int_{\Omega} \Theta\,\mathrm{d}\Omega \tag{7.1.1}$$

where Θ is the total charge density and $\boldsymbol{\nu}$ is the outward pointing unit vector normal to the boundary of Ω. Localisation of this equation gives

$$\nabla\cdot\mathbf{d} = \Theta \qquad \text{and} \qquad \mathbf{n}\cdot[\mathbf{d}] = 0.$$

The first of these relations holds where the field $\mathbf{d}$ is regular and the second is true at its discontinuities. Here, $\mathbf{n}$ denotes a normal unit vector to the discontinuity surface Σ and $[\,\cdot\,]$ denotes the jump through the discontinuity surface.

Maxwell law We also introduce the Maxwell law to derive the system (7.0.1). In the absence of magnetic fields, Maxwell equation in finite form can be written as

$$\int_{\partial\Sigma} \mathbf{e}\cdot\mathbf{t}\,\mathrm{d}l = 0$$

where Σ is a closed surface in $\mathbb{R}^3$, $\mathbf{t}$ is the tangent versor to the boundary of Σ and $\mathbf{e}$ is the electric field. Hence, through localisation, we deduce

$$\nabla\times\mathbf{e} = \mathbf{0} \qquad \text{and} \qquad \mathbf{n}\times[\mathbf{e}] = \mathbf{0}.$$

If the electric field is regular and if the domain Ω is simply connected, these last relations imply that $\mathbf{e}$ admits a potential Φ satisfying

$$\mathbf{e} = -\nabla\Phi \tag{7.1.2}$$

The continuity equation The third fundamental law of physics necessary to derive the DD model is the continuity equation or conservation of charge. By writing the change in the electrons' number density as the sum of a bulk source term (recombination) and of the charge flow contribution, we have

$$\partial_t(\rho n) = -R_n + \frac{1}{q}\nabla\cdot\mathbf{J}_n.$$

Here q denotes the elementary (positive) charge, ρ is the mass density of the continuum being described, R_n is the volumetric electrons' recombination rate while $\mathbf{J}_n$ represents the electrons' current density. We use here the following (slightly) nonstandard notation that is motivated by the continuum mechanics framework we would like to comply with: n represents the specific number of free electrons (i.e. the number of free electrons per unit mass in the solid). An analogous equation also holds for the holes' number density, namely

$$\partial_t(\rho p) = -R_p - \frac{1}{q}\nabla \cdot \mathbf{J}_p.$$

Here all the quantities with a p-subscript instead of a n-subscript refer to holes instead of electrons. The change in the sign in front of the flow term conforms to the widely agreed upon sign conventions for the currents.

In order to guarantee the conservation of charge we will further assume that

$$R \doteq R_n = R_p \tag{7.1.3}$$

so to ensure that the total charge is conserved. Moreover, we will also assume that the reaction term R only depends on the carrier concentrations ρn and ρp and (possibly) on the position $\mathbf{x}$. Indeed, equation (7.1.3) easily implies the following law for the evolution of the total charge in the semiconductor:

$$q\partial_t(\rho(p-n)) = -\nabla \cdot \mathbf{J}.$$

Here the total current density $\mathbf{J}$ is defined by

$$\mathbf{J} \doteq \mathbf{J}_n + \mathbf{J}_p.$$

The electric displacement equation This equation relates the electric displacement to the electric field and is the first constitutive relation we introduce. We will assume that the semiconductor (usually silicon for our purposes), behaves as a linear dielectric. Denoting by $\mathbf{p}$ the electric polarisation of the medium, $\mathbf{e}$, $\mathbf{d}$ and $\mathbf{p}$ are related by (see (Griffiths, 1998, Section 4.3))

$$\mathbf{d} = \epsilon_0 \mathbf{e} + \mathbf{p}$$

where ϵ_0 is the vacuum permittivity. If we assume that the dielectric is linear and isotropic, i.e.

$$\mathbf{p} = \epsilon_0 \chi \mathbf{e}.$$

Here the quantity χ is the electric susceptibility. Collecting terms we deduce

$$\mathbf{d} = \epsilon_0 \epsilon_r \mathbf{e}$$

where ϵ_r is the relative permittivity given by $\epsilon_r = \chi + 1$. In the case of silicon, the relative permittivity is approximately equal to 11.68. In order to simplify the notation we also introduce the permittivity of the semiconductor ϵ_s given by

$$\epsilon_s \doteq \epsilon_0 \epsilon_r$$

In the general situation, when the crystalline structure has fewer symmetries (e.g. under strain), the relative dielectric permittivity (and hence the dielectric permittivity) can be represented by a second rank tensor $\boldsymbol{\epsilon}_r$. In this case, the constitutive relation for the electric displacement takes the form

$$\mathbf{d} = \epsilon_0 \boldsymbol{\epsilon}_r \mathbf{e}.$$

The charge density equation Two contributions make up the total charge in the continuum: lattice charges and free charges. As discussed in Chapter 6, apart from the clouds of free electrons and holes, one has to account for the lattice charges associated to polarised doping atoms. By denoting by N_A and N_D the specific number of acceptors and donors respectively, under the assumption of total polarisation of dopants, the total charge in the semiconductor Θ appearing in (7.1.1) can be written as

$$\Theta = -q\rho\left((n - N_D) - (p - N_A)\right).$$

It is convenient to introduce the doping profile $C(\mathbf{x})$, which summarises the distribution of dopants throughout the domain considered. In particular, the doping profile depends on the position and can be define as

$$C(\mathbf{x}) = N_D - N_A$$

thus leading to the following form for the charge density equation

$$\Theta = -q\rho\left(n - p - C\right).$$

We will always assume here that the doping profile C is a given data of the problem we are interested in,. On the other hand, the specific numbers of charges n and p will be unknown. This relation is the second constitutive relation needed in the derivation of the DD model.

The current density equation We now introduce the third and last constitutive equation we need. Indeed, in order to obtain a system in closed form, we still lack a suitable link between the currents and the other physical variables of the model. The particular form of this constitutive relation is one of the reasons for the simplicity and success enjoyed by the DD model in the last decades. We will assume that only two phenomena account for the total current densities: a

drift current and a diffusion current. To keep the initial model as simple as possible, as a first approximation, we will assume this constitutive law to be linear in its arguments. Taking into account the usual sign conventions we write

$$\begin{aligned} \mathbf{J}_n &= q\mu_n \rho n \mathbf{e} + qD_n \nabla(\rho n) \\ \mathbf{J}_p &= q\mu_p \rho p\, \mathbf{e} - qD_p \nabla(\rho p) \end{aligned} \tag{7.1.4}$$

where μ_n (resp. μ_p) is the electrons' mobility (resp. the holes' mobility) and D_n (resp. D_p) is the electrons' diffusion constant (resp. the holes' diffusion constant).

In the general setting, when the crystalline structure cannot be considered isotropic, the mobility and diffusion constants can be replaced by the more significant mobility and diffusion tensors $\boldsymbol{\mu}_n$ and $\mathbf{D}_n$ (as well as $\boldsymbol{\mu}_p$ and $\mathbf{D}_p$)

The resulting model We have now introduced all the relations needed in order to write the full DD system. Some simple computations give the following system of differential equations describing the evolution of an isotropic semiconductor

$$\begin{cases} \nabla \cdot (\epsilon_s \nabla \Phi) = q\rho\,(n - p - C) \\ \partial_t(\rho n) = \nabla \cdot\, (D_n \nabla(\rho n) - \mu_n \rho n \nabla \Phi) - R(n,p,\rho) \\ \partial_t(\rho p) = \nabla \cdot\, (D_p \nabla(\rho p) + \mu_p \rho p \nabla \Phi) - R(n,p,\rho). \end{cases} \tag{7.1.5}$$

In the case of a homogeneous body with constant density this system further simplifies to

$$\begin{cases} \epsilon_s \Delta \Phi = q\rho\,(n - p - C) \\ \partial_t n = D_n \Delta n - \mu_n \nabla n \cdot \nabla \Phi - \mu_n n \Delta \Phi - \frac{1}{\rho} R(n,p,\rho) \\ \partial_t p = D_p \Delta p + \mu_p \nabla p \cdot \nabla \Phi + \mu_p p \Delta \Phi - \frac{1}{\rho} R(n,p,\rho). \end{cases}$$

We recall that, in the general case (e.g. when the semiconductor is deformed), D_n, D_p, μ_n, μ_p and ϵ_s are tensor quantities, which can possibly depend on the strains imposed to the solid. Indeed, for a deformed silicon crystal, some symmetries are lost and anisotropic behaviour is possible. We refer to Section (7.2) below for a discussion of these phenomena.

The recombination term A few comments are still necessary before system (7.1.5) can be of practical use for applications. In particular, in order to start the analytical and numerical study of the solutions of system (7.1.5) we need some explicit expression for the recombination term. Depending on the band structure and operating conditions of the semiconductor considered, several recombination mechanisms might be relevant. In the case of silicon (and more generally for indirect semiconductors—see Chapter 6) a satisfactory expression for $R(n,p)$ is given by the Shockley-Read-Hall model (see Sze and Ng (2007)).

The Shockley-Read-Hall model, denoted shortly as SRH in the sequel (see Shockley and Read Jr (1952) and Hall (1952)), is particularly relevant when the recombination process involves carriers having different wave vectors, as it is the case in silicon (and in indirect semiconductors). This recombination mechanism invokes the existence of energy states in the middle of the band gap (the so called deep levels, which correspond to lattice defects in the crystal). These act as catalysers of the recombination reaction. In particular, in order to ensure momentum conservation, a recombination event in an indirect band semiconductor has to be a three particle event, which involves, besides the two carriers, also an interaction with the crystal (e.g. through a phonon). The just mentioned deep levels model this interaction. After some probabilistic argument, one can deduce the following expression for the recombination term given by the SRH model:

$$R(n,p,\rho) = \rho \frac{np - n_i n_i}{\tau_p(n+n_i) + \tau_n(p+n_i)} \tag{7.1.6}$$

where τ_n and τ_p are the mean recombination times for electrons and holes and where n_i is the thermal equilibrium specific number of carriers. In order to derive this expression for the (net) recombination rate, only thermal effects were taken into account (while other contributions, like radiative ones, were discarded).

We observe that the expression (7.1.6) corresponds to a source term in the conservation law for electrons and holes as soon as the concentrations of carriers are low (in particular when $np < n_i^2$), while it acts naturally as a recombination term at higher concentrations of carriers (namely when $np > n_i^2$). It might also be helpful to note that the numerator of this reaction term is exactly equal to the one, which would be expected in the description of a chemical reaction between two chemical species. In this framework, the denominator can be interpreted as a slowdown of the recombination rate due to the above-described three particle interaction mechanism involved in the SRH model.

The thermal equilibrium specific number of carriers n_i for both electrons and holes varies upon the doping of the semiconductor. For pure (undoped) silicon at room temperature (300 K) the typical value for n_i is $\rho n_i \approx 1.6 \times 10^{16}$ m^{-3}.

Einstein's relation Finally, we also discuss a relation between the coefficients appearing in (7.0.1), which leads to an important reduction in the number of parameters to be experimentally determined in the model. This is widely known under the name of Einstein's relation and states a connection between the diffusion constant and the mobility of elctrons (an analogous relation holds also for holes). Indeed, when the carriers' concentration is not too high and the doping is not too strong (that is when the semiconductor is nondegenerate), one can show that

(see (Sze and Ng, 2007, Section 1.5.5))

$$D = \frac{k_B \theta}{q} \mu \tag{7.1.7}$$

holds both for electrons and for holes. Here k_B is the Boltzmann constant, while θ is the absolute temperature of the medium. In the case of silicon, typical values for the electrons' and holes' mobilities are given by

$$\mu_n \approx 1.45 \times 10^{-1} \text{ m}^2/\text{V s} \quad \text{and} \quad \mu_p \approx 5 \times 10^{-2} \text{ m}^2/\text{V s}.$$

We observe that an analogous identity also holds for the tensor quantities.

The rationale behind this relation is that the average propagation speed of charged particles depends on the lattice properties of the crystal. These are responsible, through collisions, both for the braking of the charged particles accelerated by an electric field and for the scattering of diffusing electrons and holes. This microscopic link between drift and diffusion is the underlying reason for (7.1.7) to hold.

7.2 A brief history of strain effects on SCs' properties

The effects of strain on the electronic properties of semiconductors have been reported in pioneering results since the '50s (see Bardeen and Shockley (1950) and Smith (1954)). These coupling mechanisms were initially employed for the manufacturing of high-precision miniaturised sensors (see Smith (1954) for an early account of piezoresistance effects in silicon).

Later in the 90s, strained semiconductors became particularly attractive for a wider range of applications when geometrical scaling of the current CMOS technology started to reach its physical limits (see Sun et al. (2009) for an overview on the theoretical and technological issues involved). In order to stick with Moore's law, geometric scaling alone became insufficient and other strategies effective in enhancing the properties of the electronic circuits had to be devised. In particular, pre-strained semiconductors were found to be particularly effective in enhancing the mobilities of carriers in the channel of CMOS. Intel introduced the new concept of strain-enhanced electronic devices already in 2002 (see Sun et al. (2009) as well as Thompson et al. (2006) for an account on the introduction of the first commercial feature-enhanced devices into the market) and since then strained CMOS technology has become the standard technique to attain even higher density integrated circuits.

However, most of the research was focused on understanding and controlling the properties of silicon (or other semiconductors) at fixed strain. This is largely justified by the fact that the current silicon wafer technology does not easily allow the development and the construction of

deformable electronic circuits (sensors are the only notable exception to this otherwise general rule). The newly developed soft electronic technologies pose several questions concerning the effects of large mechanical deformation on the electronic properties of semiconductor circuits.

The goal of the remaining part of this chapter is to give an account of these effects, which can be more easily understood in terms of the band structure of semiconductors (and in particular of silicon) discussed in Chapter 6.

7.3 Strain effects in silicon

Among the mechanisms responsible of the change of the electronic properties of a strained semiconductor with respect to the unperturbed situation, we will discuss the shift in the energy bands and in the Fermi levels as well as the changes strain induces on the mobilities and on the effective masses of carriers. In turn, these effects imply other macroscopically relevant phenomena, such as changes in the amplitude of the band-gap and in the thermal equilibrium number of carriers. Moreover, the above mentioned effects are both qualitatively and quantitatively easily described taking into account the energy band structure discussed in the previous chapter.

7.3.1 Shift of the energy bands

From an atomistic point of view, the conduction and valence band in a semiconductor can be seen to arise as follows. The atomic bonds between two atoms of the same specie usually involve the combination in even number of electronic orbitals belonging to the two atoms and having the same energy. Due to fundamental quantum properties of the wave function, from an even number of orbitals of the original atoms, an equal number of molecular orbitals is expected to arise. However, these molecular orbitals do not have the same energy: usually one with lower energy than the original atomic one appears (bonding orbital) together with one with higher energy (anti-bonding orbital). We illustrate this schematically in Figure 7.1.

When considering the situation of a crystal, a similar scheme can be thought to occur, with molecular orbitals replaced by non-localised wave functions extending over the whole crystal. Thus the bonding orbital corresponds to the valence band, while the anti-bonding one to the conduction band.

We now investigate how the energy levels of the just introduced molecular orbitals depend on the relative distance of the atoms involved. One can reasonably expect that, the farther the atoms, the weaker the interaction and therefore the more the molecular orbitals should resemble to the original atomic ones. Thus as the atoms are brought apart from their equilibrium bonded position, the bonding and anti-bonding molecular orbitals should near. Viceversa, upon the closer

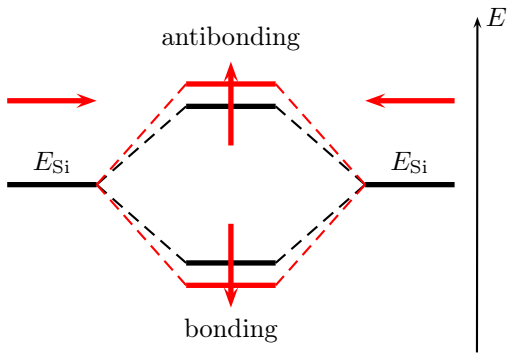


Figure 7.1: Schematic representation of the molecular orbitals arising from the interaction of two atomic orbitals having the same energy. The bonding orbital can be thought to correspond to the valence band of a semiconductor crystal, while the anti-bonding one to the conduction band. The effects of compression in the lattice direction and the consequent enhanced interaction between wave functions are represented in red. See text for description.

they are pushed, the wider the resulting gap should be.

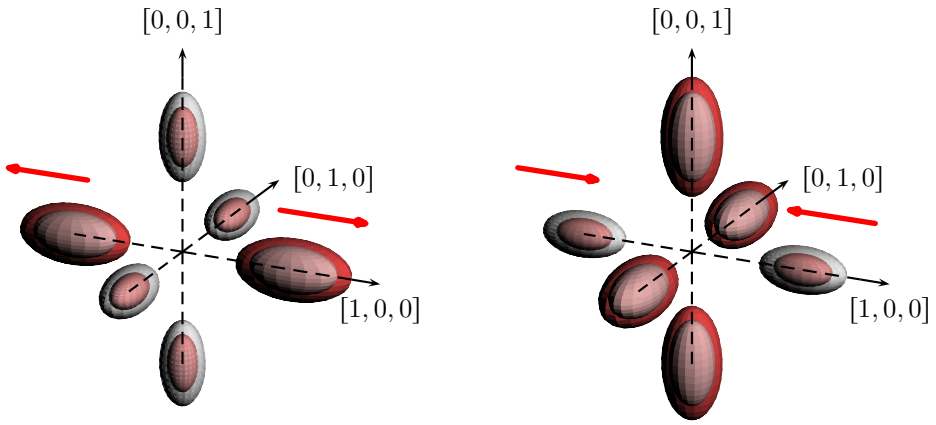
This simple picture should also translate to corresponding relative displacement in the conduction and valence bands of a semiconductor crystal upon traction and compression. Although the basic phenomena occurring are explained by this argument, one should remember that a crystal is a three dimensional structure much more complicated than a simple linear molecule.

We consider the case of silicon atoms and start our analysis by focusing on the conduction band only. For the sake of simplicity, assume that the crystal is uniformly stretched along the [100] direction and that it is free to deform in the other directions. Since the Poisson ratio of silicon is positive (from experimental results $\nu \approx 0.25$), we expect a contraction of the crystal in the [010] and [001] directions. Recalling the six-valleys model for the conduction band introduced in Chapter 6, one can expect the two valleys in the [100] direction to lower its energy, while the other four will move to (slightly) higher energies. Obviously, an opposite behaviour is to be expected in the case of compression along the [100] direction—see Figure 7.2.

Although the conduction band of silicon presents six different minima, from the above argument one can expect a linear behaviour of the energy level of each of them with respect to deformations. To be more quantitative, for each valley, the so called deformation potentials $\boldsymbol{\Xi}$ can be introduced giving rise to the following approximate law

$$\Delta E_C = \boldsymbol{\Xi}_{ij} \boldsymbol{\epsilon}_{ij}.$$

Here ΔE_C represents the shift in the energy level of one of the valleys is the conduction band. We also note that, from the macroscopic point of view we are interested in, the deformation



(a) Traction along [100] (b) Compression along [100]

Figure 7.2: The effects of uniaxial compression and deformation on the conduction band of cystalline silicon.

potentials Ξ_{ij} are material parameters, which have to be determined either experimentally or from atomistic computations. Due to the symmetries of the conduction band for the valley in the $\mathbf{k} = [100]$ direction, the tensor $\boldsymbol{\Xi}$ can only depend on two independent variables. These are known in the literature as Ξ_d for the pure dilation component and Ξ_u for the pure shear one (see Herring and Vogt (1956)). Therefore, we can write

$$\boldsymbol{\Xi} = \begin{bmatrix} \Xi_d + \Xi_u & 0 & 0 \\ 0 & \Xi_d & 0 \\ 0 & 0 & \Xi_d \end{bmatrix}.$$

For silicon, pertinent values for these deformation potentials are (see Fischetti and Laux (1996) and references therein)

$$\Xi_d = 1.1 \text{ eV}$$
$$\Xi_u = -10 \text{ eV}.$$

From these values we can estimate the shift in the edge of the conduction band as

$$\Delta E_C \approx 0.1 \text{ eV}$$

for strains of approximately 1%.

The study of the energy shift of the valence band seems to be more complicated. In order to asses the change in this part of the electronic structure of silicon under deformations, it is necessary to resort to the Luttinger Hamiltonian introduced in Section 6.1 above (see equation (6.1.2)).

