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Processus cinétiques dans les domaines à bord et quasi-stationnarité

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À ma mère,

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Résumé

Cette thèse est décomposée en trois parties, chacune portant sur des questions reliées à l'étude du processus de Langevin, qui décrit l'évolution des positions et vitesses de particules ponctuelles. Nous nous plaçons ici en dimension quelconque et l'étude menée se fait en combinant outils probabilistes et analytiques.

La première partie se concentre sur l'extension du cadre parabolique au cadre dégénéré associé à l'opérateur de Fokker-Planck cinétique sur un domaine de la forme $\mathscr{O} \times \mathbb{R}^d$, où $\mathscr{O}$ désigne un domaine borné en position, et les vitesses vivent dans $\mathbb{R}^d$. Nous obtenons dans cette partie l'existence et l'unicité de solutions classiques à l'équation de Fokker-Planck cinétique sur le domaine $\mathscr{O} \times \mathbb{R}^d$. Nous obtenons également une inégalité de Harnack ainsi qu'un principe du maximum associés à l'opérateur de Fokker-Planck cinétique. Finalement, nous obtenons un résultat de compacité dans l'ensemble des fonctions continues bornées du semigroupe du processus de Langevin absorbé au bord de $\mathscr{O} \times \mathbb{R}^d$.

Ces résultats sont utilisés dans la deuxième partie de la thèse pour prouver notamment l'existence d'une unique distribution quasi-stationnaire pour le processus de Langevin dans le domaine $\mathscr{O} \times \mathbb{R}^d$. Nous montrons également la convergence de la loi du processus conditionné à rester dans $\mathscr{O} \times \mathbb{R}^d$ durant $[0, t]$, lorsque t tend vers l'infini, vers la distribution quasi-stationnaire. Ces résultats sont obtenus de deux manières différentes : l'une portée sur des outils d'analyse fonctionnelle et l'autre reposant sur des techniques plus probabilistes. Nous étudions également la distribution quasi-stationnaire obtenue et explicitons son comportement limite lorsque le paramètre de friction dans l'équation de Langevin tend vers l'infini (régime sur-amorti).

Finalement, nous considérons dans la dernière partie la chaîne de Markov construite à partir des entrées et sorties successives du processus de Langevin dans un domaine. Nous étudions alors la stationnarité de la chaîne de Markov obtenue. Ces deux dernières parties (distribution quasi-stationnaire et entrée-sortie d'un domaine) sont motivées par l'analyse d'algorithmes d'échantillonnage des trajectoires du processus de Langevin pour des temps très longs dans le cas où ce processus est métastable.

Summary

This manuscript is divided into three parts, addressing different problems related to the study of the Langevin process, which describes the evolution of positions and velocities of point particles. We consider here an arbitrary dimension and the results rely on a combination of probabilistic tools and analytic tools.

The first part focuses on the extension of some results statisfied in the parabolic theory on smooth bounded domains to the degenerate case of the kinetic Fokker-Planck operator on a domain $\mathscr{O} \times \mathbb{R}^d$, where $\mathscr{O}$ is a bounded domain in position, and the velocities live in $\mathbb{R}^d$. We obtain in this part the existence of a unique classical solution to the kinetic Fokker-Planck equation on the domain $\mathscr{O} \times \mathbb{R}^d$ with initial conditions and homogeneous Dirichlet boundary conditions. We also obtain a Harnack inequality as well as a Maximum principle associated to the kinetic Fokker-Planck operator. Finally, we obtain a compactness result on the set of bounded continuous functions of the semigroup of the Langevin process absorbed at the boundary of $\mathscr{O} \times \mathbb{R}^d$.

The results prove to be useful in the second part to prove the existence of a unique quasi-stationary distribution for the Langevin process on the domain $\mathscr{O} \times \mathbb{R}^d$. We also obtain a weak convergence of the law of the Langevin process conditioned to stay in $\mathscr{O} \times \mathbb{R}^d$ during $[0, t]$, when t goes to infinity, towards its quasi-stationary distribution. These results are obtained using two differents approaches: the first one relying on functional analysis tools and the second one resorts to more probabilistic tools. We also consider the obtained quasi-stationary distribution and identify its weak limit when the friction parameter in the equation satisfied by the Langevin process goes to infinity (overdamped limit).