Under strain, to each of the four terms P, Q, L and M, a "deformation" counterpart has to be added. The suitable corrections are

$$\begin{aligned} P_\epsilon &= -a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \\ Q_\epsilon &= -\frac{b}{2}(\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz}) \\ L_\epsilon &= -d(\epsilon_{xz} - i\epsilon_{yz}) \\ M_\epsilon &= \frac{\sqrt{3}}{2}b(\epsilon_{xx} - \epsilon_{yy}) - id\epsilon_{xy}. \end{aligned}$$

Significant values for the parameters appearing in these expressions are (see equation (6.1.3) as well as (Sun et al., 2007, Table II))

$$a_v \approx 2.46 \text{ eV}, \qquad b \approx -2.1 \text{ eV} \quad \text{and} \quad d \approx -4.8 \text{ eV}.$$

We refer the interested reader to Sun et al. (2007) and references therein for a more detailed description of the model just introduced.

In contrast to the case of the conduction band of silicon, for the valence band, no explicit computation seems to be available to compute the effects of strain. However, due to the degeneracy of the bands, one can expect that strain has only little effects on the energy level of the conduction band. Indeed an explicit computation in the case of the reduced 4×4 Luttinger Hamiltonian gives the following expression for the energy levels as a function of the wave vector

$$E(\mathbf{k}) = -P - P_\epsilon \pm \sqrt{|Q + Q_\epsilon|^2 + |L + L_\epsilon|^2 + |M + M_\epsilon|^2}$$

For $\mathbf{k} = 0$ and for uniaxial deformations of the form

$$\boldsymbol{\epsilon} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\nu & 0 \\ 0 & 0 & -\nu \end{bmatrix} \epsilon \tag{7.3.1}$$

this expression reduces to

$$E([0,0,0]) = a_v(1 - 2\nu)\epsilon \pm \frac{b}{2}(1 + \nu)\epsilon.$$

If ϵ is of the order of 1%, the resulting shift of the energy bands amounts to $10 \div 20$meV, which can be considered smaller than the effects on the conduction band (of the order of 100meV for similar strains as discussed above).

As a result of the preceding discussion, in the following we will ignore the energy shifts of the valence band due to strain and consider only those of the conduction band. In particular, due to the six-valley model for the conduction band, for uniaxial deformation of the form (7.3.1) the

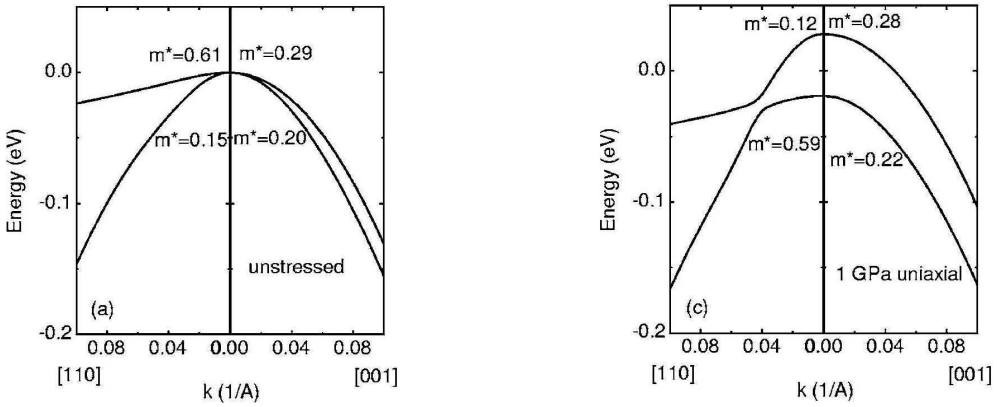


Figure 7.3: The effects of strain on the energy level of the valence band in silicon. On the left side the unstressed energy bands; only the HH and LH bands are shown for simplicity. On the right hand side the conduction band configuration for moderate uniaxial tensile strain (approximately 0.8%). Image credits Sun et al. (2007).

resulting shift of the edge of the conduction band ΔE_C is given by

$$\Delta E_C = \Delta E_g = \begin{cases} ((1-2\nu)\Xi_d + \Xi_u)\,\epsilon \approx -9\text{eV}\cdot\epsilon & \text{for } \epsilon > 0 \\ ((1-2\nu)\Xi_d - \nu\Xi_u)\,\epsilon \approx -1.5\text{eV}\cdot\epsilon & \text{otherwise} \end{cases}$$

As a consequence of the above discussion, this is also equal to the change in the energy gap, ΔE_g.

7.3.2 Changes in effective masses

We now discuss the effects of strain on the effective masses of charge carriers. As seen in equation (6.1.1), these quantities are strictly related to the shape of the energy bands. In particular, one can write

$$\frac{1}{\mathbf{m}^*_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial \mathbf{k}_i \partial \mathbf{k}_j}.$$

for the tensor valued mass and

$$m^*_{\mathbf{v}} = \mathbf{v}^T \mathbf{m}^* \mathbf{v}.$$

for the resulting effective mass in the direction of the unit vector $\mathbf{v}$.

As it was the case for the effects of strain on the shift of the band edges of silicon, also for effective masses the description of the conduction band is simpler than the one of the valence band. Indeed, in the case of the conduction band, the band warping is very slight. Hence one can consider the curvature of the energy bands to be constant under small deformations. Moreover, symmetry constraints impose the energy levels near the six energy minima (valleys) along the Δ

directions to be ellipsoids of revolution with two equal semiaxis. Considering, for example, the valley in the [100] direction, this implies that the longitudinal and transverse electronic effective masses m_l and m_t may be (and in practice are) different. We have already seen that, when the semiconductor is stretched along one of the symmetry axes, two of the six valley lower, while the other four rise. These relative shifts of energy minima trigger a redistribution of free electrons among the valleys, therefore changing the overall electrons' mass tensor, which has to be calculated as the weighted mean over the six valleys of the effective masses in a given direction. As a first approximation, we can therefore assume that the change of the electrons' effective mass under small strains is linear in the deformation. Therefore we will have

$$\mathbf{m} = \begin{bmatrix} m_l & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_t \end{bmatrix}$$

at the minimum of the conduction band in the [100] direction. As a consequence, the density of states effective mass of each valley, that is the geometric mean of the eigenvalues of $\mathbf{m}$, will be equal to

$$m_{dn} = (m_l m_t^2)^{1/3} \tag{7.3.2}$$

for the six valleys and will remain constant under small deformations. For silicon, the longitudinal and transverse effective masses are given by

$$m_l \approx 0.98 m_0 \quad \text{and} \quad m_t \approx 0.19 m_0$$

where m_0 is the rest mass of a free electron.

The situation for the valence band is much more complicated. As we saw above, the interactions between the HH, LH and split-off bands causes a strong warping of the bands and consequently a strong dependence of the holes' effective mass on deformations. These interactions are not only very significant but also strongly nonlinear as can clearly be seen by inspecting the shapes of the energy levels for the conduction band (see Figure 7.4). In order to get a precise picture of strain effects on the effective mass of holes, a solution (either approximate or numerical) of the Luttinger Hamiltonian is necessary.

Once the new holes' effective masses for the three interacting bands have been evaluated, the total density of states effective mass for the holes can be evaluated as (see (Sze and Ng, 2007, Equation 1.25))

$$m_{dp}^{3/2} = w^{lh} m_{lh}^{3/2} + w^{hh} m_{hh}^{3/2} + w^{so} m_{so}^{3/2} \tag{7.3.3}$$

where m_{lh}, m_{hh} and m_{so} represent the density of states effective mass respectively for the light holes, heavy holes and split-off bands and w^{lh}, w^{hh} and w^{so} are suitable weights given by the

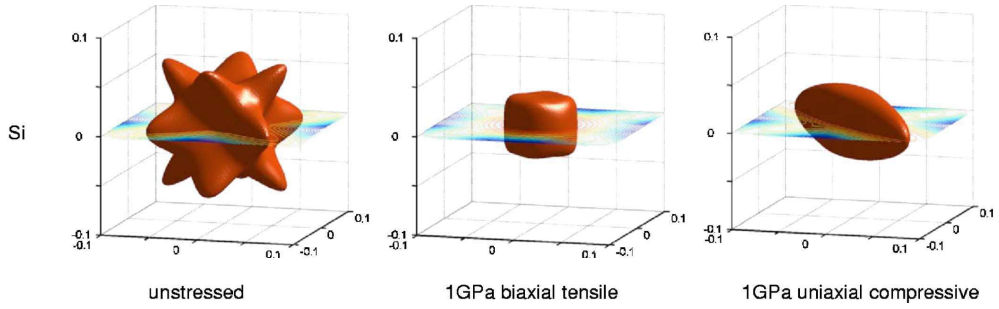


Figure 7.4: The effects of strain on the isoenergetic curves of the valence band in silicon. The very interaction between light and heavy holes bands causes significant band warping. Image credits (Sun et al., 2009, Figure 4.33).

Boltzmann statistic:

$$w^i = e^{\frac{\Delta E_V^i}{k_B \theta}}.$$

Here the relative energies of the valence bands ΔE_V^i are measured with respect to the edge of the valence band itself.

We also emphasise that the density of states effective mass will be relevant in what follows in two main respects: first, in Section 7.3.3, we will use it to evaluate the change in the Fermi level of doped semiconductors; then, in Section 7.3.5, we will discuss its effects on the mobilities of the carriers. We anticipate that the effects on the Fermi levels can be neglected at first approximation (see below), while the effects on the mobilities are relevant. Since due to the difficulties encountered in this section, we do not have an explicit estimate of the effective mass for holes in the valence band of silicon, we will introduce suitable approximate models for holes mobilities in the following.

7.3.3 Shift of the Fermi level

As discussed in Section 6.1, the Fermi level of a semiconductor is the median energy of the electrons populating its valence and conduction bands. We recall that the Fermi level for an intrinsic semiconductor is given by (see (Sapoval and Hermann, 1990, Equation IV.25))

$$E_F = \frac{1}{2}(E_c + E_v) + \frac{3}{4} k_B \theta \ln \frac{m_p}{m_n}. \tag{7.3.4}$$

In what follows, we will focus on p-n junctions, which are realised by juxtaposing two differently doped semiconductors. Therefore, in this section we will consider the effects of strain on the Fermi level of doped silicon only. In particular, in this setting, the relation (7.3.4) can be rewritten as (compare (Sapoval and Hermann, 1990, Equations IV.30 and IV.38) or (Sze and Ng,

2007, Equations 1.44 and 1.47))

$$E_F = E_C + k_B\theta \ln \frac{N_D}{N_C} \tag{7.3.5}$$

for n-doped semiconductors

$$E_F = E_V + k_B\theta \ln \frac{N_V}{N_A} \tag{7.3.6}$$

in the p-doped case. Here, N_V and N_C are the effective specific number of states in the valence and conduction bands respectively. In order to evaluate this unknown quantities, we recall two further equations (see (Sapoval and Hermann, 1990, Equations IV.16 and IV.18) as well as (Sze and Ng, 2007, Equations 1.18 and 1.24))

$$N_C = 2\left(\frac{2\pi m_{dn} k_B \theta}{h^2}\right)^{3/2} M_C \tag{7.3.7}$$

$$N_V = 2\left(\frac{2\pi m_{dp} k_B \theta}{h^2}\right)^{3/2} \tag{7.3.8}$$

where M_C is the weighted number of valleys in the conduction band of the semiconductor. In the case of silicon, M_C is defined by

$$M_C = \sum_{i=1}^{6} e^{-\frac{\Delta E_C^i}{k_B\theta}},$$

where ΔE_C^i are the relative energies of the six valleys measured with respect to the edge of the conduction band. We note that in the unstrained case, all ΔE_C^i are equal to zero and this expression reduces to the expected $M_C = 6$, as expected for the six valleys model.

We now try to estimate the effects of deformations on the Fermi level. Indeed, in the case of n-doped silicon, only the above expressions for the conduction band are relevant. Since from Section 7.3.2 the density of states effective mass m_{dn} is not affected by deformation, we need to evaluate only the changes to the Fermi level due to the weighted number of valleys M_C. However, due to the six-valleys model discussed before, this changes from six to four or two depending on the particular stress state imposed to the material. Since this factor enters in (7.3.5) through a logarithm, we can estimate the maximum shift in the Fermi level with respect to the conduction band edge as

$$\Delta_{\max}(E_F - E_C) = k_B\theta \ln 3 \approx 28\text{meV}$$

which is small when compared to the global shift in the conduction band (which is of the order of 100meV as discussed above).

In the case of the valence band, a different effect has to be taken into account. In particular, in this case the effective mass m_{dp} is greatly decreased by strain due to the decoupling of the HH and LH valence bands. From the data in Figure 7.3 (see also Sun et al. (2007)), we can

trace down to a factor $2 \div 3$ this reduction (note however, that due to the high anisotropy of the isoenergetic curves, this factor might be much larger along selected directions). This corresponds to a maximum shift in the Fermi level with respect to the valence band edge of a few tens of meVs, which can again be neglected when compared to the overall changes in the size of the band-gap.

7.3.4 Changes in the thermal equilibrium specific number of carriers

We can now discuss the effects of strain on the thermal equilibrium specific number of carriers n_i. These are a consequence of the changes in the effective specific number of states of the valence and conduction bands as well as in the size of the band gap. Due to the Fermi-Dirac distribution of electrons in the semiconductor, these effects can be summarised by the following expression for n_i in terms of the (see (Sapoval and Hermann, 1990, equation IV.22))

$$n_i^2 = N_C N_V e^{-\frac{E_g}{qU_T}}.$$

From the analysis above, the variation of term at exponent is approximately given by

$$\frac{\Delta E_g}{qU_T} \approx 2 \div 3$$

while the effects on the effective specific number of states bring each a reduction of a factor 3 to the thermal equilibrium specific number. Altogether these effects roughly compensate. As a consequence we will neglect the effect of strain on n_i and hence on the reaction term R appearing in the DD system (7.0.1).

7.3.5 Changes in mobilities

Finally, we investigate the effects of the strain upon the mobilities of the charge carriers. This requires to delve again in the electronic structure of silicon. As before, the situation for the conduction and the valence bands is quite different.

Two main effects contribute to the mobility changes in the deformed conduction band: redistribution of electrons in the different valleys due to energy shift of the minima of the conduction band and changes in the scattering of electrons between valleys (see Dhar et al. (2005)). In order to evaluate the first contribution we write

$$\boldsymbol{\mu}_n = \sum_{i=1}^{6} \pi^i \boldsymbol{\mu}_n^i$$

where $\boldsymbol{\mu}_n^i$ represents the mobility tensor for the i-th valley of the conduction band, while π^i is the fraction of free electrons in the i-th valley. The π^is may be easily computed from the Boltzmann

statistics and are given by

$$\pi^i = \frac{\exp\left(\frac{\Delta E_C^i}{k_B\theta}\right)}{\sum_{j=1}^{6}\exp\left(\frac{\Delta E_C^j}{k_B\theta}\right)}.$$

On the other hand, the tensor mobilities $\boldsymbol{\mu}_n^i$ can be written as the product of a scalar mobility and a scaled inverse mass tensor (see (Dhar et al., 2005, Equations 5–7))

$$\boldsymbol{\mu}_n^i = \mu_{ns}\left(\widehat{\mathbf{m}}_n^i\right)^{-1}.$$

Here the mass matrix are different for the different valleys. Up to symmetries we have

$$\widehat{\mathbf{m}}_n^{[100]} = \frac{1}{m_0}\begin{bmatrix} m_l & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_t \end{bmatrix}.$$

as well as analogous expressions for the minima in the [010] and [001] directions. The electrons' scalar mobility μ_{ns} summarises here all the contributions due to scattering phenomena. Among these, momentum relaxation due to intravalley scattering, intervalley scattering and impurity scattering should be considered. We recall that the intervalley scattering depends on the shift of the conduction bands, while the impurity scattering is sensible to the doping concentration. For the sake of simplicity we will assume this scalar mobility to be constant throughout the material and we will set

$$\mu_{ns} = \frac{qt_n}{m_0}$$

where t_n is a suitable relaxation time summarising all scattering events. Assuming this parameter to be independent of strain, from the discussion of the preceding paragraphs, due to the relative shifts of the valleys in the conduction band, we conclude that, in silicon, the mobility-strain relation is not differentiable for zero strains. However, in the case of uniaxial stresses, a reasonable first approximation is to consider μ_n as a piecewise linear function of the deformation, with a kink at the origin (cf. Figure 7.5). In particular, for strains of the form (7.3.1), and for ϵ small (up to 1%) we will assume

$$\mu_n(\epsilon) = \begin{cases} \mu_{n0} + \alpha\epsilon & \text{for } \epsilon > 0 \\ \mu_{n0} + \beta\epsilon & \text{otherwise} \end{cases} \tag{7.3.9}$$

where μ_{n0} is the electrons' (longitudinal) mobility in the unstrained case and is given by

$$\mu_{n0} \approx 1.45 \times 10^{-1}\ \mathrm{m}^2/\mathrm{V\ s}.$$

The parameters α and β can be estimated from Figure 7.5 as follows

$$\alpha \approx 1.5 \times 10^{1}\ \mathrm{m}^2/\mathrm{V\ s} \quad \text{and} \quad \beta \approx 5\ \mathrm{m}^2/\mathrm{V\ s}.$$

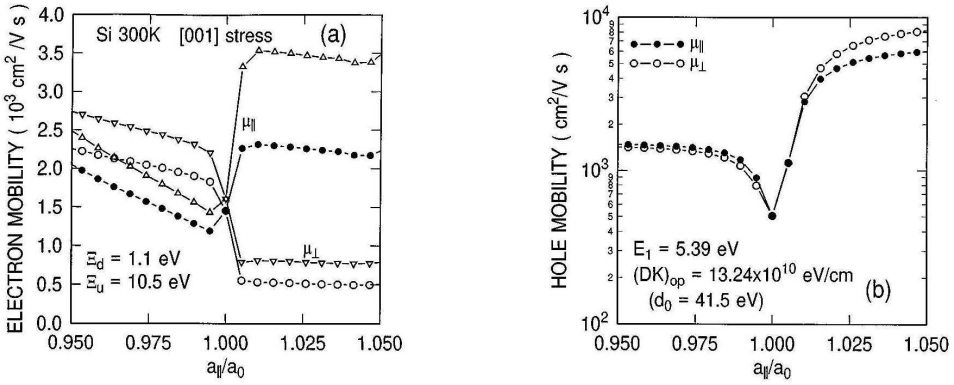


Figure 7.5: An semi-empirical computation of the electrons' and holes' mobilities in uniaxially strained silicon. the dots refer to to the longitudinal mobilities, while the circles to the transverse ones. The triangles corresponds to results obtained following a different approach (see Jacoboni et al. (1981)). Image credits (Fischetti and Laux, 1996, Figure 10).

The dependence of the holes' mobility with respect to strain is again more complicated due to the strong effect of band warping on the final mobility. A possible approach, which explicitly accounts for scattering kernels, can be found in Fischetti and Laux (1996) (see, in particular Equations 16 and 19). From the qualitative point of view, we observe that as soon as the semiconductor is strained, the HH and LH bands decouple, hence leading to a reduced effective mass for the carriers and to an enhanced mobility. Incidentally, we remark that this (relevant) effect has been one of the main reasons for the study of the properties of strained p-doped silicon for applications to very large scale integration (VLSI) in the '90s.

The most relevant results of the approach in Fischetti and Laux (1996), which can be used both for electrons and holes, are summarised in Figure 7.5. In particular, in the case of the uniaxial strain given by (7.3.1), we will assume

$$\mu_p(\epsilon) = \mu_{p0} + \alpha'|\epsilon| \tag{7.3.10}$$

where μ_{p0} is the holes' mobility in the unstrained case and is given by

$$\mu_{p0} \approx 5 \times 10^{-2}\ \mathrm{m}^2/\mathrm{V\ s}.$$

Moreover, the parameter α' can be estimated again from Figure 7.5 as follows

$$\alpha' \approx 1.5 \times 10^{1}\ \mathrm{m}^2/\mathrm{V\ s}.$$

Summarising the discussion of this section, the strain effects on the electronic properties of a semiconductor described by the DD model can be modelled through suitable expressions for the

mobilities of electrons and holes. In the next chapter we will investigate what are the consequences of this coupling for a fundamental electronic component as the p-n junction. In particular we will study how the characteristic of the junction is affected by strain and whether the reverse coupling between electronic and mechanical properties is relevant or not in this kind of applications.

Bibliography

Bardeen, J. & Shockley, W. (1950). Deformation potentials and mobilities in non-polar crystals. *Physical Review*, 80(1):72.

Bosia, S., Constantinescu, A., Jabbour, M., & Triantafyllidis, N. On the modelling of strained semiconductors. in preparation.

Dhar, S., Kosina, H., Palankovski, V., Ungersboeck, S., & Selberherr, S. (2005). Electron mobility model for strained-Si devices. *Electron Devices, IEEE Transactions on*, 52(4):527–533.

Fischetti, M. & Laux, S. (1996). Band structure, deformation potentials, and carrier mobility in strained Si, Ge, and SiGe alloys. *Journal of Applied Physics*, 80(4):2234–2252.

Griffiths, D. J. (1998). *Introduction to Electrodynamics (3rd Edition)*. Benjamin Cummings.

Hall, R. N. (1952). Electron-hole recombination in germanium. *Physical Review*, 87(2):387.

Herring, C. & Vogt, E. (1956). Transport and deformation-potential theory for many-valley semiconductors with anisotropic scattering. *Physical Review*, 101(3):944.

Jacoboni, C., Nava, F., Canali, C., & Ottaviani, G. (1981). Electron drift velocity and diffusivity in germanium. *Physical Review B*, 24(2):1014.

Markowich, P. A., Ringhofer, C. A., & Schmeiser, C. (1990). *Semiconductor equations*. Springer-Verlag.

Poupaud, F. (1988). *Etude mathématique et simulations numériques de quelques équations de Boltzmann*. PhD thesis, Université Paris 6.

Sapoval, B. & Hermann, C. (1990). *Physique des Semi-conducteurs*. Ellipses.

Shockley, W. & Read Jr, W. (1952). Statistics of the recombinations of holes and electrons. *Physical Review*, 87(5):835.

Smith, C. S. (1954). Piezoresistance effect in germanium and silicon. *Physical review*, 94(1):42.

Sun, Y., Thompson, S., & Nishida, T. (2007). Physics of strain effects in semiconductors and metal-oxide-semiconductor field-effect transistors. *Journal of applied physics*, 101(10):104503–104503.

Sun, Y., Thompson, S., & Nishida, T. (2009). *Strain effect in semiconductors: theory & device applications*. Springer.

Sze, S. & Ng, K. (2007). *Physics of semiconductor devices*. Wiley-Interscience publication. Wiley-Interscience.

Thompson, S. E., Sun, G., Choi, Y. S., & Nishida, T. (2006). Uniaxial-process-induced strained-si: extending the cmos roadmap. *Electron Devices, IEEE Transactions on*, 53(5):1010–1020.

Van Roosbroeck, W. (1950). Theory of flow of electrons and holes in germanium and other semiconductors. *Bell Syst. Tech. J*, 29(4):560–607.

CHAPTER 8

P-N junctions under strain

Outline

We study the effects of strain on the electronic properties of the p-n junction. After reviewing the physics of this electronic device, the Shockley relation for strained junctions is deduced. Hence a simple (semi-empirical) expression for the strain-dependent characteristic curve of a p-n junction is obtained. The assumptions leading to this result are then verified a posteriori. This enables us to evaluate also the Maxwell stresses at the interface between p- and n-doped semiconductors. As a result we conclude that Maxwell stresses as well as the reverse coupling between electronic effects and mechanical properties can be neglected at a first approximation.

In contemporary solid state electronics technology, p-n junctions (also known as diodes) represent a simple, but at the same time fundamental device. This can easily be seen as one of the few basic bricks constituting most of the electronic devices being developed today. From a macroscopic point of view, a p-n junction is an "asymmetric" device, enabling a current flow only in one direction and being essentially an open circuit in the opposite one (see Figure 8.4).

The basic functioning of diodes was first understood by Shockley in the '40s (see Shockley (1949) and Shockley et al. (1963)). Since then the theory has developed along many different directions both proposing refined models describing the behaviour of p-n junction in particular settings and deducing the Shockley relation in more rigourous way from the general models describing semiconductors. Among these we recall the approaches through rigourous asymptotics in Markowich et al. (1990).

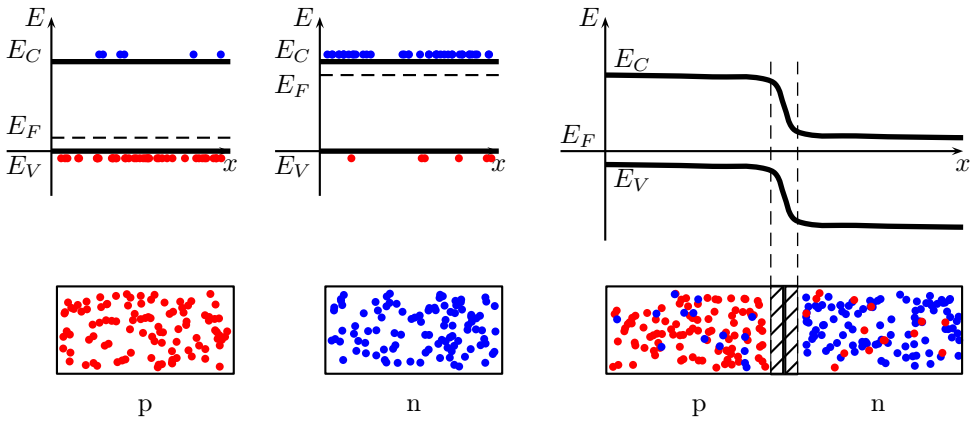
In this section we will focus on the relation between strain and the current-voltage characteristic of the p-n junction. As it has been discussed in the previous chapter, the mechanical coupling may take place through the variation in the band gap, through the changes in the equilibrium electrons' and holes' number densities n_p^0 and p_n^0 as well as through the diffusion (or mobility) constants. From equations (8.2.6) and(8.2.8) below, in order to understand the dependence of n_p^0 and p_n^0 on strain we further have to discuss the dependence on deformations of the energy bands and Fermi levels as well as of the effective masses of electrons and holes. In order to simplify the following discussion and to keep in touch with our main application to solar cells, we will focus on the case of doped silicon only (see Sun et al. (2007)).

The plan of this chapter is as follows. In Section 8.1 we briefly review the physics explaining the functioning of p-n junctions. Then we derive the Shockley relation for a uniaxially strained junction. Our approach involves several ansatz, which are motivated by physical consideration. Finally, in Section 8.3 we verify that all our assumptions are verified in the present setting. Moreover we discuss the possible reverse coupling describing the mechanical effects of the strong electric fields encountered in the device.

8.1 P-N junctions in operation

A p-n junction is an electronic device built by matching two differently doped semiconductors. In the simplest design, a p-doped and a n-doped semiconductor are combined. In practice, this can be achieved by diffusing some dopants (e.g. donors) on top of a uniformly doped (e.g. p-doped) silicon. This leads to a (sharp) gradient in the doping profile of the device (see, e.g., Jäger (2002) for an overview of integrated circuits fabrication technologies).

Due to the properties of doped semiconductors discussed in Section 6.1.2, the concentrations of electrons and holes in a p- and in a n-doped semiconductor are significantly different. When such materials are at contact, diffusion will cause electrons originating from the conduction band in the n-doped semiconductor to flow towards the p-doped domain. At the same time, their hole counterparts will diffuse in the opposite direction in compliance with the concentration gradient. The net imbalance of charges through the interface will then generate an electric field at the junction, which will prevent the flow of further charges through the contact. In particular, the process reaches a stationary configuration when the relative energies (Fermi levels) of the charge carriers at both sides of the junction are equal. In Figure 8.1 we have depicted the stationary equilibrium state for an unperturbed p-n junction. The drift effects are here easily visualised recalling that in Figure 8.1b, the electrons move downward while the holes naturally try to rise in the energy diagram.



(a) Isolated p- and n- doped silicon (b) A p-n junction at equilibrium

Figure 8.1: A representation of the ideal sharp p-n junction. On the left hand side, the energy diagram for the isolated doped semiconductors, on the right hand side the resulting energy diagram for the whole junction. In these diagrams, electrons are represented as blue dots, while holes as red ones. Note that in this diagram, electrons tend to lower energy levels due to electric drift, while holes move in the opposite direction. A net difference of potential (built-in potential) develops through the device. The hatched area indicates the depletion zone. See text for details.

As a result of the net movement of charges between the differently doped semiconductors, an electric field develops through the junction. Eventually, the n-doped semiconductor will have an higher potential than the p-doped one (recall that, according to the usual sign conventions, the electric potential is opposite to the energy bands for electrons depicted in figure 8.1b). Recalling the expressions for the Fermi level in a doped semiconductor (see equations (7.3.5) and (7.3.6)), the built-in potential difference through the junction is given by

$$\phi_{bi} = \frac{E_g}{q} + \frac{k_B \theta}{q} \ln \frac{N_A N_D}{N_C N_D}.$$

Since in a nondegenerate semiconductor the doping concentrations N_A and N_D are smaller than the density of states N_C and N_D, we immediately see that the build-in potential is (slightly) smaller than the bandgap. For a silicon p-n junction and for standard doping profiles, ϕ_{bi} is approximately given by 0.7 V.

We can think that the resulting (strong) electric field at the junction is able to wipe away all remaining free charges near the interface between the n- and the p-doped semiconductor. Therefore a region depleted of electrons and holes arises at the junction, which is called depletion zone. Therefore, we can approximate the electric field at a p-n junction at equilibrium by assuming that, in the depletion zone, the specific charge density is given by N_D on its n-doped side and by N_A on the other one. A simple 1D computation assuming a piecewise constant right hand side in

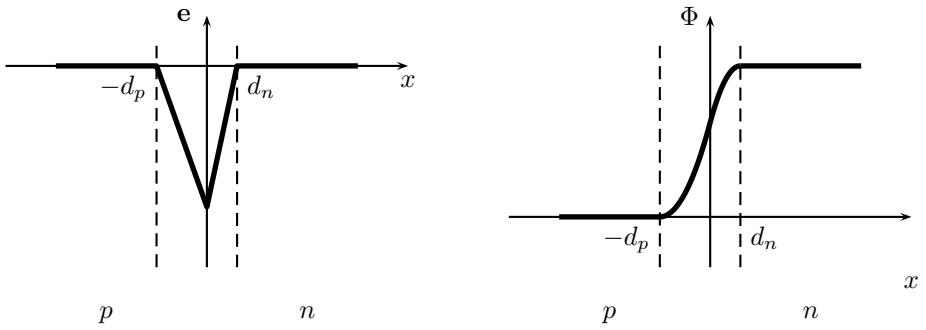


Figure 8.2: The approximate solution for the electric field **e** and for the electric potential Φ at a p-n junction given by equation (8.1.1).

the first equation of (7.0.1) leads to the following approximate expression for the electric field **e**

$$e = \begin{cases} -\frac{q\rho N_A}{\epsilon_0\epsilon_r}(x + d_p) & \text{for } x \in [-d_p, 0], \\ \frac{q\rho N_D}{\epsilon_0\epsilon_r}(x - d_n) & \text{for } x \in [0, d_n]. \end{cases} \tag{8.1.1}$$

Here d_n (resp. d_p) is the depth of the depletion zone in the n-doped (resp. p-doped) part of the device. These are given by (see (Sapoval and Hermann, 1990, Section VII.2)

$$d_n = \left(\frac{2\epsilon_0\epsilon_r\phi}{q\rho}\right)^{1/2}\left(\frac{N_A}{N_D(N_A + N_D)}\right)^{1/2}$$
$$d_p = \left(\frac{2\epsilon_0\epsilon_r\phi}{q\rho}\right)^{1/2}\left(\frac{N_D}{N_A(N_A + N_D)}\right)^{1/2}$$

where ϕ is the difference of the electric potential through the junction. As a first approximation, the total width of the junction is therefore given by

$$d_n + d_p = \left(\frac{2\epsilon_0\epsilon_r\phi}{q\rho}\right)^{1/2}\left(\frac{N_A + N_D}{N_A N_D}\right)^{1/2}.$$

In particular we observe that this quantity is closely related to the Debye length

$$l_{\text{Debye}} = \sqrt{\frac{\epsilon_0\epsilon_r U_T}{q\rho\overline{C}}}$$

which arises naturally in the nondimensionalisation of the Gauss equation for the electric potential (see the first equation of (7.0.1) again). Here U_T is the thermal voltage given by

$$U_T = \frac{k_B\theta}{q} \approx 25\text{mV} \qquad \text{at room temperature.}$$

and $\overline{C}$ is the characteristic value of the doping profile. Indeed, in the case of a symmetric junction, the quantity $\frac{N_A+N_D}{N_A N_D}$ is equal to $\frac{2}{\overline{C}}$ and therefore, $d_n + d_p$ is proportional to the Debye length up

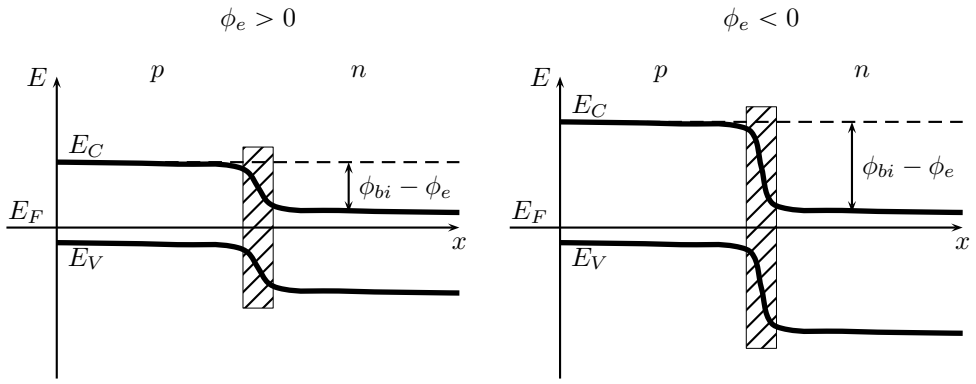


Figure 8.3: The effects of an external bias on the energy bands diagram of a p-n junction. In the case of direct external voltage (i.e., when the potential of the p-doped region is lifted), the energy barrier is reduced and hence many more charge carriers can diffuse through the junction. In the case of reverse bias the opposite phenomenon occurs.

to the substitution of the external electric field with the thermal voltage. We also recall that the Debye length (or Debye radius) arises in the context of multi-body interactions as a measure of the radius of the nonlocal electromagnetic interaction among charges (electrons and holes) within the semiconductor (see Lifshitz et al. (1981) for an introduction to plasma physics).

We conclude this section by quickly reviewing the effects of an external applied voltage between the two extrema of the p-n junction. We will denote by ϕ_e this external applied voltage. In particular, ϕ_e will be positive if it raises the potential of the p-doped region with respect to the one of the n-doped domain. In order to understand the effects of this applied potential on the operations of the p-n junction we refer to Figure 8.3. When ϕ_e is positive we will say that the junction is directly biased. The applied voltage opposes to the built-in potential and therefore, the drift current at the junction is significantly reduced. As we will discuss quantitatively in the next section, the resulting effect is an exponentially increasing current through the junction as a function of the external voltage (see equation (8.2.7)).

In the opposite case, for $\phi_e < 0$ (reverse bias), the field at the interface is strengthened. Electrons could easily move from the p side to the n side of the junction (and holes move in the reverse direction), but only very few such charge carriers are available there. Therefore, only a little current is seen to flow through the junction at reverse bias (this is the so called saturation current).

The usual characteristic curve for a p-n junction (diode) as given by equation (8.2.7) is represented in Figure 8.4.

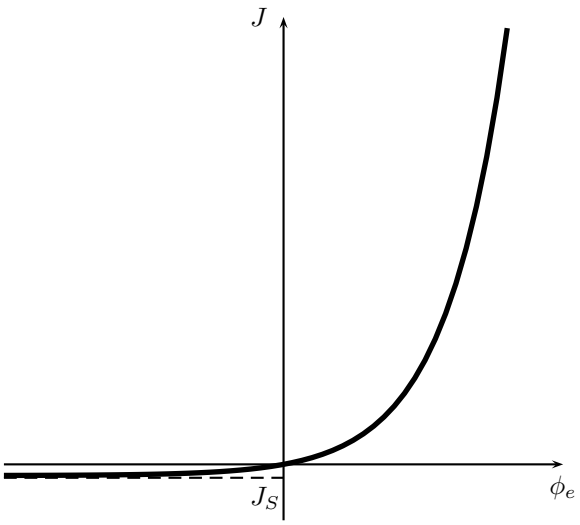


Figure 8.4: Characteristic curve for a p-n junction. Remark the different behaviour under direct and reverse external voltage. The saturation current density J_s is clearly identifiable for reverse applied external voltages.

8.2 The Shockley relation with strain effects

We will now discuss the operation of the biased p-n junction in more detail. In particular, in this section we will derive the current-voltage characteristic of this device (the so called Shockley relation). In doing this we will be careful in underlying the possible effects of strain on our arguments. Our approach will be a standard physical one (see, e.g., Sapoval and Hermann (1990)). We refer also the interested reader to Markowich et al. (1990) for a different perspective on this problem based on rigourous asymptotic expansions of the solution near the interface.

We will assume that the material properties of the p-n junction can be modeled though the drift-diffusion system (7.0.1) described in the previous chapter. We also assume that the domain representing the area occupied by the device is divided into two adjacent parts on which the doping profile is (essentially) constant. The doping profile will change abruptly (we do not make assumptions on whether continuously or with a jump) at the contact between the two domains. In order to derive the Shockley relation, in this section we make the following two assumption:

- a depletion region exists. By this we mean that there is a region surrounding the boundary between the p- and n-doped regions of the device where the two fields n and p appearing in (7.0.1) are small with respect to the reference values of the doping profile. Moreover, we will assume that the concentration of charges, n and p, as well as the electric potential Φ vary quickly in this area;

- in the remaining part of the device the zero charge approximation holds. Our assumption is that the Gauss law for the electric potential (the first equation in (7.0.1)) can be substituted by the simpler algebraic relation

$$n - p - C = 0.$$

As it was discussed in the previous chapter, in order to capture the most relevant effects of strain on the functioning of the p-n junction, one has to assume strain-dependent mobilities and band gap. In the case of an unknown displacement field, this implies that these quantities may depend on the position. To fix ideas we will assume that the strain field through the junction is uniform plus a perturbation, which is localised near the junction. Moreover, we will assume that the density is constant (for example, considering a linear elastic continuum). This accounts for the possible inverse coupling effects linking the strong electric fields to additional mechanical stresses on the material. We will check in Section 8.3 that the implicit assumption of smallness for these terms is verified a posteriori using the results we will deduce in this section.

The first step in our argument moves from the assumption that a depletion region exists. We assume that the junction coincides with $x = 0$, that the n-doped region extends for positive values of the coordinate x and that for $x < 0$ the semiconductor is p-doped. The depletion zone will extend from $x = -d_p$ to $x = d_n$. Outside this region we will assume that the zero charge approximation (essentially) holds (see Figure 8.3).

In particular, in the depletion zone we expect a sharp gradient in the variables n, p and Φ. Recall the constitutive equation for the electrons' current

$$\mathbf{J}_n = \mu\rho\left(k_B\theta\nabla n - qn\nabla\Phi\right)$$

From the above discussion on the form of the electric potential through the junction, we expect the drift and the diffusion currents to be opposite and much larger than the total resulting electrons' current. In particular we assume

$$|\mathbf{J}_n| \ll |\mu\rho qn\nabla\Phi| \approx |\mu\rho k_B\theta\nabla n| \tag{8.2.1}$$

In the 1D case, the above current equation reduces to

$$\mu\rho\left(k_B\theta n' - qn\Phi'\right) \approx 0 \tag{8.2.2}$$

which is satisfied for any $\mu = \mu(x)$ if

$$k_B\theta n' = qn\Phi'.$$

Upon integration this relation gives

$$n(x) = C\exp\frac{q\Phi(x)}{k_B\theta} \tag{8.2.3}$$

where the constant C can be determined by the "boundary conditions" for n and Φ at the limits of the depletion zone. From (8.2.3) we further deduce

$$n(-d_p) = n(d_n) \exp \frac{-q(\Phi(d_n) - \Phi(-d_p))}{k_B \theta}$$

We recall that the potential difference through the junction is given by $\Phi(d_n) - \Phi(-d_p) = \phi_{bi} - \phi_e$. Moreover, at $x = d_n$ the concentration of electrons has essentially reached the equilibrium value imposed by the doping concentration of donors, i.e. $n(d_n) = N_D$ holds. Therefore the concentration of electrons on the p-side of the junction is

$$n(-d_p) = N_D \exp - \frac{q(\phi_{bi} - \phi_e)}{k_B \theta}. \tag{8.2.4}$$

We note that in this passage, no information is required on the size of the depletion zone, except that it exists.