Finally, we consider in the last part a Markov chain obtained from the successive entry and exit points of a domain for the Langevin process. We then study the stationarity of this Markov chain. These last two parts are motivated by algorithms which are used in computational statistical physics in order to simulate the Langevin dynamics over very long times, when these dynamics are metastable.

List of submissions

- [59] (with T. Lelièvre, J. Reygner). *A probabilistic study of the kinetic Fokker-Planck equation in cylindrical domains* (arXiv:2010.10157)

- [60] (with T. Lelièvre, J. Reygner). *Quasi-stationary distribution for the Langevin process in cylindrical domains, part I: Existence, uniqueness and long time convergence.* (arXiv:2101.11999)

- [69] *Quasi-stationary distribution for the Langevin process in cylindrical domains, part II: overdamped limit.* (arXiv:2103.00338).

CONTENTS

CHAPITRE 1 INTRODUCTION

Cette thèse est consacrée à l'étude du processus de Langevin dans des domaines à bord. Nous introduisons cette étude dans les sections 1.1 et 1.2 et présentons nos principaux résultats dans la section 1.3. Quelques perspectives sont esquissées dans la section 1.4.

1.1 Physique statistique computationnelle en grande dimension et changement d'échelle de temps

L'étude de phénomènes naturels complexes a longtemps été au centre des préoccupations des physiciens. Décrire précisément le mouvement des astres par exemple, à travers un cadre mathématique universel, a pendant longtemps echappé aux scientifiques du domaine. Ainsi si les gens observaient le mouvement elliptique des planètes autour du soleil ils ne savaient pas l'expliquer ou le formaliser. Ce ne fut qu'en 1686 que I. Newton théorisa pour la première fois le mouvement gravitationnel des corps, ou "mécanique newtonienne". Ces équations permettaient de décrire la trajectoire d'un ensemble de N planètes, étoiles, comètes, etc. Des méthodes de résolution approchées furent ensuite développées afin d'approcher ces solutions du mieux possible. C'est ainsi que dès 1791, J. Delambre appliqua la méthode numérique plus connue sous le nom de schéma de Verlet aux équations posées par I. Newton, afin de construire une trajectoire discrète du mouvement des astres. Les premières utilisations de l'ordinateur comme outil de résolution numérique arrivèrent plus tard, en 1941. Ensuite, l'intérêt des méthodes numériques s'étendit alors très vite aux mouvements microscopiques également, comme par exemple le mouvement d'atomes et/ou de molécules qui est décrit par des équations similaires. L'intérêt fondamental étant que ces simulations numériques pouvaient se substituer à l'observation microscopique de ces phénomènes dans les bonnes conditions de températures, pression, etc. La recherche en simulation numérique et en modélisation de l'évolution de système moléculaire s'est ainsi grandement développée durant le vingtième siècle menant notamment à plusieurs prix Nobel décernés à des physiciens pionniers dans ce nouveau domaine. Citons par exemple des chercheurs comme W. Kohn, récompensé en 1998 pour ses développements de la théorie de la fonctionnelle de la densité, ainsi que J. A. Pople récompensé la même année pour son développement de méthodes informatiques appliquées à la chimie quantique.