We estimate the electrons' current through the junction by evaluating the effect of the just computed electron density being injected on the p-side of the junction. To do this we derive a suitable approximation of the drift-diffusion system holding true in the bulk of the n- and p-doped regions. In particular, linearising the conservation of charge for holes around the state $p \equiv N_D$ we deduce the equation

$$D_n n'' - \frac{n - n_p^0}{\tau_n} = 0$$

where n_p^0 is the equilibrium specific number of electrons in the p-doped semiconductor. It is important to emphasise that this approximation holds true only if the concentration of the injected minority carriers is small when compared to the doping profile, i.e., when

$$n_p^0 \ll N_A \qquad \text{and respectively} \qquad p_n^0 \ll N_D \tag{8.2.5}$$

hold in the n-doped (resp. p-doped) parts of the domain. We also recall that the general expression for the equilibrium concentration of carriers is and is given by (see (Sapoval and Hermann, 1990, equation IV.15))

$$n^0 = N_C \exp - \frac{E_C - E_F}{k_B \theta}. \tag{8.2.6}$$

As discussed before, here we assume that the mobilities (and hence the diffusion terms) are constant with respect to the space variable (uniform strain). From this equation and from the boundary data $n(-d_p)$ computed above we deduce the following expression for the profile of the density of the injected electrons in the p-doped part od the device

$$n(x) = n_p^0 + (n(-d_p) - n_p^0) \exp - \frac{-d_p - x}{\sqrt{D_n \tau_n}} \qquad \text{for } x < -d_p.$$

In this part of the device, from the zero space charge approximation we deduce that the electric potential has to be linear. Moreover, we assume that it varies slowly with respect to the space

variable. Therefore, the expression for the electrons' current reduces to

$$J_n = D_n q \rho n'.$$

Hence, at $x = -d_p$ we obtain

$$J_n(-d_p) = q\rho\sqrt{\frac{D_n}{\tau_n}}(n(-d_p) - n_p^0)$$

Some care is now needed to rewrite the term $n(-d_p) - n_p^0$ in order to simplify this expression. In particular we would like to factor out the term n_p^0. Indeed, evaluating expression (8.2.6) on both sides of the junction, we obtain

$$\frac{n_p^0}{n_n^0} = \frac{N_{Cp}}{N_{Cn}} \exp \frac{E_{Cp} - E_{Cn}}{k_B\theta}$$

where we have used the fact that the Fermi level is the same at the two side of a junction at equilibrium. We also observe that the difference $E_{Cp} - E_{Cn}$ is proportional to the voltage difference through the junction equilibrium ϕ_{bi} and that $n_n^0 = N_D$. Since the strain in the device is assumed to be constant plus perturbation concentrated in the depletion zone, we can further assume that the specific number of states N_{Cn} and N_{Cp}, though possible different from the unstrained values, are equal at both sides of the junction. Therefore, we deduce

$$N_D = n_n^0 = n_p^0 \exp \frac{q\phi_e}{k_B\theta}$$

so that the electrons' current can be rewritten as

$$J_n(-d_p) = q\rho n_p^0\sqrt{\frac{D_n}{\tau_n}}(e^{\frac{q\phi_e}{k_B\theta}} - 1).$$

We emphasise that this result is independent of the particular profile of the mobility as soon as μ does not vary too much in the depletion zone and that the approximation (8.2.2) holds true. We will check this assumption a posteriori in Section 8.3.

An analogous expression can be deduced for the current of the holes through the junction. Taking into account the usual sign conventions we have

$$J_p(d_n) = q\rho p_n^0\sqrt{\frac{D_p}{\tau_p}}(e^{\frac{q\phi_e}{k_B\theta}} - 1).$$

Therefore, the total current through the biased junction is given by

$$J = J_n + J_p = q\rho\left(n_p^0\sqrt{\frac{D_n}{\tau_n}} + p_n^0\sqrt{\frac{D_p}{\tau_p}}\right)(e^{\frac{q\phi_e}{k_B\theta}} - 1) = J_s(e^{\frac{q\phi_e}{k_B\theta}} - 1). \tag{8.2.7}$$

Here J_s is the so called saturation current and corresponds to the theoretical maximum current density that can flow through a p-n junction under reverse bias and is given by

$$J_s = q\rho\left(n_p^0\sqrt{\frac{D_n}{\tau_n}} + p_n^0\sqrt{\frac{D_p}{\tau_p}}\right).$$

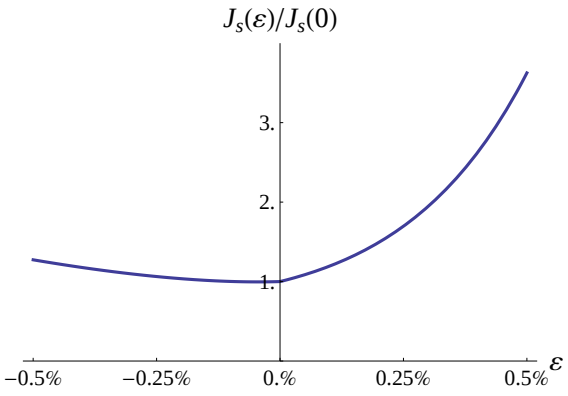


Figure 8.5: The ratio of the normalised saturation current density $J_S(\epsilon)/J_S(0)$ versus the strain ϵ in the case of a p-n junction under uniaxial strain. See text for description.

Relation (8.2.7) is known as Shockley relation. In particular, it follows from the above discussion that it may depend upon strain only through the mobilities (or diffusion coefficients) and through the changes in the equilibrium specific number of minority carriers in the bulk of the semiconductor. These last are given by (8.2.6) and by

$$p^0 = N_V \exp -\frac{E_F - E_V}{k_B \theta}. \tag{8.2.8}$$

Moreover, in order to assess the effects of strain on the characteristic curve of the p-n junction, we should take into account (7.3.7) and (7.3.8) as well as (7.3.9) and (7.3.10). The resulting dependence of J_s on strain in the case of a uniaxial load is depicted in Figure 8.5.

We observe that the effects of enhanced mobilities and reduced band-gap, both contribute to the increase of the saturation current. However, this is more relevant in the case of tension rather than under compression. This prediction of our model is due both to the asymmetric behaviour of the electrons' mobility and to the stronger reduction of the band-gap under traction rather than under compressione. Experimental verification of the model proposed is currently under investigation.

8.3 Maxwell stresses and reverse coupling

In this section we will check a posteriori all the assumptions that let us derive the Shockley relation (8.2.7) for a strained p-n junction. We can evaluate the reverse coupling contribution of electric on mechanical properties introducing the so called Maxwell stresses (see (Kovetz, 2000, Chapter 15). In the case of a linear dielectric and neglecting the contribution of the displacement

current (stationary case), the Maxwell stresses can be written as

$$\boldsymbol{\sigma}_M = \epsilon_0(2\epsilon_r - 1)\mathbf{e} \otimes \mathbf{e} - \frac{\epsilon_0}{2}|\mathbf{e}|^2\mathbf{I}.$$

In order to estimate the order of magnitude of these stresses and compare them to the usual loads experienced by real thin film devices, we have to derive an estimate for the maximum value of the electric field $\mathbf{e}$. However, this can be easily achieved by considering the approximate expression (8.1.1) deduced above. In particular, the maximum electric field at the junction is given by

$$|e|_{\max} = \frac{q\rho N_A}{\epsilon_0\epsilon_r}d_p = \frac{q\rho N_D}{\epsilon_0\epsilon_r}d_n.$$

We recall that the relative permittivity of silicon is $\epsilon_r = 11.9$. Moreover, for standard doping concentrations, we may assume that ρN_A and ρN_D do not exceed 10^{25} m^{-3}, while the built in potential ϕ_{bi} is approximately equal to 0.7 V. This leads to the following approximations from below for the size of the depletion zone

$$d_n \approx d_p \approx 10^{-8} \text{ m},$$

for the maximum value of the electric field

$$|\mathbf{e}|_{\max} \approx 10^8 \text{ V/m}$$

and for the intensity of Maxwell stresses

$$|\boldsymbol{\sigma}_M|_{\max} \approx 2\epsilon_0\epsilon_r|\mathbf{e}|^2_{\max} \approx 2 \text{ MPa}.$$

Recalling that the Young modulus of silicon is approximately given by

$$E \approx 150 \text{ GPa}$$

the electric field induced strains can be estimated by

$$\epsilon_M \approx 10^{-5}.$$

These are at least a couple of order of magnitude smaller than the usual strains considered for flexible electronic devices (usually up to 1% deformation).

Our assumption that the strain field through a strained p-n junction can be considered uniform plus a small perturbation localised at the interface is therefore a posteriori verified. However, we still have to check whether assumption (8.2.1) holds true and if the injected minority carrier concentrations are small with respect to the doping profile (see equation (8.2.5)).

Concerning the concentrations of injected minority carriers, from equation (8.2.4) we have

$$\rho n(-d_p) \approx 10^{13} \text{ m}^{-3}.$$

Moreover, an analogous estimate also holds for the injected holes on the n-side of the junction. These values are much smaller than the typical concentrations of dopants in the current silicon based technology, which usually range in the interval $10^{19} \div 10^{25}$ m^{-3}. Therefore, also assumption (8.2.1) is verified a posteriori

Finally, we have to consider the relative sizes of the drift and diffusion current densities. We recall that the typical values for the mobilities of carriers in silicon range in the interval $0.5 \div 5 \times 10^{-1}$ m^2/V s. Therefore, considering the electrons concentration at the middle of the junction given by (8.2.3) ($n \approx 10^{18}$), we have

$$J_{\text{drift}} \approx 10^6 \text{ A/m}^2.$$

Moreover, by construction, the diffusion current has a similar order of magnitude. On the other hand, recalling that the typical life-time for carriers in silicon is $\tau_n \approx 10^{-3}$ s, the current densities as given by equation (8.2.7) can be estimated as

$$J \approx 10^{-6} \text{ A/m}^2.$$

Again, the a priori assumption (8.2.1) seems to be widely confirmed a posteriori.

Therefore, we conclude that the reverse coupling effects of the electronic properties on the mechanical deformations in a semiconductor can be neglected at first approximation. However, an energetic framework seems necessary in order to assess the thermodynamical consistency of the models considered in this chapter and in the previous one. This would also lead to a firmer justification of the computations proposed in this section. Such a development will be the focus of further investigation (see Bosia et al.).

Bibliography

Bosia, S., Constantinescu, A., Jabbour, M., & Triantafyllidis, N. On the modelling of strained semiconductors. in preparation.

Jäger, R. (2002). *Introduction to Microelectronic Fabrication.* Modular Series on Solid State Deviced, Vol 5. Prentice Hall PTR.

Kovetz, A. (2000). *Electromagnetic Theory.* Oxford Lecture Series in Mathematics and Its Applications. Clarendon Press.

Lifshitz, E. M., Pitaevskii, L. P., & Landau, L. D. (1981). *Physical kinetics*, volume 60. Pergamon press Oxford.

Markowich, P. A., Ringhofer, C. A., & Schmeiser, C. (1990). *Semiconductor equations*. Springer-Verlag.

Sapoval, B. & Hermann, C. (1990). *Physique des Semi-conducteurs*. Ellipses.

Shockley, W. (1949). The theory of p-n junctions in semiconductors and p-n junction transistors. *Bell System Technical Journal*, 28(3):435–489.

Shockley, W. et al. (1963). *Electrons and holes in semiconductors*, volume 1. van Nostrand.

Sun, Y., Thompson, S., & Nishida, T. (2007). Physics of strain effects in semiconductors and metal-oxide-semiconductor field-effect transistors. *Journal of applied physics*, 101(10):104503–104503.

Part III

High cycle fatigue in alloys

Summary

In the third part of this manuscript is dedicated to a possible dynamical system approach to the estimate of the time to failure in alloys subjected to periodic loading. The proposed model, though introducing some additional flexibility with respect to the existing literature, is still amenable to explicit analytical study.

From the point of view of applications, the model considered conjugates both a greater flexibility in accommodating experimental data with only a small overhead in computing time when compared to similar explicit methods known in the literature.

Notation used in Part III

$\mathbf{A}$	localisation tensor (number)	p.232
$\mathbf{b}$	mesoscopic kinematical hardening vector (Pa)	p.233
$\mathbf{C}$	macroscopic elasticity tensor (Pa)	p.231
$\mathbf{c}$	mesoscopic elasticity tensor (Pa)	p.231
c	kinematic hardening parameter (number)	p.235
$\mathbf{E}$	macroscopic strain tensor (number)	p.231
$\mathbf{E}^p$	macroscopic plastic strain tensor (number)	p.231
f_{-1}	fatigue limit under fully reversed tension compression (pascal)	p.244
$\mathbf{L}$	macroscopic compliance tensor (Pa^{-1})	p.231
$\mathbf{l}$	mesoscopic compliance tensor (Pa^{-1})	p.231
$\mathbf{m}$	slip direction (number)	p.233
$\mathbf{n}$	normal versor to the slip plane (number)	p.233
p	mesoscopic hydrostatic stress (pascal)	p.234
$S^H_{\max}$	maximal hydrostatic stress during one loading cycle (pascal)	p.243
$\mathbf{T}$	maximal hydrostatic stress during one loading cycle (pascal)	p.233
ΔT	amplitude of the macroscopic resolved shear stress (pascal)	p.237
ΔT_0	limit amplitude of the macroscopic resolved shear on the critical plane (pascal)	p.235
T_a	amplitude of the mesoscopic resolved shear stress (pascal)	p.244
t_{-1}	fatigue limit under fully reversed torsion (pascal)	p.244
Γ	cumulated plastic mesostrain (number)	p.232
$\widetilde{\Gamma}$	failure limit for the cumulated plastic mesostrain (number)	p.232
$\boldsymbol{\gamma}^p$	mesoscopic shear plastic strain vector (number)	p.235

$\boldsymbol{\epsilon}$	mesoscopic strain tensor (number)	p.231
$\boldsymbol{\epsilon}^p$	mesoscopic plastic tensor (number)	p.231
$\boldsymbol{\epsilon}^p_d$	deviatoric part of the mesoscopic plastic strain tensor (number)	p.234
$\boldsymbol{\epsilon}^{pc}$	cumulated mesoscopic plastic strain tensor (number)	p.234
λ	Lamé first parameter (Pa)	p.233
μ	shear modulus (Pa)	p.233
$\boldsymbol{\Sigma}$	macroscopic stress tensor (Pa)	p.231
$\boldsymbol{\sigma}$	mesoscopic stress tensor (Pa)	p.231
σ^m_{xx}	mean normal stress in the x direction (Pa)	p.244
σ^a_{xx}	amplitude of the normal stress in the x direction (Pa)	p.244
$\boldsymbol{\tau}$	mesoscopic resolved shear stress vector (Pa)	p.233
τ_y	shear yield limit of a crystal (Pa)	p.233
τ^a_{xy}	amplitude of xy shear component of stress tensor (Pa)	p.244

CHAPTER 9

Fast time-scale average for a mesoscopic high cycle fatigue criterion

Outline

This chapter discusses the lifetime prediction of structures in high-cycle fatigue based on the two-scale fatigue criteria of Dang Van type and several of its extensions in finite lifetime regime. The main assumptions for this criteria are (i) the material is polycrystalline and undergoes localised plasticity in one of the misoriented grains and (ii) crack initiation arises as a consequence of cumulated plasticity in this grain.

The model proposed has two distinguishing features. On the one hand a generalisation of mesoscopic plasticity model is presented, on the other a fast time scale average is introduced for tracking the cyclic material behaviour and the subsequent evolution of damage. The tracking method is based on the split between a quick quasi-periodic response of the system to the cyclic load and a slow evolution of the internal hardening and damage parameters of the material at the mesoscopic scale. Moreover, a comparison between predicted and experimental lifetimes is presented. The results are discussed in terms of prediction capabilities and also in terms of the identification procedure of parameters of the mesoscopic model.

A class of fatigue prediction models for the cyclic behaviour of structures is based on multiscale analysis. These try to bridge the gap between the fine evolution of the defects at the scale of the microstructure and the load transmitted from the macroscopic scale of the structure. The analysis usually involves homogenisation techniques for the smaller scales and is based on the concept of shakedown. This amounts to characterising the cyclic behaviour through an asymptotic limit cycle, which is either plastic or elastic denoting

respectively presence or absence of dissipation.

This chapter addresses the question of finite lifetime in the *high cycle fatigue* (HCF) regime for metallic polycristalline materials. Within HCF, it is common to assume that the structure is in elastic shakedown at the macroscospic scale but undergoes elastic or plastic shakedown at the mesoscale (i.e. scale of the grains) for infinite or finite lifetime respectively. In the case of finite lifetime, we will refer to the time to failure of the material with the expression *lifetime*.

In this general framework, the fatigue criterion proposed by Dang Van (DVK) in Dang-Van (1993) (and extended in Papadopoulos (1987, 1993, 1995); Papadopoulos et al. (1997); Papadopoulos (1998)) has been highly successful in predicting failure or endurance of structures. The DVK fatigue criterion decides whether or not the structure will have an infinite lifetime by considering the shakedown limit of the slip system in the different grains. This approach was expressed later in a more general term through the Melan-Koiter shakedown theorem (see Dang Van (1999); Nguyen (2003) and references therein). The hydrostatic stress is considered in order to account for the local heterogenous structure. This has only recently been justified using a precise homogenisation procedure Monchiet et al. (2006); Charkaluk et al. (2002).

In order to give quantitative estimates of the lifetime, several extensions of the DVK criterion have been proposed. Among others we recall the models of Morel Morel (1998, 2000) and of Maitournam et al. Jabbado (2006); Maitournam et al. (2011). In the first case, a simple mesoscopic plastic model is introduced. The evolution of the cumulated plastic strain up to final failure at the mesoscopic level is evaluated to effectively predict lifetime under cyclic and variable loading. The second model differs from this approach by (i) proposing a mesoscopic plastic model depending on the hydrostatic stress component to account for the damage process; (ii) estimating the plastic shakedown cycle at the mesoscopic scale using a classical fatigue criterion based on the range of plastic strain.

The extension discussed in this chapter is constructed under similar assumptions to those of Morel's model Morel (1998, 2000). However, it is grounded on a generalisation of the mesoscopic plasticity model and introduces a new fast time scale average for tracking the cyclic material behaviour and the subsequent evolution of damage. This separation of time scales is justified by the great number of cycles usually considered in HCF experiments (10^4–10^7 cycles). The cyclic material behaviour can be viewed as the succession of (a) a short hardening (or softening) transient up to a saturation point, (b) a long phase close to a stable cycle and (c) a final brief softening leading to failure. The long transient observed in the second phase above can be described through the theory of dynamical systems as the presence of a saddle-node ghost (see Strogatz (1994) and references therein) and is therefore amenable to precise analytical study.

The chapter starts with a short presentation of the two scale model used in the HCF theory.

We then introduce three different constitutive laws and the relative techniques to compute lifetimes. In particular we discuss: (i) Maitournam's et al., (ii) Morel's and (iii) the present model. Sections 2 and 3 discuss the main analytical tools from dynamical systems theory, namely separation of time-scales and saddle-node ghost estimates. In Section 4 the identification method for the parameters of the model is detailed. Finally Sections 5 and 6 present the prediction capabilities for experiments extracted from literature and conclusions. An appendix completes the presentation with an extended computation of the lifetime using the saddle-node ghost estimates.

9.1 The models at the mesoscopic scale

In the framework of HCF for metallic polycristalline materials, one can assume that only a few grains of the material undergo plastic deformations whilst most of the material remains elastic. We can therefore consider the material point at the macroscopic scale as a representative elementary volume (REV) at the mesoscopic scale. This volume is a non-homogeneous medium, which can be assimilated under the given assumptions to an elastic matrix and an elasto-plastic inclusion (grain).

The loading of the REV, i.e. macroscopic stresses $\mathbf{\Sigma}$ and strains $\mathbf{E}$, can be computed in the framework of the standard continuum theory (macroscale) and will be considered as given here. In order to evaluate the mesoscopic state, i.e. mesoscopic stresses $\boldsymbol{\sigma}$ and strains $\boldsymbol{\epsilon}$, several homogenisation techniques have been considered in the literature. The models of Bui, Lin-Taylor, Kröner-Budansky-Wu and Sachs have been described in relation with the DVK fatigue criterion for example in Cano et al. (2004); Dang Van (1999); Jabbado (2006); Maitournam et al. (2011).

Without restraining the generality, we shall adopt here the Lin-Taylor homogenisation scheme, which is based on the equality of macroscopic and mesoscopic strain:

$$\boldsymbol{\epsilon} = \mathbf{E}.$$

As pointed out by Dang Van (see Dang Van (1971, 1999) and references therein), when dealing with the description of HCF, Lin-Taylor's approximation is particularly effective as it permits to accept the existence of mesoscopic plastic strain and residual stress fields. Therefore, we will limit the presentation to this particular case.

Let us denote by $\mathbf{C}$ and $\mathbf{c}$ the macroscopic and mesoscopic elasticity tensor, and by $\mathbf{L}$ and $\mathbf{l}$ the macroscopic and mesoscopic compliance tensors. For completeness reasons we also introduce both the mesoscopic plastic strain tensor $\boldsymbol{\epsilon}^p$ and the macroscopic plastic strain tensor $\mathbf{E}^p$. However, as in HCF the structure is in elastic shakedown at the macroscopic level, it follows that

$$\mathbf{E}^p = \mathbf{0}.$$

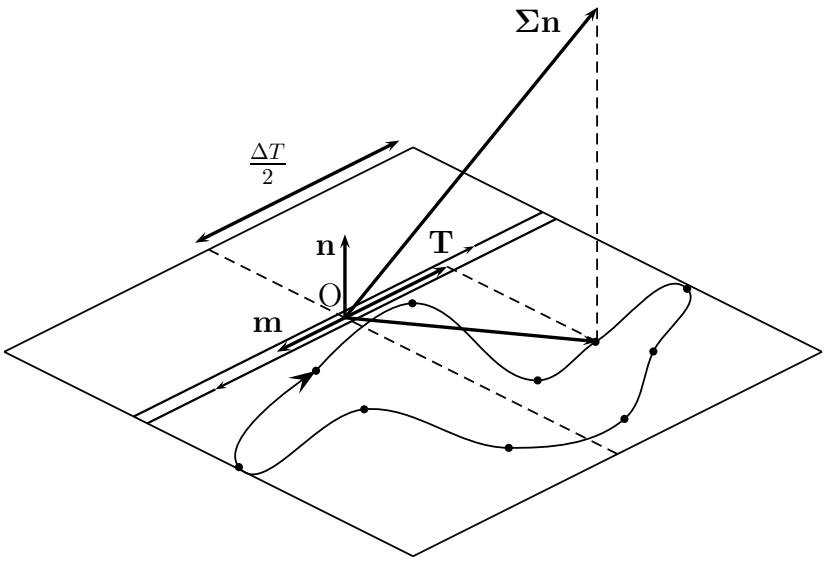


Figure 9.1: Path of the macroscopic shear stress on the material plane identified by $\mathbf{n}$ at the point O and the corresponding path of the macroscopic resolved shear stress $\mathbf{T}$ acting on a glide direction.

With this notation the main assumptions of Lin-Taylor model are equality of macroscopic and mesoscopic elasticity tensors and equality of the respective strains:

$$\mathbf{C} = \mathfrak{c} \qquad \mathbf{E} = \boldsymbol{\epsilon}.$$

Assuming that the behaviour at the macroscopic scale is purely elastic, from the expressions of the elastic Hooke's law at the macroscopic and mesoscopic scale we deduce

$$\boldsymbol{\sigma} = \mathbf{A}\boldsymbol{\Sigma} - \mathbf{AC}(\boldsymbol{\epsilon}^p - \mathbf{E}^p) \tag{9.1.1}$$

where the fourth-order tensor $\mathbf{A}$ is the localisation tensor defined by

$$\mathbf{A} \doteq \mathbf{c} : \mathbf{L}.$$

The next step in the modelling is the introduction of a suitable material behaviour at the mesoscopic scale in order to take into account fatigue. The experimental evidence leads to consider a three-phase model involving an initial hardening (or softening) phase, followed by a stable saturation phase and a final softening Morel and Petit (1996); Morel (1998, 2000) as schematically displayed in Figure 9.2. Under these assumptions, failure corresponds to vanishing mesoscopic yield limit. As the yield limit is directly related to the cumulated plastic mesostrain, denoted by Γ hereafter (see equation (9.1.8) below), one can also express failure as limit of cumulated

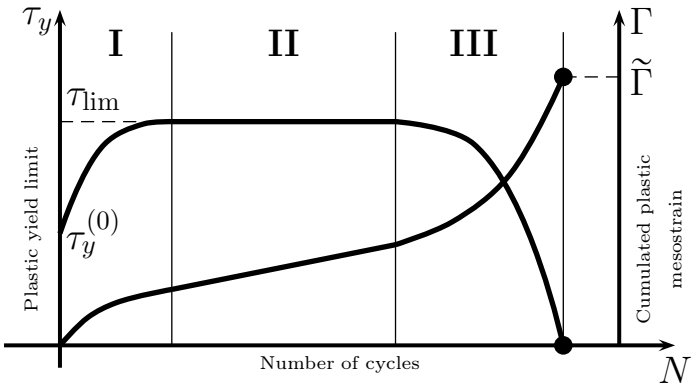


Figure 9.2: Scheme for the evolution of the yield limit (continuous line) and of the damage (cumulated plastic mesostrain—dashed line) in function of the number of cycles. The material behavior involves a hardening phase (I), a saturation phase (II) and a final softening (III). Recall that under periodic loading, number of cycles and time are equivalent up to a constant factor.

plastic mesostrain $\widetilde{\Gamma}$:

$$\Gamma = \widetilde{\Gamma}.$$

We recall that cumulated plastic mesostrain is a monotonic increasing function of the number of loading cycles the system has endured and that the plastic models considered here are rate independent. Therefore, it can be appropriately chosen as an independent variable to represent the evolution of the yield limit instead of time or of number of cycles. This approach will be followed in the present formulation (see also Figure 9.3 later on).

Assuming further that only one glide plane is active for any plastically deforming inclusion of the medium (grain), it has been shown in Papadopoulos (1993) that relation (9.1.1) for a perfectly elastic matrix can be reduced to

$$\boldsymbol{\tau} = \mathbf{T} - \mu\gamma^p\mathbf{m} \tag{9.1.2}$$

where $\mathbf{T}$ and $\boldsymbol{\tau}$ are the macroscopic and mesoscopic resolved shear stresses acting along the slip direction $\mathbf{m}$ of the plane identified by its normal $\mathbf{n}$ and μ is the shear modulus of the λ, μ Lamè constants Constantinescu and Korsunsky (2007); Germain (1962). Explicitly the later are defined by:

$$\mathbf{T} = (\mathbf{m}\otimes\mathbf{n} : \boldsymbol{\Sigma})\mathbf{m}$$
$$\boldsymbol{\tau} = (\mathbf{m}\otimes\mathbf{n} : \boldsymbol{\sigma})\mathbf{m}.$$

Denoting by $\mathbf{b}$ the mesoscopic kinematical hardening vector and by τ_y the shear limit of a crystal, the mesoscopic plastic model is now determined by defining:

- the yield function $f(\boldsymbol{\tau}, \mathbf{b}, \tau_y)$

- the hardening rule, assumed to be in the general form

$$\dot{\tau_y} = g(\Gamma)\dot{\Gamma} \tag{9.1.3}$$

which implies by integration that

$$\tau_y = G(\Gamma) \tag{9.1.4}$$

where G is a suitable primitive function of g.

If this plastic model is brought into the three-phase description of cyclic material behaviour previously introduced, one has to require G to be a concave function increasing when Γ is small and decreasing for larger values of the mesoscopic shear plastic strain. Moreover there will be a unique value for the cumulated plastic mesostrain denoted by $\widetilde{\Gamma}$ for which the following hold:

$$G(\widetilde{\Gamma}) = 0, \qquad G(\widetilde{\Gamma})' < 0. \tag{9.1.5}$$

In this terms, the *lifetime* defined as the failure of the REV, or equivalently as the initiation of a macroscopic crack is defined as the unique time instant $\widetilde{t}$ for which

$$\Gamma(\widetilde{t}) = \widetilde{\Gamma}.$$

As a consequence of the definition of $\widetilde{\Gamma}$, one can equally express the lifetime by a vanishing plastic yield at the mesoscale (see (9.1.4)).

A large panel of choice for the definition of the yield function f and for the evolution of the yield limit τ_y is possible. Among the different models proposed in the literature, we shall only recall the proposals of Maitournam et al. and the one of Morel.

Maitournam's model Maitournam et al. (2011)

The proposal of this model is to consider a plastic material behaviour at the mesoscale with a dependence of the yield function not only on the deviatoric part of the stress but also on the hydrostatic part. A kinematic hardening under the assumptions of associative plasticity is also considered. The mesoscopic yield function can therefore be written as

$$f(\boldsymbol{\sigma}, \boldsymbol{\epsilon}_d^p, p) \doteq \sqrt{\frac{1}{2}(\boldsymbol{\sigma} - h\boldsymbol{\epsilon}_d^p) : (\boldsymbol{\sigma} - h\boldsymbol{\epsilon}_d^p)} - k(p)$$

with

$$k(p) = \beta - \alpha p(t) \qquad \text{or} \qquad k(p) = \begin{cases} \beta - \alpha p & \text{if } p \geqslant 0 \\ \beta - \gamma p & \text{if } p < 0 \end{cases}$$

and where p is the mesoscopic hydrostatic stress, $\boldsymbol{\epsilon}_d^p$ is the deviatoric part of the mesoscopic plastic strain tensor and α, β, γ and h are suitable parameters.

The underlying hypothesis of this model consider that the mesostructure can be computed from the macroscopic structure. Fatigue will then be determined from the plastic shakedown cycle and from a phenomenological fatigue law linking lifetime and cumulated mesoscopic plastic strain $\boldsymbol{\epsilon}^{pc}$:

$$N = g(\boldsymbol{\epsilon}^{pc}).$$

which is a Manson-Coffin type fatigue criterion.

Morel's model Morel (1998), Morel (2000)

This model considers a complete description for the mesoscopic plastic yield limit as introduced above. Three sharply separated phases account for the hardening of the mesoscopic inclusion. The dependence of the yield limit on plastic strain is piece-wise linear (see Figure 9.3). Moreover, the yield function is defined in terms of the resolved shear stress and has both isotropic and kinematic hardening terms:

$$f(\boldsymbol{\tau}, \mathbf{b}, \tau_y) = (\boldsymbol{\tau} - \mathbf{b}) \cdot (\boldsymbol{\tau} - \mathbf{b}) - \tau_y^2. \tag{9.1.6}$$

In this case, the three phase of the plastic inclusion are defined as:

$$\dot{\tau_y} = \begin{cases} g\dot{\Gamma} & \text{during hardening;} \\ 0 & \text{during the saturation phase;} \\ -h\dot{\Gamma} & \text{during softening;} \end{cases} \tag{9.1.7}$$

$$\dot{\mathbf{b}} = c\dot{\boldsymbol{\gamma}}^p$$

where $\boldsymbol{\gamma}^p$ is the mesoscopic shear plastic strain, c is the kinematic hardening parameter and Γ is the cumulated plastic mesostrain given by

$$\dot{\Gamma} \doteq \sqrt{\dot{\boldsymbol{\gamma}}^p \cdot \dot{\boldsymbol{\gamma}}^p}. \tag{9.1.8}$$

Power law model

The model proposed here replaces the piecewise-linear dependence in the evolution of the yield limit with a power law. When compared with the model of Morel, one immediately notices the advantages arising from the piecewise-linear description. Indeed, in this latter case, for periodic macroscopic loadings it is possible to obtain explicitly the lifetime (see Morel (1998)). However, the hardening rule (9.1.7) is a rough approximation of the actual behaviour of materials, for which the sharp transitions between hardening and saturation regimes as well as from saturation to softening regimes are difficult to justify.

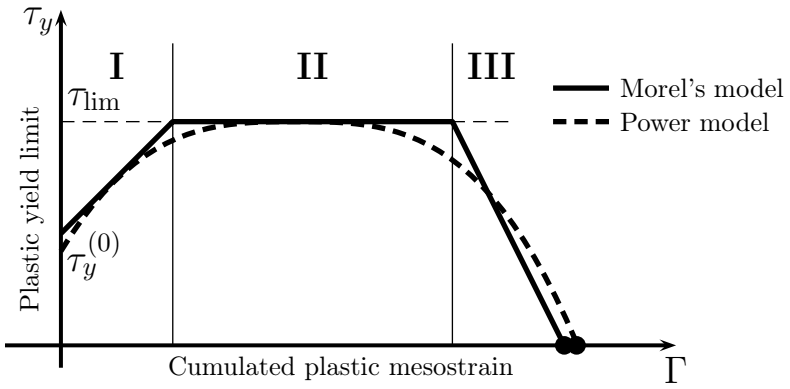


Figure 9.3: The three-phase evolution of the plastic yield limit. Comparison between the piecewise linear model (Morel—continuous line) and the power model (dashed line).

An alternative model is given by the following constitutive power law

$$G(\Gamma) \doteq \frac{\Delta T_0}{2} - \frac{|\Gamma - \Gamma_0|^\alpha}{\beta} \tag{9.1.9}$$

with $\alpha > 1$, which naturally satisfies the constraints of concavity and monotonicity introduced above (see Figure 9.3). Th term ΔT_0 appearing in the last relation is the amplitude of the macroscopic resolved shear stress on the critical plane for limit loading.

When compared with the piecewise linear model of Morel, one cannot hope to retrieve exact lifetime estimates for this model. However, as we shall see below, precise a-priori analytical estimates can be derived in this setting under mild regularity assumption on the behaviour of the function G, which are satisfied by the power law (9.1.9). Before delving into the details of such estimates, we will derive a suitable approximation for the just introduced constitutive laws in the case of periodic loadings. In particular we now want to consider a time-average over each cycle of the loading.

9.2 Separation of time scales

In the regime of HCF we can distinguish between a quick quasi-periodic response of the system to the cyclic charge and a slow evolution of the inner parameter describing the hardening and damage of the material itself. This separation of time scales is justified by the great number of cycles usually considered in HCF experiments ($10^4 - 10^7$ cycles). It seems therefore sound to look for a slowly-varying approximation for this internal variable and for the cumulated plastic mesostrain Γ, by averaging out the periodic behaviour of the system. This process is also known as "time-homogenization" (see Bender and Orszag (1999); Guckenheimer and Holmes (1990)).

By differentiating the yield function (9.1.6) with respect to time we obtain:

$$\dot{f} = 2(\boldsymbol{\tau} - \mathbf{b}) \cdot \dot{\boldsymbol{\tau}} + 2(\mathbf{b} - \boldsymbol{\tau}) \cdot \dot{\mathbf{b}} - 2\tau_y \dot{\tau_y}.$$

Since during plastic deformations the yield function f is constant ($f \equiv 0$), by recalling relation (9.1.2), we deduce

$$\dot{T} - \mu\dot{\gamma^p} - c\dot{\gamma^p} = g(\Gamma)\dot{\Gamma}$$

where we have set

$$\boldsymbol{\gamma}^p = \gamma^p \mathbf{m}.$$

From definition (9.1.8) we have

$$\dot{\Gamma} = |\dot{\gamma^p}|$$

and therefore

$$\dot{\Gamma} = \frac{|\dot{T}|}{g(\Gamma) + c + \mu},$$

which represents the evolution law for the cumulated plastic mesostrain during plastic deformations. Obviously Γ is constant during the elastic part of the loading so that we can deduce the following ordinary differential equation describing the evolution of the cumulated plastic mesostrain

$$\dot{\Gamma} = \begin{cases} \frac{|\dot{T}|}{g(\Gamma)+c+\mu} & \text{when } f = 0, \\ 0 & \text{when } f < 0. \end{cases} \tag{9.2.1}$$

We recall that the cumulated plastic mesostrain Γ is a nondecreasing function of time also if the resolved plastic mesostrain γ^p oscillates. Indeed, Γ accounts for all the plastic deformations the material has endured up to the current time.

We now want to simplify the evolution law (9.2.1) in the special case of cyclic loadings. By the above discussion it is easy to see that under a periodic loading of equivalent amplitude comparable to ΔT_0, the plastic mesostrain changes only slightly during one charge/discharge cycle. Therefore, the increase per cycle of the cumulated plastic mesostrain is small when compared with the variation of the mesoscopic strain. This justify us stating that the evolution of cumulated plastic strain is slow with respect to the evolution of the mesoscopic strain. As a consequence, we can assume that Γ constant during each cycle.

By considering Γ as constant during one period of the forcing term, we can decouple the quick dynamic of the elasto-plastic response of the material to the external loading and the slow evolution of the internal damaging mechanism (i.e. the slow drift of Γ). We denote by ΔT the amplitude of the macroscopic resolved shear stress. In order to integrate (9.2.1) on a single cycle, we observe that during a complete unloading-loading phase from $-\Delta T/2$ to $\Delta T/2$, the mesoscopic

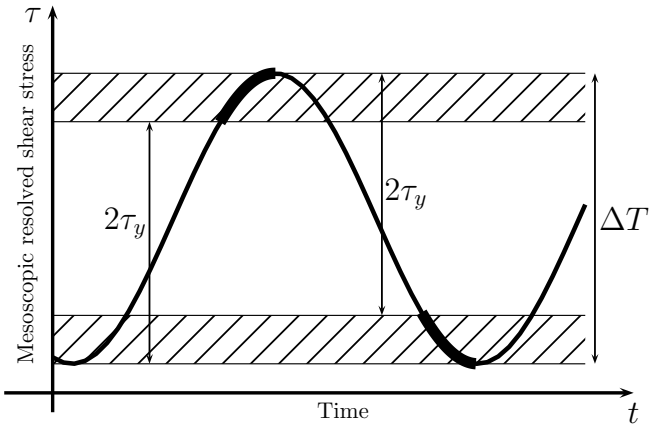


Figure 9.4: Illustration of the relation between the periodic resolved plastic shear stress and the evolution of the cumulated plastic mesostrain. Notice that only the heavily thickened part of the loading cycle contributes to plastic deformations. The amplitude of the hatched regions has been emphasise for clarity of expositions.

inclusion will be in elastic regime ($f < 0$) up to $T = -\Delta T/2 + 2\tau_y$. therefore, we obtain (see Figure 9.4 and (Morel, 2000, Appendix A))

$$\int_{f=0} \dot{T} = \frac{\Delta T}{2} - \left(-\frac{\Delta T}{2} + 2\tau_y\right) = \Delta T - 2\tau_y.$$

By taking into account the second half of the loading cycle (i.e. the transition of T from $\Delta T/2$ to $-\Delta T/2$), and using this result in (9.2.1) we finally have

$$\Delta_{\text{cycle}}\Gamma = \int_{\text{cycle}} \dot{\Gamma} = \frac{4}{\mu + c + g(\Gamma)} \left(\frac{\Delta T}{2} - \tau_y\right).$$

where $\Delta_{\text{cycle}}\Gamma$ represents the (small) change in Γ during a single complete loading cycle.

The behaviour of the simple system we are studying can therefore be reduced to a system of an ordinary differential equation and a difference equation

$$\begin{cases} \Delta_{\text{cycle}}\Gamma = \frac{4}{\mu+c+g(\Gamma)} \left(\frac{\Delta T}{2} - \tau_y(\Gamma)\right) \\ \dot{\tau_y} = g(\Gamma)\dot{\Gamma}. \end{cases}$$

If we consider an adimensionalized time period equal to 1 for the cycle forcing term $\Delta_{\text{cycle}}t = 1$ (i.e. if we measure time by the number of cycles of the periodic loading the system has undergone), we can average the evolution equation for the cumulated plastic mesostrain getting the following ordinary differential equation system

$$\begin{cases} \dot{\Gamma} \approx \frac{\Delta_{\text{cycle}}\Gamma}{\Delta_{\text{cycle}}t} = \frac{4}{\mu+c+g(\Gamma)} \left(\frac{\Delta T}{2} - \tau_y(\Gamma)\right) \\ \dot{\tau_y} = g(\Gamma)\dot{\Gamma}. \end{cases}$$

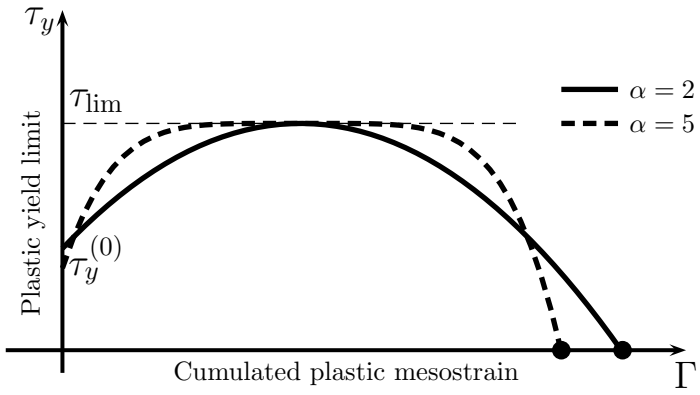


Figure 9.5: The dependence of the mesoscopic hardening law on the the "flatness" parameter α. Note that for larger αs (dashed line) the plateau is longer.

Recalling the integral relation (9.1.4) for the shear limit τ_y, we finally get the following ordinary differential equation describing the evolution of our medium

$$\dot{\Gamma} = \frac{4}{\mu + c + g(\Gamma)} \left(\frac{\Delta T}{2} - G(\Gamma) \right). \tag{9.2.2}$$

We recall that the proposed power law model for mesoscopic hardening is determined by 5 parameters. As we will discuss later, of these ΔT_0 can be directly identified by knowing the characteristic of the loading. Of the remaining parameters, α has a clear physical significance representing the "flatness" of the hardening law (see Figure 9.5). This parameter with the other remaining three, namely Γ_0, β and the sum $\mu + c$ will be identified through a fitting procedure.