Les défis en simulation moléculaire demeurent cependant très nombreux. La physique statistique nous enseigne qu'il faut simuler des systèmes comportant un nombre très important de particules sur des temps très longs pour avoir accès aux quantités macroscopiques d'intérêt. Les finalités sont diverses : évaluer certaines quantités lorsque le système est à l'équilibre (appelées quantités thermodynamiques), ou considérer des quantités dynamiques dépendant de la loi des trajectoires du système. Dans ce deuxième cas par exemple, il convient d'approcher la trajectoire réelle du système par une trajectoire discrète en temps de manière suffisamment précise. Présentons maintenant une dynamique typique utilisée en pratique pour simuler l'évolution d'un système moléculaire, et qui sera l'objet d'étude de cette thèse. Soit un ensemble de N particules (penser à des atomes) décrites chacune par leur vecteur position $q \in \mathbb{R}^3$ ainsi que leur vecteur moment cinétique $p \in \mathbb{R}^3$. Le système complet est alors décrit par le vecteur $(q,p) = (q_1,\ldots,q_n,p_1,\ldots,p_n) \in \mathbb{R}^{2d}$ où $d = 3n$. Au temps $t \geq 0$, nous noterons (q_t,p_t) la position et le moment du système complet. En principe, la physique statistique nous enseigne que pour atteindre la limite thermodynamique, le nombre d'atomes doit être de l'ordre de grandeur du nombre d'Avogadro, soit 10^{23}. En pratique, les simulations utilisent plutôt un nombre N entre 10^6 et 10^9, heureusement déja suffisant pour observer nombre de propriétés macroscopiques. Notons $V(q)$ le potentiel d'interaction s'appliquant sur le système composé des N particules, et $\gamma > 0$ le terme de friction décrivant la fréquence de collision avec le bain thermostatique, i.e. des degrés de liberté non simulés mais qui fixent la température du système, notée T. L'évolution de ce système peut alors être décrite par l'équation différentielle stochastique suivante (EDS) portant sur le processus $(q_t,p_t)_{t\geq 0}$:

$$\begin{cases} \mathrm{d}q_t = M^{-1}p_t\mathrm{d}t, \\ \mathrm{d}p_t = -\nabla V(q_t)\mathrm{d}t - \gamma M^{-1}p_t\mathrm{d}t + \sigma \mathrm{d}B_t, \end{cases} \tag{1.1}$$

où $\sigma = \sqrt{2\gamma\beta^{-1}}$, $\beta^{-1} = k_BT$ (k_B étant la constante de Boltzmann), $M \in \mathbb{R}^{d\times d}$ la matrice diagonale donnant la masse de chaque particule et $(B_t)_{t\geq 0}$ le mouvement brownien, traduisant ici l'agitation thermique au sein du système. Le processus $(q_t,p_t)_{t\geq 0}$ est appelé dans la littérature processus de Langevin. On voit également souvent apparaître dans la littérature un processus relié appelé le processus de Langevin suramorti, qui lui n'est décrit que par une coordonnée de position $\overline{q}_t \in \mathbb{R}^d$ au cours du temps. L'EDS suivie par le processus de Langevin suramorti est donnée de la manière suivante dans le cas où M est la matrice identité :

$$\mathrm{d}\overline{q}_t = -\nabla V(\overline{q}_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t. \tag{1.2}$$

D'ailleurs, il est possible de retrouver sur un intervalle de temps de durée $T_{max} > 0$, la loi du processus de Langevin suramorti $(\overline{q}_t)_{t\in[0,T_{max}]}$ cf. [56], en faisant tendre le coefficient de friction γ vers l'infini dans la loi de la position du processus de Langevin changée d'échelle de temps $(q_{\gamma t})_{t\in[0,T_{max}]}$.

La distribution stationnaire du processus de Langevin (1.1) est bien connue et elle est donnée par la mesure suivante dans $\mathbb{R}^{2d}$:

$$\nu(\mathrm{d}q\mathrm{d}p) = \frac{\mathrm{e}^{-\beta\left(\frac{1}{2}p\cdot M^{-1}p + V(q)\right)}}{Z}\mathrm{d}q\mathrm{d}p, \tag{1.3}$$