9.3 Lifetime estimates in HCF

In the discussion of the previous section no explicit reference to the analytic form of the constitutive relation $G(\Gamma)$ has been made. We now want to particularize the above results by choosing as constitutive hardening relation the power model (9.1.9) introduced above.

In this case, equation (9.2.2) exhibits a threshold behaviour controlled by the value of ΔT. If $\frac{\Delta T}{2}$ is smaller than $\frac{\Delta T_0}{2}$ (i.e. if it is smaller than the maximum value attained by $G(\Gamma)$), then the system will undergo elastic shakedown and be in an infinite endurance regime. If, otherwise, $\frac{\Delta T}{2}$ is above this value, then the material will eventually fail (i.e. $G(\Gamma) \to 0$).

Due to the hypothesis of concavity and regularity on $G(\Gamma)$, for values of ΔT near the threshold value, the system will show a very long transient regime, which is proceeded and followed by two phases of faster evolution. The time span of this transient regime will constitute the fundamental element for our estimate of the lifetime of the material in HCF regime. Incidentally, we observe

that this kind of estimates will essentially be unaffected by changes of the expression of $G(\Gamma)$ far away from its maximal value.

Starting from (9.1.9), we immediately deduce

$$g(\Gamma) = -\frac{\alpha}{\beta}|\Gamma - \Gamma_0|^{\alpha-1}\operatorname{sgn}(\Gamma - \Gamma_0)$$

so that our model (9.2.2) reduces to

$$\begin{cases} \dot{\Gamma} = \frac{4}{\mu+c-\frac{\alpha}{\beta}|\Gamma-\Gamma_0|^{\alpha-1}\operatorname{sgn}(\Gamma-\Gamma_0)}\left(\frac{\Delta T-\Delta T_0}{2} + \frac{|\Gamma-\Gamma_0|^{\alpha}}{\beta}\right) \\ \Gamma(0) = 0. \end{cases} \tag{9.3.1}$$

From the mathematical theory of dynamical systems an explicit lower (i.e. conservative) estimate can be deduced for the lifetime of the material (see Section 9.4):

$$\widetilde{t} \geqslant \frac{\gamma_{\text{opt}}+1}{\gamma_{\text{opt}}}\frac{\pi(\mu+c)}{2\alpha\sin\frac{\pi}{\alpha}}\beta^{\frac{1}{\alpha}}\left(\frac{\Delta T-\Delta T_0}{2}\right)^{\frac{1-\alpha}{\alpha}} - \frac{\alpha}{4(\alpha-1)}\frac{1}{\gamma_{\text{opt}}-1} - \frac{\beta(\mu+c)}{4(\alpha-1)}\Gamma_0^{1-\alpha} \tag{9.3.2}$$

where γ_{opt} is given by

$$\gamma_{\text{opt}} = \frac{\pi\left(\frac{2}{\beta(\Delta T-\Delta T_0)}\right)^{\frac{\alpha-1}{\alpha}} + \sqrt{\pi\frac{\alpha^2}{\beta(\alpha-1)(\mu+c)}\left(\frac{2}{\beta(\Delta T-\Delta T_0)}\right)^{\frac{\alpha-1}{\alpha}}\sin\frac{\pi}{\alpha}}}{\pi\left(\frac{2}{\beta(\Delta T-\Delta T_0)}\right)^{\frac{\alpha-1}{\alpha}} - \frac{\alpha^2}{\beta(\alpha-1)(\mu+c)}\sin\frac{\pi}{\alpha}}. \tag{9.3.3}$$

In order to get some insight in this expression, we can consider its limit for great values of α, that is when the plateau of the saturation phase becomes flat. This corresponds to the setting of Morel's works (see Morel (1998) and Morel (2000)). Indeed, we obtain

$$\lim_{\alpha\to\infty}\gamma_{\text{opt}} = \frac{2+\sqrt{2\frac{\beta(\Delta T-\Delta T_0)}{\mu+c}}}{2-\frac{\Delta T-\Delta T_0}{\mu+c}} \approx 1$$

and

$$\lim_{\alpha\to\infty}\widetilde{t} \geqslant \frac{\gamma_{\text{opt}}+1}{\gamma_{\text{opt}}}\frac{\mu+c}{\Delta T-\Delta T_0} - \frac{1}{4}\frac{1}{\gamma_{\text{opt}}-1} \approx \frac{2(\mu+c)}{\Delta T-\Delta T_0}$$

where the approximations at the end of the previous computations hold for small $\Delta T - \Delta T_0$. This estimate corresponds to (Morel, 2000, Equation (A9)).

Unfortunately, no simple and efficient expression could be derived for an analytical upper bound on the lifetime for our model.

9.4 A priori estimates

In this section we will derive the bound (9.3.2), (9.3.3) for the dynamical system (9.3.1). In order to simplify the notation and focus on the main analytical argument, we will consider the following

equivalent Cauchy problem

$$\begin{cases} \dot{y} = h(y) \doteq \frac{\epsilon + A|y|^\alpha}{1 - B|y|^{\alpha-1}\operatorname{sgn} y} \\ y(0) = y_0. \end{cases} \tag{9.4.1}$$

with $y_0 \leqslant 0$. We observe that all the results of this section can be readily adapted to our original model (9.3.1) by setting:

$$\begin{aligned} \epsilon &= \frac{4}{\mu + c}\frac{\Delta T - \Delta T_0}{2} \\ A &= \frac{4}{\mu + c}\frac{1}{\beta} \\ B &= \frac{1}{\mu + c}\frac{\alpha}{\beta} \\ y_0 &= -\Gamma_0. \end{aligned}$$

We start by rigourously defining the lifetime for our system.

Definition 9.4.1. The *lifetime* for system (9.4.1) is the time $t^{\xi}_{y_0}$ that is necessary for any solution to travel from y_0 to ξ where ξ is the vertical asymptote of h, given by the (unique) real root of

$$1 - B|\xi|^{\alpha-1}\operatorname{sgn}\xi = 0.$$

Before stating the main estimate, we recall an elementary result, which will be very important in the following. (see (Strogatz, 1994, Exercise 4.3.10)).

Theorem 9.4.1. *The time required for a solution of the differential equation*

$$\dot{y} = \epsilon + Ay^\alpha$$

to go from $-\infty$ to $+\infty$ is given by

$$t^{+\infty}_{-\infty} = \frac{\pi}{\frac{\alpha}{2}\sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}}.$$

Consider now equation (9.4.1). In order to estimate the lifetime from below (conservative estimate of the endurance of the material) we will consider the following approximation from above of h:

$$h(y) \leqslant \widetilde{h}(y) \doteq \begin{cases} \epsilon + A|y|^\alpha & \text{if } y \leqslant 0 \\ \gamma(\epsilon + A|y|^\alpha) & \text{if } 0 \leqslant y \leqslant x_1 \\ +\infty & \text{otherwise} \end{cases}$$

where x_1 is defined by:

$$\gamma(\epsilon + A|x_1|^\alpha) = h(x_1), \quad x_1 \in (0, \xi) \qquad \text{i.e} \quad x_1 = \left(\frac{\gamma - 1}{B\gamma}\right)^{\frac{1}{\alpha-1}} \tag{9.4.2}$$

and γ will be determined later. Since solutions of the dynamical system associated to $\widetilde{h}$ travel slower than those of (9.4.1), we immediately deduce that

$$t^{\xi}_{y_0} = t^{0}_{y_0} + t^{x_1}_{0} + t^{\xi}_{x_1} \geqslant \tilde{t}\,{}^{0}_{y_0} + \tilde{t}\,{}^{x_1}_{0}$$

where with $\tilde{t}\,{}^{b}_{a}$ we denote the time required by a solution of the dynamical system

$$\dot{y} = \widetilde{h}(y)$$

to travel from a to b.

We start by estimating $\tilde{t}\,{}^{0}_{y_0}$, always from below. We consider the further approximation

$$\dot{y} = \widetilde{\widetilde{h}}_A(y) \doteq A|y|^{\alpha}. \tag{9.4.3}$$

Reasoning as above, we deduce

$$\tilde{t}\,{}^{0}_{y_0} = \tilde{t}\,{}^{0}_{-\infty} - \tilde{t}\,{}^{y_0}_{-\infty} \geqslant \tilde{t}\,{}^{0}_{-\infty} - \tilde{\tilde{t}}_A\,{}^{y_0}_{-\infty}$$

By symmetry, Theorem 9.4.1 implies

$$\tilde{t}\,{}^{0}_{-\infty} = \frac{\pi}{\alpha \sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}}$$

whereas a direct integration of equation (9.4.3) gives

$$\tilde{\tilde{t}}_A\,{}^{y_0}_{-\infty} = \frac{1}{A}\frac{1}{\alpha-1}|y_0|^{1-\alpha}$$

from which we deduce

$$\tilde{t}\,{}^{0}_{y_0} \geqslant \frac{\pi}{\alpha \sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}} - \frac{1}{A}\frac{1}{\alpha-1}|y_0|^{1-\alpha}.$$

We now consider the lower approximation of the travelling time $\tilde{t}\,{}^{\xi}_{0}$ from 0 to ξ (failure). Arguing as before we deduce:

$$\tilde{t}\,{}^{\xi}_{0} \geqslant \tilde{t}\,{}^{+\infty}_{0} - \tilde{\tilde{t}}_{\gamma A}\,{}^{+\infty}_{x_1} = \frac{\pi}{\alpha\gamma \sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}} - \frac{1}{\gamma A}\frac{1}{\alpha-1} x_1^{1-\alpha}$$

Using the definition of x_1 given above (see (9.4.2)) we finally get

$$\tilde{t}\,{}^{\xi}_{0} \geqslant \frac{\pi}{\alpha\gamma \sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}} - \frac{B}{A(\alpha-1)}\frac{1}{\gamma-1}$$

which is minimised when

$$\gamma = \gamma_{\text{opt}} \doteq \frac{\pi\left(\frac{A}{\epsilon}\right)^{\frac{\alpha-1}{\alpha}} + \sqrt{\pi B \frac{\alpha}{\alpha-1}\left(\frac{A}{\epsilon}\right)^{\frac{\alpha-1}{\alpha}} \sin\frac{\pi}{\alpha}}}{\pi\left(\frac{A}{\epsilon}\right)^{\frac{\alpha-1}{\alpha}} - \frac{\alpha}{\alpha-1} B \sin\frac{\pi}{\alpha}}$$

for ϵ small enough.

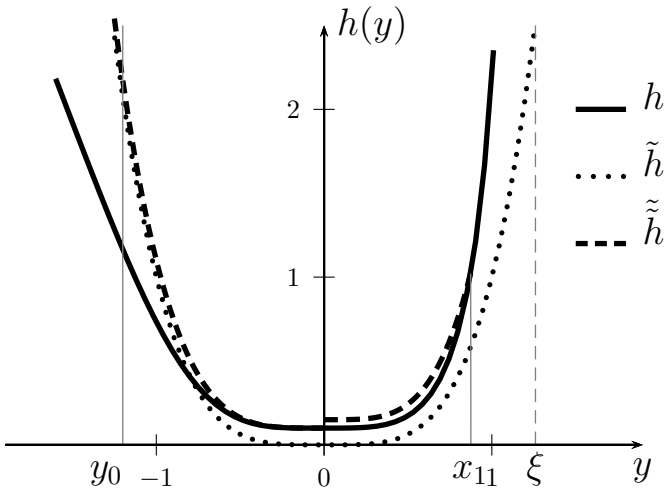


Figure 9.6: The approximations to the function $h(y)$ used in deriving the lower bound on the failure time for system (9.4.1).

Putting all the above results together we finally obtain the following estimate from below to the lifetime of our model:

$$t^{\xi}_{y_0} \geqslant \frac{\gamma_{\text{opt}}+1}{\gamma_{\text{opt}}}\frac{\pi}{\alpha \sin\frac{\pi}{\alpha}} A^{-\frac{1}{\alpha}} \epsilon^{\frac{1-\alpha}{\alpha}} - \frac{B}{A(\alpha-1)}\frac{1}{\gamma_{\text{opt}}-1} - \frac{1}{A}\frac{1}{\alpha-1}|y_0|^{1-\alpha}.$$

After substitution of the values for A, B, ϵ and y_0 arising in our model, we finally deduce the desired estimate on the lifetime.

9.5 Identification of parameters from fatigue experiments

In the constitutive relation (9.1.9) for $G(\Gamma)$ and in equation (9.2.2), five different parameters appear: namely $\mu+c$, ΔT_0, Γ_0, α and β. Moreover, since our model is essentially one-dimensional, ΔT has also to be evaluated starting from each 3D macroscopic loading state of interest.

In order to evaluate ΔT and ΔT_0 we adopt the same approach used by Morel in Morel (1998). Starting from the Dang Van criterion (see Dang Van (1971) and Dang-Van (1993)), we assume that the material undergoes elastic shakedown if

$$\Delta T + A S^H_{\max} \leqslant B,$$

where $S^H_{\max}$ is the maximum value reached by the mesoscopic (and macroscopic) hydrostatic stress

during the periodic loading, while ΔT is a suitable measure of the resolved shear stress acting along the most solicited slip direction plane. In particular, we will use the following definition (see Morel Morel (1998) and Papadopoulos Papadopoulos (1993))

$$\Delta T = \max_{\theta,\phi} T_\sigma(\theta,\phi)$$

where

$$T_\sigma(\theta,\phi) = \sqrt{\int_0^{2\pi} \left(T_a(\theta,\phi,\psi)\right)^2 \, \mathrm{d}\psi}.$$

Here θ and ϕ are angular variables used to identify the plane orthogonal to the versor

$$\mathbf{n} = \begin{pmatrix} \sin\theta\,\cos\phi \\ \sin\theta\,\sin\phi \\ \cos\theta \end{pmatrix},$$

in the physical space, ψ is an angle parametrizing all possible direction $\mathbf{m}$ in the slide plane identified by $\mathbf{n}$ and $T_a(\theta,\phi,\psi)$ is the amplitude of the variation of the mesoscopic resolved shear stress $\boldsymbol{\tau}$ defined above.

The material parameters A and B can be related to the fatigue limits under fully reversed tension compression f_{-1}, and under fully reversed torsion t_{-1}:

$$A = \frac{\sqrt{\pi}\left(t_{-1} - \frac{f_{-1}}{2}\right)}{\frac{f_{-1}}{3}}, \qquad B = \sqrt{\pi}\, t_{-1}.$$

In the simple case of sinusoidal loading, that is for loadings in the form

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma^m_{xx} + \sigma^a_{xx}\sin(\omega t) & \tau^a_{xy}\sin(\omega t+\varphi) & 0 \\ \tau^a_{xy}\sin(\omega t+\varphi) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{9.5.1}$$

for a suitable reference frame, where σ^m_{xx} is the mean normal stress in the x direction, σ^a_{xx} and τ^a_{xy} are the amplitude of the normal and shear stresses, ΔT and ΔT_0 can be explicitly computed and are given by the following expressions:

- In phase tension and torsion ($\varphi = 0°$)

$$\Delta T_0 = \frac{t_{-1}f_{-1} - \left(t_{-1} - \frac{f_{-1}}{2}\right)\sigma^m_{xx}}{f_{-1} + \left(t_{-1} - \frac{f_{-1}}{2}\right)\frac{\sigma^a_{xx}}{\sqrt{\frac{(\sigma^a_{xx})^2}{4} + (\tau^a_{xy})^2}}}$$

$$\Delta T = \frac{t_{-1}f_{-1} - \left(t_{-1} - \frac{f_{-1}}{2}\right)\sigma^m_{xx}}{f_{-1}\left((\sigma^a_{xx})^2 + (\tau^a_{xy})^2\right) + 2\left(t_{-1} - \frac{f_{-1}}{2}\right)(\sigma^a_{xx})^2} \cdot \sqrt{\frac{(\sigma^a_{xx})^2 + (\tau^a_{xy})^2}{2}}\sqrt{(\sigma^a_{xx})^2 + (\tau^a_{xy})^2 + \left|(\sigma^a_{xx})^2 - 3(\tau^a_{xy})^2\right|}$$

- Out of phase tension and torsion ($\varphi = 90^\circ$)

$$\Delta T_0 = \sqrt{\frac{(\sigma^m_{xx})^2}{4} + (\tau^a_{xy})^2}$$
$$\Delta T = \frac{\sqrt{(\sigma^a_{xx})^2 + (\tau^a_{xx})^2}}{2\sqrt{2}\sigma^a_{xx}} \sqrt{(\sigma^a_{xx})^2 + (\tau^a_{xy})^2 + |(\sigma^a_{xx})^2 - 3(\tau^a_{xy})^2|}$$

We now consider the other modelling parameters. We observe that the kinematic hardening parameter c and the Lamè shear modulus μ may in principle be considered material constants already known from other experiments. However, here we will identify them together with the other material constants appearing in (9.1.9) and (9.2.2): Γ_0, α and β. We note, moreover, that μ and c always appear together in the above expressions (in particular, see equation (9.2.2)) so that only a joint estimate of the sum $\mu + c$ can be obtained with this model. The identification of these four remaining parameters will be achieved through optimisation of a suitable cost function (see e.g. Maitournam et al. (2011)). Two choices seem natural in this context:

- minimising the sum of the squared errors between the experimental lifetimes and the simulated ones;

- minimising the sum of the squared relative errors between the experimental lifetimes and the simulated ones.

These two approaches have led to very similar results in the experimental validation of our model of the next sections. Following Maitournam et al. (2011), we will therefore report only the results using the first of the two approaches.

9.6 Results and discussion

In order to assess the efficiency of the estimate for the predicted lifetime obtained above, we compared the numerical solution of system (9.2.2) describing the evolution of the cumulated mesoscopic plastic strain, to the analytical approximation of lifetime given by estimates (9.3.2) and (9.3.3). The complete integration of (9.2.2) was performed using a high-order Runge-Kutta scheme (in particular a Runge Kutta $(4, 5)$ method was used—see (The MathWorks Inc., 2011, routine `ode45`)). We emphasise that the estimate (9.3.2) is a lower bound for the lifetime and therefore it is a theoretical conservative estimate.

On account of the many different tests done, we report in Figure 9.7 the results of some numerical experiments showing a good agreement of approximation (9.3.2) for physically meaningful parameters, when the "flatness" parameter α is large enough. In order to assess the efficiency of

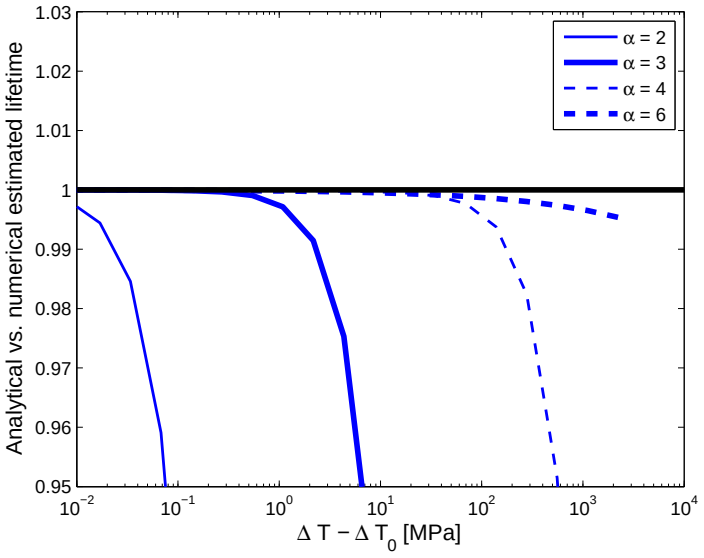


Figure 9.7: The dependence of the efficiency ratio η (ratio between the analytical estimate (9.3.2) and the lifetime obtained by numerical integration of (9.3.1), see text) vs. the load $\Delta T - \Delta T_0$ for different values of the parameter α of the model. See text for description.

the analytical approximation deduced previously, we introduce the following efficiency ratio

$$\eta = \frac{\text{lifetime given by (9.3.2)}}{\text{lifetime obtained by numerical integration of (9.3.1)}}.$$

We observe that values of η near 1 correspond to efficient estimates and that if $\eta < 1$ the analytical bound is conservative. In particular, as soon as α is greater than 4 or 5, the approximation is efficient for all the values of $\Delta T - \Delta T_0$, which arise in experiments and which can be accounted for with this kind of model (usually $\Delta T - \Delta T_0 \approx 10^0 \div 10^3$MPa for metallic materials). In order to keep the discussion as simple as possible, only integer values of α were considered here. However, α can be any real number greater than 1.