où $Z = \int_{\mathbb{R}^{2d}} \mathrm{e}^{-\beta\left(\frac{1}{2}p\cdot M^{-1}p+V(q)\right)}\mathrm{d}q\mathrm{d}p$ est supposé fini. Les propriétés thermodynamiques du système peuvent être caractérisées par des fonctionnelles du processus à l'équilibre pouvant s'écrire sous la forme $\int_{\mathbb{R}^{2d}} \varphi(q,p)\nu(\mathrm{d}q\mathrm{d}p)$. Evaluer ces intégrales par des quadratures numériques représente un défi en soi lorsque l'on considère un nombre important de particules en raison de la malédiction de la dimension ($d = 3n$ devient très grand). Il est dès lors nécessaire de recourir à d'autres méthodes. L'une de ces approches alternatives consiste à discrétiser en temps la dynamique (1.1) pour simuler la trajectoire par une chaine de Markov, puis d'utiliser un résultat de convergence de la distribution de cette chaine vers sa mesure stationnaire comme prouvé dans [40].

En pratique, le pas de temps utilisé pour les simulations numériques de dynamiques moléculaires est de l'ordre de la femtoseconde (10^{-15} s) tandis que les phénomènes macroscopiques apparaissant sur le système peuvent se produire au bout d'un temps allant de la microseconde (10^{-6} s) à l'heure (10^3 s), voire beaucoup plus pour certaines transitions de phase. La simulation de ces phénomènes nécessite donc un nombre gigantesque d'itérations du schéma numérique souvent irréalisable en pratique avec les puissances de calcul actuelles, en tout cas en utilisant un algorithme naïf basé sur une simple discrétisation de (1.1) (on discutera en Section 1.2.3 un exemple de méthodes numériques permettant de contourner cette difficulté).

Cette différence d'échelles de temps entre les comportements microscopique et macroscopique est liée à un phénomène bien connu appelé la métastabilité. On dit qu'un processus est métastable si

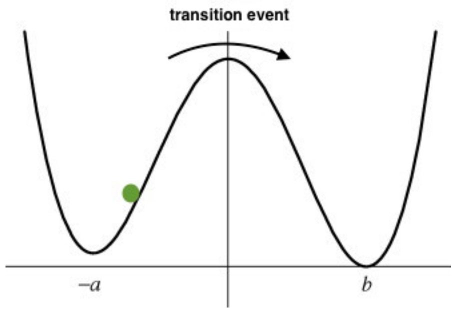

FIGURE 1.1 : Particule dans un potentiel à double-puits

il reste piégé dans des zones de l'espace pendant des temps très longs. Ces zones sont appelées des états métastables. Un exemple très simple d'une telle situation est donné dans la Figure 1.1 ci-dessus et expliqué ci-dessous.

Considérons une particule suivant le processus de Langevin (1.1) en une dimension ($d = 1$) avec le potentiel V représenté sur la Figure 1.1. Si la position de la particule correspond à la boule verte, alors celle-ci va osciller pendant un temps très long autour du minimum local $q = -a$ avant d'effectuer un saut vers le puits de potentiel centré en $q = b$. Dans cette situation l'état métastable correspond à un puits de potentiel. Le système oscille très longtemps avant de franchir la barrière énergétique nécessaire pour quitter son état présent. Cependant, d'autres types de métastabilité existent, par exemple la métastabilité "entropique" où la transition ne nécessite pas de franchir une barrière énergétique mais de s'aventurer par un passage très étroit. L'étude des processus métastables basée sur la distribution quasi-stationnaire, qui est la motivation de ce travail de thèse, s'applique à la fois à des métastabilités énergétique et entropique.

1.2 Metastabilité, distributions quasi-stationnaires et méthodes numériques associées

L'objectif de cette section est de présenter, sur le cas simple de la dynamique de Langevin suramortie (1.2), la notion de distribution quasi-stationnaire (DQS), ainsi que son utilité pour simuler des processus métastables sur des temps longs. Un objectif de la thèse est d'étendre cette approche à la dynamique de Langevin (1.1), ce qui sera l'objet de la prochaine section, où nous présenterons les résultats principaux de cette thèse.