In Figure 9.7 the behaviour of η with respect to the load $\Delta T - \Delta T_0$ is shown. The different lines correspond to the representative values for α, $\alpha = 2, 3, 4$ and 6. All other parameters are physically relevant and have been kept constant to ease comparison. In particular we have considered $\Gamma_0 = 66$, $\mu + c = 2800000$MPa, $\beta = 70000\text{MPa}^{-1}$ $\Delta T_0 = 445$MPa. The horizontal line at height 1 represents a perfect estimate. As expected, the analytical estimate derived above is confirmed to be conservative.

We have finally checked the effectiveness of our model in fitting experimental results and in predicting failure. To this end, we use some of the experimental data which can be found in the literature (see Dubar et al. (1992); Jabbado (2006); Lee (1985); Morel and Petit (1996);

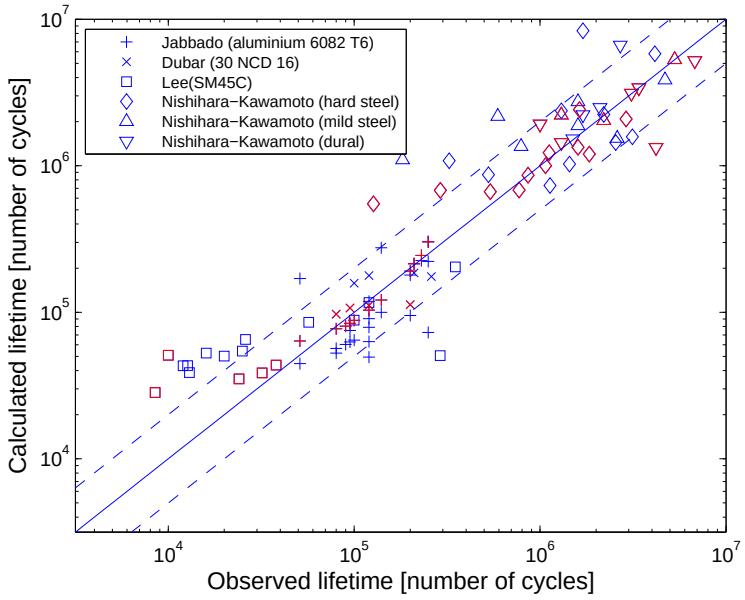


Figure 9.8: The computed versus observed lifetimes from different fatigue tests. The data used to fit the model for each material are highlighted in red (training points) while the other observations used to check the validity of the approximation are in blue (control points).

Nishihara and Kawamoto (1945)). In each case, we have used the data coming from simple tension compression tests (called training points in the sequel) to fit the parameters of the model and to make predictions for the other observations. The results of these experiments (predicted endurance limit vs. experimental values) can be found in Figure 9.8. Data used to fit the model (training points) are highlighted in red, while the remaining observation used to check the model (control points) are in blue. In this plot the diagonal represents perfect agreement between the model and the experimental values, whereas the two dashed limes represent a factor 2 acceptable tolerance.

As can be seen from Figure 9.8, the agreement between estimated and observed lifetimes is quite satisfactory. Most of the experimental points fall between the two dashed tolerance lines for a wide range of the experimental parameters and a variety of materials considered. Scatter of experimental data up to 3-5 times that of the fatigue curve is indeed typical of HCF, which is due to individual properties of the material local zones. That is why, scatter of data presented in Figure 9.8 can be considered as regular if individual properties of the specimen are not taken into account.

9.7 Conclusions

We have proposed a new model for the lifetime of materials in the HCF regime. This model is a refinement of the one introduced by Morel in Morel (2000) based on the DVK criterion. In oarticular, it provides a more thorough understanding of the basic phenomena and gives an explanation of the long transient behaviour observed in material between the initial accomodation and the final breakdown (or crack initialisation).

Our approach allows us to consider a richer mesoscopic hardening rule than already done in the literature. As in Morel (1998, 2000) our model involves an initial hardening, a long saturation phase and a final softening leading to failure. The nonlinear power law proposed depends on 5 different parameters. The a priori analysis and the numerical tests reveal that the most relavant among the parameters is α, which describes the "flatness" of the hardening law. Moreover, α is directly related to the lifetime estimate (9.3.2). All the parameters of the mesoscopic model can be estimated using a simple and efficient least-square optimisation procedure. Nevertheless, study of the relations between more refined microscopic models and the parameters should be performed in the future.

The additional detail of description introduced has only a minor impact on the computational cost of the model. Indeed, when studying crack initiation problems, the main computational tasks are related to the solution of stresses and strains on the whole structure of interest. Therefore, any algebraic criterion for failure detection (in opposition to more complex local relations) is practically equivalent from the point of view of computational costs.

The lifetime estimates obtained account well for the experiments. The residual unpredicted variability is consistent with the usual scattering of HCF experimental data.

The main advantage of the proposed method based on dynamical systems techniques is the possibility of extending it to a large class of local material behaviour involving not only plasticity, but also crack and damage evolution, while keeping a simple closed-form formula for the prediction of the lifetime.

Finally we note that the extension of this approach to more complex periodic and quasi-periodic multiaxial loadings and to a larger base of materials constitute interesting fields of research, which are relevant for applications and which remain still largely unexplored.

Bibliography

Bender, C. M. & Orszag, S. A. (1999). *Advanced mathematical methods for scientists and engineers. I.* Springer-Verlag. Asymptotic methods and perturbation theory, Reprint of the 1978 original.

Cano, F., Constantinescu, A., & Maitournam, H. (2004). Critère de fatigue polycyclique pour des matériaux anisotropes: application aux monocristaux. *Comptes Rendus Mecanique*, 332(2):115–121.

Charkaluk, E., Bignonnet, A., Constantinescu, A., & Dang Van, K. (2002). Fatigue design of structures under thermomechanical loadings. *Fatigue & Fracture of Engineering Materials & Structures*, 25(12):1199–1206.

Constantinescu, A. & Korsunsky, A. (2007). *Elasticity with Mathematica ®: An Introduction to Continuum Mechanics and Linear Elasticity*. Cambridge University Press.

Dang Van, K. (1971). *Sur la résistance à la fatigue des métaux*. PhD thesis.

Dang-Van, K. (1993). Macro-micro approach in high-cycle multiaxial fatigue. *ASTM Special Technical Publication*, 1191:120–120.

Dang Van, K. (1999). Introduction to fatigue analysis in mechanical design by the multiscale approach.

Dubar, L. et al. (1992). Fatigue multiaxiale des aciers. passage de l'endurance à l'endurance limitée. Prise en compte des accidents géométriques.

Germain, P. (1962). *Mécanique des milieux continus*. Cours de physique à l'usage de la licence. Masson.

Guckenheimer, J. & Holmes, P. (1990). *Nonlinear oscillations, dynamical systems, and bifurcations of vector fields*, volume 42 of *Applied Mathematical Sciences*. Springer-Verlag. Revised and corrected reprint of the 1983 original.

Jabbado, M. (2006). *Fatigue polycyclique des structures métalliques : durée de vie sous chargements variables*. PhD thesis, Ecole Polytechnique.

Lee, S. (1985). A criterion for fully reversed out-of-phase torsion and bending. In: *ASTM,*, pages 553–568.

Maitournam, M., Krebs, C., & Galtier, A. (2011). A multiscale fatigue life model for complex cyclic multiaxial loading. *International Journal of Fatigue*, 33:232–240.

The MathWorks Inc. (2011). Matlab version 7.12.0 (r2011a).

Monchiet, V., Charkaluk, E., & Kondo, D. (2006). Plasticity-damage based micromechanical modelling in high cycle fatigue. *Comptes Rendus Mecanique*, 334(2):129–136.

Morel, F. (1998). A fatigue life prediction method based on a mesoscopic approach in constant amplitude multiaxial loading. *Fatigue & Fracture of Engineering Materials & Structures*, 21(3):241–256.

Morel, F. (2000). A critical plane approach for life prediction of high cycle fatigue under multiaxial variable amplitude loading. *International journal of fatigue*, 22(2):101–119.

Morel, F. & Petit, J. (1996). *Fatigue multiaxiale sous chargement d'amplitude variable*. PhD thesis.

Nguyen, Q.-S. (2003). On shakedown analysis in hardening plasticity. *Journal of the Mechanics and Physics of Solids*, 51(1):101 – 125.

Nishihara, T. & Kawamoto, M. (1945). The strength of metals under combined alternating bending and torsion with phase difference. *Memories of the College of Engineering, Kyoto Imperial University*, 11(85):112.

Papadopoulos, I. (1987). *Fatigue polycyclique des métaux: une nouvelle approche*. PhD thesis, Ecole nationale des ponts et chaussées (France).

Papadopoulos, I. (1993). *Fatigue limit of metals under multiaxial stress conditions: the microscopic approach*. Joint Research Centre, ISEI.

Papadopoulos, I. (1995). A high-cycle fatigue criterion applied in biaxial and triaxial out-of-phase stress conditions. *Fatigue & Fracture of Engineering Materials & Structures*, 18(1):79–91.

Papadopoulos, I. (1998). Critical plane approaches in high-cycle fatigue: on the definition of the amplitude and mean value of the shear stress acting on the critical plane. *Fatigue & Fracture of Engineering Materials & Structures*, 21(3):269–285.

Papadopoulos, I., Davoli, P., Gorla, C., Filippini, M., & Bernasconi, A. (1997). A comparative study of multiaxial high-cycle fatigue criteria for metals. *International Journal of Fatigue*, 19(3):219–235.

Strogatz, S. (1994). *Nonlinear dynamics and chaos*. Addison-Wesley Reading, MA.

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Bibliography

Abels, H. (2009a). Existence of weak solutions for a diffuse interface model for viscous, incompressible fluids with general densities. *Comm. Math. Phys.*, 289(1):45–73.

Abels, H. (2009b). Longtime behavior of solutions of a Navier-Stokes/Cahn-Hilliard system. In: *Nonlocal and abstract parabolic equations and their applications*, volume 86 of *Banach Center Publ.*, pages 9–19. Polish Acad. Sci. Inst. Math., Warsaw.

Abels, H. (2009c). On a diffuse interface model for two-phase flows of viscous, incompressible fluids with matched densities. *Arch. Ration. Mech. Anal.*, 194(2):463–506.

Abels, H. & Feireisl, E. (2008). On a diffuse interface model for a two-phase flow of compressible viscous fluids. *Indiana Univ. Math. J.*, 57(2):659–698.

Abels, H. & Kassmann, M. (2007). An analytic approach to purely nonlocal Bellman equations arising in models of stochastic control. *J. Differential Equations*, 236(1):29–56.

Abels, H. & Wilke, M. (2007). Convergence to equilibrium for the Cahn-Hilliard equation with a logarithmic free energy. *Nonlinear Anal.*, 67(11):3176–3193.

Abels, H. & Wilke, M. (2013). Well-posedness and qualitative behaviour of solutions for a two-phase Navier-Stokes-Mullins-Sekerka system. *Interfaces Free Bound.*, 15(1):39–75.

Adams, R. A. (1975). *Sobolev Spaces*. Academic Press, New York, San Francisco, London.

Anderson, D. M., McFadden, G. B., & Wheeler, A. A. (1998). Diffuse-interface methods in fluid mechanics. volume 30 of *Annu. Rev. Fluid Mech.*, pages 139–165. Annual Reviews.

Aristotelous, A. C., Karakashiany, O. A., & Wise, S. M. (2012). A mixed discontinuous Galerkin, convex splitting scheme for a modified Cahn–Hilliard equation. Preprint.

Babin, A. V. & Vishik, M. I. (1992). *Attractors of evolution equations*, volume 25 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co. Translated and revised from the 1989 Russian original by Babin.

Badalassi, V. E., Ceniceros, H. D., & Banerjee, S. (2003). Computation of multiphase systems with phase field models. *J. Comput. Phys.*, 190(2):371–397.

Ball, J. M. (1997). Continuity properties and global attractors of generalized semiflows and the Navier-Stokes equations. *J. Nonlinear Sci.*, 7(5):475–502.

Ball, J. M. (1998). Erratum: "Continuity properties and global attractors of generalized semiflows and the Navier-Stokes equations". *J. Nonlinear Sci.*, 8(2):233.

Bardeen, J. & Shockley, W. (1950). Deformation potentials and mobilities in non-polar crystals. *Physical Review*, 80(1):72.

Bates, P. W. & Han, J. (2005). The Neumann boundary problem for a nonlocal Cahn-Hilliard equation. *J. Differential Equations*, 212(2):235–277.

Bender, C. M. & Orszag, S. A. (1999). *Advanced mathematical methods for scientists and engineers. I.* Springer-Verlag. Asymptotic methods and perturbation theory, Reprint of the 1978 original.

Bergh, J. & Löfström, J. (1976). *Interpolation Spaces*. Springer.

Bogdan, K., Burdzy, K., & Chen, Z.-Q. (2003). Censored stable processes. *Probab. Theory Related Fields*, 127(1):89–152.

Bosia, S. (2012). Well-posedness and long term behavior of a simplified Ericksen-Leslie non-autonomous system for nematic liquid crystal flows. *Commun. Pure Appl. Anal.*, 11(2):407–441.

Bosia, S., Constantinescu, A., Jabbour, M., & Triantafyllidis, N. On the modelling of strained semiconductors. in preparation.

Boyer, F. (1999). Mathematical study of multi-phase flow under shear through order parameter formulation. *Asymptot. Anal.*, 20(2):175–212.

Boyer, F. (2001). Nonhomogeneous Cahn-Hilliard fluids. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 18(2):225–259.

Brézis, H. (1973). *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*. North-Holland Publishing Co. North-Holland Mathematics Studies, No. 5. Notas de Matemática (50).

Brezis, H. (2011). *Functional analysis, Sobolev spaces and partial differential equations*. Universitext. Springer.

Bulíček, M., Ettwein, F., Kaplický, P., & Pražák, D. (2010). On uniqueness and time regularity of flows of power-law like non-Newtonian fluids. *Math. Methods Appl. Sci.*, 33(16):1995–2010.

Cahn, J. W. (1961). On spinodal decomposition. *Acta Metallurgica*, 9(9):795 – 801.

Cahn, J. W., Elliott, C. M., & Novick-Cohen, A. (1996). The Cahn-Hilliard equation with a concentration dependent mobility: motion by minus the Laplacian of the mean curvature. *European J. Appl. Math.*, 7(3):287–301.

Cahn, J. W. & Hilliard, J. E. (1958). Free energy of a nonuniform system. i. interfacial free energy. *The Journal of Chemical Physics*, 28(2):258–267.

Cano, F., Constantinescu, A., & Maitournam, H. (2004). Critère de fatigue polycyclique pour des matériaux anisotropes: application aux monocristaux. *Comptes Rendus Mecanique*, 332(2):115–121.

Carvalho, A. N., Langa, J. A., & Robinson, J. C. (2013). *Attractors for infinite-dimensional non-autonomous dynamical systems*, volume 182 of *Applied Mathematical Sciences*. Springer.

Casey, H. (1999). *Devices for integrated circuits: silicon and III-V compound semiconductors*. John Wiley.

Charkaluk, E., Bignonnet, A., Constantinescu, A., & Dang Van, K. (2002). Fatigue design of structures under thermomechanical loadings. *Fatigue & Fracture of Engineering Materials & Structures*, 25(12):1199–1206.

Chepyzhov, V. V. & Vishik, M. I. (1997). Evolution equations and their trajectory attractors. *J. Math. Pures Appl. (9)*, 76(10):913–964.

Chepyzhov, V. V. & Vishik, M. I. (2002). *Attractors for equations of mathematical physics*, volume 49 of *American Mathematical Society Colloquium Publications*. American Mathematical Society.

Cherfils, L., Miranville, A., & Zelik, S. (2011). The Cahn-Hilliard equation with logarithmic potentials. *Milan J. Math.*, 79(2):561–596.

Chill, R. (2003). On the łojasiewicz-Simon gradient inequality. *J. Funct. Anal.*, 201(2):572–601.

Choksi, R., Maras, M., & Williams, J. F. (2011). 2D phase diagram for minimizers of a Cahn-Hilliard functional with long-range interactions. *SIAM J. Appl. Dyn. Syst.*, 10(4):1344–1362.

Colli, P., Frigeri, S., & Grasselli, M. (2012). Global existence of weak solutions to a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Math. Anal. Appl.*, 386(1):428–444.

Colli, P., Krejčí, P., Rocca, E., & Sprekels, J. (2007). Nonlinear evolution inclusions arising from phase change models. *Czechoslovak Math. J.*, 57(132)(4):1067–1098.

Constantinescu, A. & Korsunsky, A. (2007). *Elasticity with Mathematica ®: An Introduction to Continuum Mechanics and Linear Elasticity*. Cambridge University Press.

Dang Van, K. (1971). *Sur la résistance à la fatigue des métaux*. PhD thesis.

Dang-Van, K. (1993). Macro-micro approach in high-cycle multiaxial fatigue. *ASTM Special Technical Publication*, 1191:120–120.

Dang Van, K. (1999). Introduction to fatigue analysis in mechanical design by the multiscale approach.

Denisova, I. V. & Solonnikov, V. A. (1991). Solvability in Hölder spaces of a model initial-boundary value problem generated by a problem on the motion of two fluids. *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)*, 188(Kraev. Zadachi Mat. Fiz. i Smezh. Voprosy Teor. Funktsii. 22):5–44, 186.

Dhar, S., Kosina, H., Palankovski, V., Ungersboeck, S., & Selberherr, S. (2005). Electron mobility model for strained-Si devices. *Electron Devices, IEEE Transactions on*, 52(4):527–533.

Dubar, L. et al. (1992). Fatigue multiaxiale des aciers. passage de l'endurance à l'endurance limitée. Prise en compte des accidents géométriques.

Eden, A., Foias, C., Nicolaenko, B., & Temam, R. (1994). *Exponential attractors for dissipative evolution equations*, volume 37 of *RAM: Research in Applied Mathematics*. Masson.

Efendiev, M., Miranville, A., & Zelik, S. (2000). Exponential attractors for a nonlinear reaction-diffusion system in $\mathbf{R}^3$. *C. R. Acad. Sci. Paris Sér. I Math.*, 330(8):713–718.

Efendiev, M., Zelik, S., & Miranville, A. (2005). Exponential attractors and finite-dimensional reduction for non-autonomous dynamical systems. *Proc. Roy. Soc. Edinburgh Sect. A*, 135(4):703–730.

Elliott, C. M. & French, D. A. (1987). Numerical studies of the Cahn-Hilliard equation for phase separation. *IMA J. Appl. Math.*, 38(2):97–128.

Elliott, C. M. & Garcke, H. (1996). On the Cahn-Hilliard equation with degenerate mobility. *SIAM J. Math. Anal.*, 27(2):404–423.

Elliott, C. M., Stinner, B., Styles, V., & Welford, R. (2011). Numerical computation of advection and diffusion on evolving diffuse interfaces. *IMA J. Numer. Anal.*, 31(3):786–812.

Fabes, E., Mendez, O., & Mitrea, M. (1998). Boundary layers on Sobolev-Besov spaces and Poisson's equation for the Laplacian in Lipschitz domains. *J. Funct. Anal.*, 159(2):323–368.

Feireisl, E. & Pražák, D. (2010). *Asymptotic behavior of dynamical systems in fluid mechanics*, volume 4 of *AIMS Series on Applied Mathematics*. American Institute of Mathematical Sciences (AIMS), Springfield, MO.

Fischetti, M. & Laux, S. (1996). Band structure, deformation potentials, and carrier mobility in strained Si, Ge, and SiGe alloys. *Journal of Applied Physics*, 80(4):2234–2252.

Foias, C. & Temam, R. (1987). The connection between the navier-stokes equations, dynamical systems, and turbulence theory. *Directions in partial differential equations*, pages 55–73.

Folland, G. B. (1999). *Real analysis*, (second ed.). Pure and Applied Mathematics (New York). John Wiley & Sons Inc. Modern techniques and their applications, A Wiley-Interscience Publication.

Frigeri, S. & Grasselli, M. (2012a). Global and trajectory attractors for a nonlocal Cahn-Hilliard-Navier-Stokes system. *J. Dynam. Differential Equations*, 24(4):827–856.

Frigeri, S. & Grasselli, M. (2012b). Nonlocal Cahn-Hilliard-Navier-Stokes systems with singular potentials. *Dyn. Partial Differ. Equ.*, 9(4):273–304.

Gajewski, H. & Zacharias, K. (2003). On a nonlocal phase separation model. *J. Math. Anal. Appl.*, 286(1):11–31.

Gal, C. G. & Grasselli, M. (2010a). Asymptotic behavior of a Cahn-Hilliard-Navier-Stokes system in 2D. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(1):401–436.

Gal, C. G. & Grasselli, M. (2010b). Trajectory attractors for binary fluid mixtures in 3D. *Chin. Ann. Math. Ser. B*, 31(5):655–678.

Gal, C. G. & Grasselli, M. (2011). Instability of two-phase flows: a lower bound on the dimension of the global attractor of the Cahn-Hilliard–Navier-Stokes system. *Phys. D*, 240(7):629–635.

Germain, P. (1962). *Mécanique des milieux continus*. Cours de physique à l'usage de la licence. Masson.

Giacomin, G. & Lebowitz, J. L. (1997). Phase segregation dynamics in particle systems with long range interactions. I. Macroscopic limits. *J. Statist. Phys.*, 87(1-2):37–61.

Giacomin, G. & Lebowitz, J. L. (1998). Phase segregation dynamics in particle systems with long range interactions. II. Interface motion. *SIAM J. Appl. Math.*, 58(6):1707–1729.

Giga, Y. & Sohr, H. (1991). Abstract L^p estimates for the Cauchy problem with applications to the Navier-Stokes equations in exterior domains. *J. Funct. Anal.*, 102(1):72–94.

Grasselli, M. & Pražák, D. (2011). Longtime behavior of a diffuse interface model for binary fluid mixtures with shear dependent viscosity. *Interfaces Free Bound.*, 13:507–530.

Griffiths, D. J. (1998). *Introduction to Electrodynamics (3rd Edition)*. Benjamin Cummings.

Guckenheimer, J. & Holmes, P. (1990). *Nonlinear oscillations, dynamical systems, and bifurcations of vector fields*, volume 42 of *Applied Mathematical Sciences*. Springer-Verlag. Revised and corrected reprint of the 1983 original.

Gurtin, M. E., Polignone, D., & Viñals, J. (1996). Two-phase binary fluids and immiscible fluids described by an order parameter. *Math. Models Methods Appl. Sci.*, 6(6):815–831.

Hall, R. N. (1952). Electron-hole recombination in germanium. *Physical Review*, 87(2):387.

Heida, M., Málek, J., & Rajagopal, K. (2012). On the development and generalizations of Cahn–Hilliard equations within a thermodynamic framework. *Zeitschrift für Angewandte Mathematik und Physik (ZAMP)*, 63:145–169.

Herring, C. & Vogt, E. (1956). Transport and deformation-potential theory for many-valley semiconductors with anisotropic scattering. *Physical Review*, 101(3):944.

Hohenberg, P. C. & Halperin, B. I. (1977). Theory of dynamic critical phenomena. *Rev. Mod. Phys.*, 49:435–479.

Huo, Y., Jiang, X., Zhang, H., & Yang, Y. (2003). Hydrodynamic effects on phase separation of binary mixtures with reversible chemical reaction. *J. Chem. Phys.*, 118:9830–9837.

Huo, Y., Zhang, H., & Yang, Y. (2004). Effects of reversible chemical reaction on morphology and domain growth of phase separating binary mixtures with viscosity difference. *Macromol. Theory Simul.*, 13(3):280–289.

Jabbado, M. (2006). *Fatigue polycyclique des structures métalliques : durée de vie sous chargements variables*. PhD thesis, Ecole Polytechnique.

Jacoboni, C., Nava, F., Canali, C., & Ottaviani, G. (1981). Electron drift velocity and diffusivity in germanium. *Physical Review B*, 24(2):1014.

Jäger, R. (2002). *Introduction to Microelectronic Fabrication*. Modular Series on Solid State Deviced, Vol 5. Prentice Hall PTR.

Jendoubi, M. A. (1998). A simple unified approach to some convergence theorems of L. Simon. *J. Funct. Anal.*, 153(1):187–202.

Kay, D., Styles, V., & Welford, R. (2008). Finite element approximation of a Cahn-Hilliard-Navier-Stokes system. *Interfaces Free Bound.*, 10(1):15–43.

Kim, J., Kang, K., & Lowengrub, J. (2004). Conservative multigrid methods for Cahn-Hilliard fluids. *J. Comput. Phys.*, 193(2):511–543.

Kim, N., Consiglieri, L., & Rodrigues, J. F. (2006). On non-Newtonian incompressible fluids with phase transitions. *Math. Methods Appl. Sci.*, 29(13):1523–1541.

Kloeden, P. E. (2000). Pullback attractors in nonautonomous difference equations. *J. Differ. Equations Appl.*, 6(1):33–52.

Kovetz, A. (2000). *Electromagnetic Theory*. Oxford Lecture Series in Mathematics and Its Applications. Clarendon Press.

Ladyzhenskaya, O. (1967). New equations for the description of the motions of viscous incompressible fluids, and global solvability for their boundary value problems. *Trudy Matematicheskogo Instituta im. VA Steklova*, 102:85–104.

Lamorgese, A., Molin, D., & Mauri, R. (2011). Phase field approach to multiphase flow modeling. *Milan J. Math.*, 79:597–642.

Langa, J. A., Miranville, A., & Real, J. (2010). Pullback exponential attractors. *Discrete Contin. Dyn. Syst.*, 26(4):1329–1357.

Lee, S. (1985). A criterion for fully reversed out-of-phase torsion and bending. In: *ASTM,*, pages 553–568.

Leray, J. (1934). Sur le mouvement d'un liquide visqueux emplissant l'espace. *Acta Math.*, 63(1):193–248.

Lifshitz, E. M., Pitaevskii, L. P., & Landau, L. D. (1981). *Physical kinetics*, volume 60. Pergamon press Oxford.

Lions, J.-L. (1969). *Quelques méthodes de résolution des problèmes aux limites non linéaires*. Dunod.

Liu, C. & Shen, J. (2003). A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. *Phys. D*, 179(3-4):211–228.

Luttinger, J. M. (1956). Quantum theory of cyclotron resonance in semiconductors: General theory. *Phys. Rev.*, 102:1030–1041.

Luttinger, J. M. & Kohn, W. (1955). Motion of electrons and holes in perturbed periodic fields. *Phys. Rev.*, 97:869–883.

Maitournam, M., Krebs, C., & Galtier, A. (2011). A multiscale fatigue life model for complex cyclic multiaxial loading. *International Journal of Fatigue*, 33:232–240.

Málek, J., Nečas, J., & Ružička, M. (2001). On weak solutions to a class of non-Newtonian incompressible fluids in bounded three-dimensional domains: the case $p \geqslant 2$. *Adv. Differential Equations*, 6(3):257–302.

Markowich, P. A., Ringhofer, C. A., & Schmeiser, C. (1990). *Semiconductor equations*. Springer-Verlag.

The MathWorks Inc. (2011). Matlab version 7.12.0 (r2011a).

Meirmanov, A. M. (1992). *The Stefan problem*, volume 3 of *de Gruyter Expositions in Mathematics*. Walter de Gruyter & Co. Translated from the Russian by Marek Niezgódka and Anna Crowley, With an appendix by the author and I. G. Götz.

Miranville, A. (2011). Asymptotic behavior of the Cahn-Hilliard-Oono equation. *J. Appl. Anal. Comput.*, 1(4):523–536.

Miranville, A. & Zelik, S. (2004). Robust exponential attractors for Cahn–Hilliard type equations with singular potentials. *Math. Methods Appl. Sci.*, 27(5):545–582.

Miranville, A. & Zelik, S. (2008). Attractors for dissipative partial differential equations in bounded and unbounded domains. In: *Handbook of differential equations: evolutionary equations. Vol. IV*, Handb. Differ. Equ., pages 103–200. Elsevier/North-Holland, Amsterdam.

Monchiet, V., Charkaluk, E., & Kondo, D. (2006). Plasticity-damage based micromechanical modelling in high cycle fatigue. *Comptes Rendus Mecanique*, 334(2):129–136.

Morel, F. (1998). A fatigue life prediction method based on a mesoscopic approach in constant amplitude multiaxial loading. *Fatigue & Fracture of Engineering Materials & Structures*, 21(3):241–256.

Morel, F. (2000). A critical plane approach for life prediction of high cycle fatigue under multiaxial variable amplitude loading. *International journal of fatigue*, 22(2):101–119.

Morel, F. & Petit, J. (1996). *Fatigue multiaxiale sous chargement d'amplitude variable*. PhD thesis.

Morro, A. (2010). Phase-field models of Cahn–Hilliard fluids and extra fluxes. *Adv. Theor. Appl. Mech*, 3:409–424.

Nguyen, Q.-S. (2003). On shakedown analysis in hardening plasticity. *Journal of the Mechanics and Physics of Solids*, 51(1):101 – 125.

Nishihara, T. & Kawamoto, M. (1945). The strength of metals under combined alternating bending and torsion with phase difference. *Memories of the College of Engineering, Kyoto Imperial University*, 11(85):112.

Oono, Y. & Puri, S. (1987). Computationally efficient modeling of ordering of quenched phases. *Physical review letters*, 58(8):836–839.

Papadopoulos, I. (1987). *Fatigue polycyclique des métaux: une nouvelle approche*. PhD thesis, Ecole nationale des ponts et chaussées (France).

Papadopoulos, I. (1993). *Fatigue limit of metals under multiaxial stress conditions: the microscopic approach*. Joint Research Centre, ISEI.

Papadopoulos, I. (1995). A high-cycle fatigue criterion applied in biaxial and triaxial out-of-phase stress conditions. *Fatigue & Fracture of Engineering Materials & Structures*, 18(1):79–91.

Papadopoulos, I. (1998). Critical plane approaches in high-cycle fatigue: on the definition of the amplitude and mean value of the shear stress acting on the critical plane. *Fatigue & Fracture of Engineering Materials & Structures*, 21(3):269–285.

Papadopoulos, I., Davoli, P., Gorla, C., Filippini, M., & Bernasconi, A. (1997). A comparative study of multiaxial high-cycle fatigue criteria for metals. *International Journal of Fatigue*, 19(3):219–235.

Park, S.-I., Ahn, J.-H., Feng, X., Wang, S., Huang, Y., & Rogers, J. A. (2008). Theoretical and experimental studies of bending of inorganic electronic materials on plastic substrates. *Advanced Functional Materials*, 18(18):2673–2684.

Pata, V. & Zelik, S. (2007). A result on the existence of global attractors for semigroups of closed operators. *Commun. Pure Appl. Anal.*, 6:481–486.

Poupaud, F. (1988). *Etude mathématique et simulations numériques de quelques équations de Boltzmann*. PhD thesis, Université Paris 6.

Robinson, J. C. (2001). *Infinite-dimensional dynamical systems*. Cambridge Texts in Applied Mathematics. Cambridge University Press. An introduction to dissipative parabolic PDEs and the theory of global attractors.

Rogers, J. A., Someya, T., & Huang, Y. (2010). Materials and mechanics for stretchable electronics. *Science*, 327(5973):1603–1607.

Sapoval, B. & Hermann, C. (1990). *Physique des Semi-conducteurs*. Ellipses.

Schmalfuss, B. (1992). Backward cocycles and attractors of stochastic differential equations. In: *International Seminar on Applied Mathematics-Nonlinear Dynamics: Attractor Approximation and Global Behaviour*, pages 185–192.

Sell, G. R. (1996). Global attractors for the three-dimensional Navier-Stokes equations. *J. Dynam. Differential Equations*, 8(1):1–33.

Shen, J. & Yang, X. (2010). Energy stable schemes for Cahn-Hilliard phase-field model of two-phase incompressible flows. *Chin. Ann. Math. Ser. B*, 31(5):743–758.

Shockley, W. (1949). The theory of p-n junctions in semiconductors and p-n junction transistors. *Bell System Technical Journal*, 28(3):435–489.

Shockley, W. et al. (1963). *Electrons and holes in semiconductors*, volume 1. van Nostrand.

Shockley, W. & Read Jr, W. (1952). Statistics of the recombinations of holes and electrons. *Physical Review*, 87(5):835.

Showalter, R. E. (1997). *Monotone Operators in Banach Space and Nonlinear Partial Differential Equations*, volume 49 of *Mathematical Surveys and Monographs*. American Mathematical Society.

Shur, M. & Hack, M. (1984). Physics of amorphous silicon based alloy field-effect transistors. *Journal of Applied Physics*, 55(10):3831–3842.

Shur, M., Hack, M., & Shaw, J. (1989). A new analytic model for amorphous silicon thin-film transistors. *Journal of Applied Physics*, 66(7):3371–3380. cited By (since 1996)85.

Siggia, E. D. (1979). Late stages of spinodal decomposition in binary mixtures. *Phys. Rev. A*, 20:595–605.

Silvestre, L. (2007). Regularity of the obstacle problem for a fractional power of the Laplace operator. *Comm. Pure Appl. Math.*, 60(1):67–112.

Simon, J. (1990). Sobolev, Besov and Nikolskiĭ fractional spaces: imbeddings and comparisons for vector valued spaces on an interval. *Ann. Mat. Pura Appl. (4)*, 157:117–148.

Smith, C. S. (1954). Piezoresistance effect in germanium and silicon. *Physical review*, 94(1):42.

Starovoitov, V. (1997). The dynamics of a two-component fluid in the presence of capillary forces. *Mathematical Notes*, 62(2):244–254.

Street, R. A. (2005). *Hydrogenated amorphous silicon*. Cambridge University Press.

Strogatz, S. (1994). *Nonlinear dynamics and chaos*. Addison-Wesley Reading, MA.

Sun, Y., Thompson, S., & Nishida, T. (2007). Physics of strain effects in semiconductors and metal-oxide-semiconductor field-effect transistors. *Journal of applied physics*, 101(10):104503–104503.

Sun, Y., Thompson, S., & Nishida, T. (2009). *Strain effect in semiconductors: theory & device applications*. Springer.

Sze, S. & Ng, K. (2007). *Physics of semiconductor devices*. Wiley-Interscience publication. Wiley-Interscience.

Temam, R. (1984). *Navier-Stokes equations*, (third ed.), volume 2 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co. Theory and numerical analysis, With an appendix by F. Thomasset.

Temam, R. (1995). *Navier-Stokes equations and nonlinear functional analysis*, (second ed.), volume 66 of *CBMS-NSF Regional Conference Series in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM).

Temam, R. (1997). *Infinite-dimensional dynamical systems in mechanics and physics*, (second ed.), volume 68 of *Applied Mathematical Sciences*. Springer-Verlag.

Teramoto, T. & Nishiura, Y. (2002). Double gyroid morphology in a gradient system with nonlocal effects. *J. Phys. Soc. Jpn.*, 71(7):1611–1614.

Thompson, S. E., Sun, G., Choi, Y. S., & Nishida, T. (2006). Uniaxial-process-induced strained-si: extending the cmos roadmap. *Electron Devices, IEEE Transactions on*, 53(5):1010–1020.

Van Roosbroeck, W. (1950). Theory of flow of electrons and holes in germanium and other semiconductors. *Bell Syst. Tech. J*, 29(4):560–607.

Villain-Guillot, S. (2010). 1D Cahn–Hilliard equation for modulated phase systems. *Journal of Physics A: Mathematical and Theoretical*, 43:205102.

Vishik, M. I., Zelik, S. V., & Chepyzhov, V. V. (2010). A strong trajectory attractor for a dissipative reactor-diffusion system. *Dokl. Akad. Nauk*, 435(2):155–159.

Visintin, A. (1996). *Models of phase transitions*. Progress in Nonlinear Differential Equations and their Applications, 28. Birkhäuser Boston Inc.

Vv.Aa. Electronic archive, New Semiconductor Materials. Characteristics and Properties.

Zeidler, E. (1990). *Nonlinear functional analysis and its applications. II/A*. Springer-Verlag.

Zhao, L., Wu, H., & Huang, H. (2009). Convergence to equilibrium for a phase-field model for the mixture of two viscous incompressible fluids. *Commun. Math. Sci.*, 7(4):939–962.

Summary

This work discusses a series of modelling problems in continuum mechanics. The first part is devoted to the mathematical analysis of some diffuse interface models in phase separation of binary mixtures (e.g., coarsening of alloys or bistable polymeric fluids). The second part discusses the function of electronic devices (in particular p-n junctions) under mechanical deformations. The third part presents a model for lifetime predictions in polycrystalline metals under periodic loading.

A typical phase separation model is the well-known model H, constructed by coupling the convective Cahn-Hilliard equation with the Navier-Stokes system through the so-called Korteweg force. Here we consider some variants of the model which account, e.g., for shear dependent viscosity or chemically reacting components. We first study basic issues like existence, uniqueness and regularity of solutions. Then we analyze the long-time behaviour of the infinite dimensional dissipative dynamical systems generated by the systems studied. More precisely, we prove the existence of global attractors, exponential attractors, pullback attractors and trajectories attractors for the corresponding dynamical systems. Also, we discuss the robustness of such invariant sets with respect to perturbations of some parameters of the model. The results obtained represent natural extensions of the properties known for single fluid flows, whose features are considered a benchmark for all new techniques proposed in the literature. Finally, as a more realistic description of phase separation phenomena, we introduce a Cahn-Hilliard equation accounting for nonlocal interactions through a singular kernel. In this case some well-posedness and regularity results are demonstrated.

The second part of this work is devoted to the study of the coupling effects between mechanical and electronic properties in semiconductors. The modelling of the electronic device is based on the drift-diffusion model for electrons and holes. The device is viewed as a standard macroscopic continuum and the objective is to understand the effects of mechanical strain on the electronic properties of the semiconductor and in particular its effects on the characteristic curve of a p-n junction. This permits to propose a variational formulation of the classical drift-diffusion system and to derive a thermodynamically consistent model for the coupled electromechanical phenomena. The strain mainly influences the mobility coefficients and the generation/recombination term. Two approximate solutions are discussed, one based on only physical assumptions and one involving asymptotic expansions. This part of the work is a preliminary step towards the understanding of the properties of flexible electronic devices.

The final part of the thesis presents an application of the theory of dynamical systems to predict the lifetime of polycrystalline metals undergoing a high cycle fatigue regime. A new model is proposed and compared with the existing literature.

Résumé

Ce travail de thèse affronte l'étude de divers problèmes surgissant de la mécanique du milieu continu. La première partie du manuscrit est dédiée à l'étude mathématique de certains modèles à interfaces diffuses qui décrivent la séparation de phase de mixtures binaires (par exemple, le grossissement de la taille des grains dans un alliage ou bien l'écoulement des fluides polymériques bistables). La seconde partie examine le fonctionnement de certains dispositifs électroniques, comme les jonctions p-n, sous l'effet de déformations mécaniques. La troisième partie présente un model pour la prédiction de la durée de vie pour des métaux polycristallins en régime de chargement cyclique.

Un modèle typique de séparation de phase est le modèle H, qui est constitué d'une équation de Cahn-Hilliard convective couplée avec le système de Navier-Stokes par la force dite de Korteweg. On considère des variations de ce modèle qui tiennent compte, par exemple, d'une viscosité du fluide dépendante du cisaillement ou de constituants réagissant chimiquement entre eux. Tout d'abord, on étudie des questions de base comme l'existence, l'unicité et la régularité des solutions. Par la suite, on analyse le comportement asymptotique des systèmes dynamiques infini-dimensionnels générés par les systèmes étudiés. Plus précisément, on démontre l'existence d'attracteurs globaux, d'attracteurs exponentiels, d'attracteurs pullback et d'attracteurs de trajectoires pour les systèmes dynamique correspondants. On discute aussi la robustesse de ces ensembles invariants par rapport à des perturbations de certains paramètres du modèle. Nos résultats constituent une extension naturelle des propriétés connues pour le cas de l'écoulement d'un fluide simple qui représentent le cas de référence pour toute nouvelle technique proposée en littérature. Enfin, comme description plus précise des phénomènes de séparation de phase, on considère une équation de Cahn-Hilliard modélisant des interactions non-locales à travers un noyau singulier. En ce cas, des résultats d'existence et de régularité sont donnés.

La seconde partie de cette thèse est dédiée à l'étude des effets de couplage entre les propriétés mécaniques et électroniques des semi-conducteurs. La modélisation des dispositifs électroniques choisie se base sur le modèle de diffusion et transport pour les électrons et les trous. Le dispositif est décrit comme un continu macroscopique standard avec, pour objectif, la compréhension des effets des déformations sur les propriétés électroniques du semi-conducteur et, en particulier, sur la caractéristique d'une jonction p-n. Ceci permet de proposer une formulation variationelle du système classique de diffusion et transport et de dériver un modèle thermodynamiquement consistent pour les effets électromécaniques couplés. Les déformations ont des effets en particulier sur les coefficients de mobilité et sur le terme de génération et recombinaison des porteurs. Deux solutions approximées sont étudiées : une développé à partir d'hypothèses physiques et l'autre qui comporte une expansion asymptotique. Ces résultats constituent une étape préalable pour la compréhension des dispositifs électroniques flexibles.

La dernière partie de la thèse présente une application de la théorie des systèmes dynamiques à la prédiction de la durée de vie des métaux polycristallins sous chargement périodique pour grand nombre de cycle de chargement. Un nouveaux model est proposé et ses prévisions comparées avec les résultats connus dans la littérature.