Soit $d \geq 1$. Soit $(\Omega, \mathscr{F}, (\mathscr{F}_t)_{t\geq 0}, \mathbb{P})$ un espace de probabilité filtré et $(B_t)_{t\geq 0}$ un $(\mathscr{F}_t)_{t\geq 0}$-mouvement Brownien dans $\mathbb{R}^d$. Soit $F : \mathbb{R}^d \mapsto \mathbb{R}^d$. A partir de cette section nous considérerons le processus de Langevin suramorti $(\overline{q}_t)_{t\geq 0}$, solution de l'EDS :

$$\mathrm{d}\overline{q}_t = F(\overline{q}_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t, \tag{1.4}$$

où F ne s'écrit pas nécessairement sous forme gradient. Son générateur infinitésimal $\overline{\mathscr{L}}$ est donné par

$$\overline{\mathscr{L}} := F \cdot \nabla + \beta^{-1}\Delta.$$

Soit à présent $\mathscr{O}$ un sous ensemble de $\mathbb{R}^d$. Nous faisons les hypothèses suivantes sur F et $\mathscr{O}$:

Hypothèse (F1). $F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$.

Hypothèse (O1). *$\mathscr{O}$ est un ouvert $\mathscr{C}^2$ borné de $\mathbb{R}^d$.*

Hypothèse (O2). *L'ensemble $\mathscr{O}$ est connexe.*

Pour $A \in \mathscr{F}$, $q \in \mathscr{O}$, notons $\mathbb{P}_q(A)$ la probabilité de l'événement A sous la condition $\overline{q}_0 = q$. Si θ est une mesure de probabilité sur $\mathscr{O}$, nous noterons $\mathbb{P}_\theta(A) = \int_{\mathscr{O}} \mathbb{P}_q(A)\theta(\mathrm{d}q)$. On notera $\overline{\tau}_\partial$ le premier temps de sortie du processus $(\overline{q}_t)_{t\geq 0}$ du domaine $\mathscr{O}$,

$$\overline{\tau}_\partial := \inf\{t > 0 : \overline{q}_t \notin \mathscr{O}\}.$$

1.2.1 Processus absorbé

Definition 1.2.1 (Processus absorbé)**.** *Sous les hypothèses (F1) et (O1), le processus $(\overline{q}_t)_{0\leq t\leq \overline{\tau}_\partial}$ est appelé processus suramorti absorbé.*

Nous rappelons brièvement dans cette section certains résultats bien connus sur le processus suramorti absorbé dans un domaine borné régulier [36, 50, 19, 30, 32, 33, 31]. Ces résultats seront en particulier utiles pour introduire la DQS associé au processus absorbé. Nous commençons par rappeler qu'il existe une unique solution classique (i.e. $\mathscr{C}^{1,2}(\mathbb{R}_+^* \times \mathscr{O}) \cap \mathscr{C}^b(\mathbb{R}_+ \times \overline{\mathscr{O}} \setminus (\{0\} \times \partial\mathscr{O}))$) au problème suivant avec une condition initiale $\overline{f} \in \mathscr{C}^b(\mathscr{O})$ et une condition au bord du domaine, $\overline{g} \in \mathscr{C}^b(\partial\mathscr{O})$:

$$\begin{cases} \partial_t \overline{u}(t,q) = \overline{\mathscr{L}}\overline{u}(t,q), & t > 0, \quad q \in \mathscr{O}, \\ \overline{u}(0,q) = \overline{f}(q), & q \in \mathscr{O}, \\ \overline{u}(t,q) = \overline{g}(q), & t > 0, \quad q \in \partial\mathscr{O}. \end{cases} \tag{1.5}$$

Ce résultat est classiquement obtenu de la manière suivante :

1. construire une solution faible $\overline{u}$ à partir d'une approche variationnelle ;
2. déduire de la régularisation parabolique (l'opérateur $\overline{\mathscr{L}}$ est elliptique) que les solutions faibles sont en réalité régulières ;
3. utiliser la régularité de $\overline{u}$ pour appliquer la formule d'Itô afin d'obtenir la représentation probabiliste suivante
$$\overline{u}(t,q) = \mathbb{E}_q\left[\mathbb{1}_{\overline{\tau}_\partial > t}\overline{f}(\overline{q}_t) + \mathbb{1}_{\overline{\tau}_\partial \leq t}\overline{g}(\overline{q}_{\overline{\tau}_\partial})\right].$$
La représentation probabiliste de la solution implique en particulier l'unicité de solution classique au problème (1.5).

On peut citer Evans [30, Section 7.1] pour la preuve des deux premières étapes ainsi que Friedman [32, 33, 31] pour la dernière étape. On peut également retrouver dans ces références d'autres résultats importants sur le problème (1.5) comme l'inégalité d'Harnack ou le principe du maximum.

Les propriétés suivantes sont également bien connues pour le processus absorbé :

- pour tout $q \in \mathscr{O}$, la mesure $\overline{\mathrm{P}}_t^{\mathscr{O}}(q,\cdot) := \mathbb{P}_q(\overline{q}_t \in \cdot, \overline{\tau}_\partial > t)$ admet une densité (dite de transition) régulière $\overline{\mathrm{p}}_t^{\mathscr{O}}(q,q')$ par rapport à la mesure de Lebesgue sur $\mathscr{O}$;
- cette densité de transition satisfait les équations de Kolmogorov rétrograde et progressive sur $\mathbb{R}_+^* \times \mathscr{O} \times \mathscr{O}$
$$\partial_t \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q') = \mathscr{L}_q \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q'), \qquad \partial_t \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q') = \mathscr{L}_{q'}^* \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q'),$$
où $\mathscr{L}^*$ est l'adjoint de $\mathscr{L}$ dans $\mathrm{L}^2(\mathrm{d}x)$ et les indices q, q' dans la notation $\mathscr{L}_q$, $\mathscr{L}_{q'}^*$ indiquent sur quelle variable l'opérateur agit ;
- pour tout $t > 0$, la fonction $\overline{\mathrm{p}}_t^{\mathscr{O}}$ est strictement positive on $\mathscr{O} \times \mathscr{O}$ et admet une extension continue sur $\overline{\mathscr{O}} \times \overline{\mathscr{O}}$ qui s'annule au bord $\partial(\mathscr{O} \times \mathscr{O})$;
- pour $T > 0$, la densité de transition $\overline{\mathrm{p}}_t^{\mathscr{O}}(q,q')$ admet un majorant gaussien de la forme $\mathrm{e}^{-\alpha/(4t)|q-q'|^2}$, avec α une constante indépendante de t, sur $(0,T] \times \mathscr{O} \times \mathscr{O}$.

La dernière propriété de majoration gaussienne découle par exemple des inégalités de D.G. Aronson [4] ou du résultat de P.Baldi [6, Théorème 4.2] basé sur la méthode parametrix.

1.2.2 Metastabilité et distribution quasi-stationnaire

Revenons à la définition de la métastabilité proposée à la fin de la section 1.1. Il convient de se demander ce qu'il se passe par exemple lorsque le processus de Langevin suramorti (1.4) demeure longtemps piégé dans un état : est ce que le processus atteint un état d'équilibre "local" sur le domaine considéré ? Nous consacrons cette sous-section aux réponses qui ont été apportées dans la littérature à cette question dans le cas du processus suramorti (1.4), absorbé au bord d'un domaine $\mathscr{O}$ régulier borné.

Intuitivement, cette mesure d'équilibre local, qu'on notera $\overline{\mu}$, est à support sur l'état que nous considérons et elle est telle que si le processus $(\overline{q}_t)_{t\geq 0}$ est initialement distribué suivant $\overline{\mu}$ alors il continue de suivre la même loi $\overline{\mu}$ tant qu'il n'est pas sorti du domaine. Considérons un domaine $\mathscr{O} \subset \mathbb{R}^d$, la définition rigoureuse est la suivante :

Definition 1.2.2 (Distribution quasi-stationnaire (DQS))**.** *Une mesure de probabilité $\overline{\mu}$ sur $\mathscr{O} \subset \mathbb{R}^d$ est une DQS sur $\mathscr{O}$ pour le process $(\overline{q}_t)_{t\geq 0}$, si pour tout borélien A de $\mathscr{O}$,*

$$\forall t \geq 0, \qquad \mathbb{P}_{\overline{\mu}}(\overline{q}_t \in A, \overline{\tau}_\partial > t) = \overline{\mu}(A)\mathbb{P}_{\overline{\mu}}(\overline{\tau}_\partial > t).$$

Une littérature importante est consacrée aux DQS pour des processus de Markov à temps discret ou continu comme le cas des diffusions, citons par exemple [23] qui est un des ouvrages de référence sur ces questions. Le cas qui nous intéresse cependant est celui des DQS pour des processus de diffusion comme (1.1) ou (1.4). La littérature spécifique aux DQS pour des diffusions est également importante. Parmi les travaux sur ces questions nous pouvons citer [68, 64, 16, 50, 51, 55, 24, 21, 20]. Dans ces études, le domaine $\mathscr{O}$ associé à la DQS est borné et dispose d'une régularité $\mathscr{C}^1$ ou $\mathscr{C}^2$. De plus, les diffusions considérées sont elliptiques, ce qui est le cas de (1.4) mais pas de (1.1). Ceci à l'exception de l'article récent [20] où N. Champagnat et D. Villemonnais concentrent leur étude quant à eux, sur des processus de Markov généraux sur des domaines qui ne sont pas nécessairement bornés ni réguliers. Ils obtiennent un certain nombre de critères qui garantissent l'existence et l'unicité de la DQS, sur lesquels nous reviendrons à la section 1.3.3.

En plus de la question de l'existence et unicité d'une DQS, il convient également de se poser la question de la convergence de la loi du processus conditionné à rester dans le domaine $\mathscr{O}$, soit la loi $\mathscr{L}(\overline{q}_t|\overline{\tau}_\partial > t)$, lorsque le temps t tend vers l'infini. En particulier, nous souhaiterions une convergence vers la DQS sur $\mathscr{O}$ du processus $(\overline{q}_t)_{t\geq 0}$. Les résultats obtenus dans la littérature vont dans ce sens et traitent de ces trois questions d'existence, d'unicité et de convergence, avec des outils relativement diversifiés.

Dans [55] par exemple, F s'écrit $-\nabla V$ et l'approche utilisée se base sur le fait que le processus $(\overline{q}_t)_{t\geq 0}$ est réversible par rapport à la mesure $\overline{\nu}(\mathrm{d}q) = \frac{\mathrm{e}^{-\beta V(q)}}{Z}\mathrm{d}q$ où $Z = \int_{\mathbb{R}^d} \mathrm{e}^{-\beta V(q')}\mathrm{d}q'$ supposément finie. L'inverse de l'opérateur $\overline{\mathscr{L}}$ avec condition de Dirichlet au bord $\partial\mathscr{O}$ étant compact de $\mathrm{L}^2(\mathrm{d}\overline{\nu})$ vers $\mathrm{L}^2(\mathrm{d}\overline{\nu})$ et symétrique, il est possible d'obtenir une décomposition spectrale de $\overline{\mathscr{L}}$ avec cette condition au bord. On peut alors montrer que le vecteur propre u_1 associé à la plus grande valeur propre de $\overline{\mathscr{L}}$ avec condition de Dirichlet au bord $\partial\mathscr{O}$ est tel que $\frac{u_1\mathrm{e}^{-\beta V}}{Z}$ est la densité de la DQS. On en déduit l'existence et l'unicité de la DQS ainsi que la convergence de la loi conditionnelle vers la DQS pour le processus $(\overline{q}_t)_{t\geq 0}$ en utilisant la décomposition spectrale. Dans le cas plus général où F ne s'écrit pas comme gradient d'une fonctionnelle, l'argument de réversibilité et donc de symétrie sur $\overline{\mathscr{L}}$ ne fonctionne pas. Cependant ce cas a été traité dans [36] par exemple, en appliquant le théorème de Krein-Rutman au dual du semigroupe du processus absorbé sur l'espace de Banach

$$\{f \in \mathscr{C}^b(\mathscr{O}) : f/\mathrm{d}_\partial \text{ est uniformément continue sur } \mathscr{O}\},$$

où d_∂ désigne la distance Euclidienne au bord $\partial\mathscr{O}$, permettant d'obtenir le premier vecteur propre de ce semigroupe et donc la densité de la DQS. Une autre approche plus probabiliste a été invoquée dans [19] où les auteurs prouvent que le semigroupe du processus $(\overline{q}_t)_{t\geq 0}$ absorbé satisfait certaines estimées de gradient, une condition d'irréductibilité ainsi qu'un contrôle de la probabilité d'absorbtion près du bord $\mathscr{O}$, à partir desquelles ils sont capables de déduire l'existence d'une unique DQS ainsi que la convergence attendue de la loi conditionnelle. Nous n'avons mentionné que trois approches et d'autres preuves peuvent être trouvées par exemple dans la littérature mentionnée plus haut. Au final, les résultats obtenus dans la littérature peuvent être résumés dans le théorème ci-dessous dans le cas du processus suramorti $(\overline{q}_t)_{t\geq 0}$.

Théorème 1.2.3 ([19, 36, 55, 50])**.** *Supposons les hypothèses (F1), (O1) et (O2) satisfaites, il existe alors une unique DQS $\overline{\mu}$ sur $\mathscr{O}$ pour le processus $(\overline{q}_t)_{t\geq 0}$ satisfaisant (1.4). De plus,*

(i) il existe une fonction $\overline{\psi} \in \mathscr{C}^2(\mathscr{O}) \cap \mathscr{C}^b(\overline{\mathscr{O}})$ telle que $\overline{\mu}(\mathrm{d}q) = \overline{\psi}(q)\mathrm{d}q$, où $\mathrm{d}q$ est la mesure de Lebesgue sur $\mathbb{R}^d$,

(ii) il existe un unique couple $(\overline{\lambda}, \overline{\eta})$, à normalisation près de $\overline{\eta}$, tel que $\overline{\eta}$ est une solution positive classique dans $\mathscr{C}^2(\mathscr{O}) \cap \mathscr{C}^b(\overline{\mathscr{O}})$ du problème aux valeurs propres suivant

$$\begin{cases} \mathscr{L}^*\overline{\eta}(q) = -\overline{\lambda}\,\overline{\eta}(q), & q \in \mathscr{O}, \\ \quad\overline{\eta}(q) = 0, & q \in \partial\mathscr{O}. \end{cases}$$

De plus $\frac{\overline{\eta}}{\int_{\mathscr{O}} \overline{\eta}} = \overline{\psi}$ et $\overline{\lambda}$ est la plus petite valeur propre de $-\mathscr{L}^*$, qui satisfait de plus $\overline{\lambda} > 0$.

(iii) Il existe $C > 0$, $\alpha > 0$ tels que pour toute mesure de probabilité θ sur $\mathscr{O}$, pour tout $t \geq 0$,

$$\left\| \mathbb{P}_\theta(\overline{q}_t \in \cdot | \overline{\tau}_\partial > t) - \overline{\mu}(\cdot) \right\|_{TV} \leq C\mathrm{e}^{-\alpha t},$$

où $\| \cdot \|_{TV}$ correspond à la norme en variation totale.

La convergence de la loi du processus $(\overline{q}_t)_{t\geq 0}$ conditionné à rester dans $\mathscr{O}$ vers la DQS s'effectue donc exponentiellement vite lorsque le temps tend vers l'infini. De plus, le préfacteur C ci-dessous ne dépend pas de la distribution initiale θ. Egalement, si le paramètre α obtenu est proche de l'optimalité alors $1/\alpha$ peut être vu comme le temps caractéristique de convergence vers la DQS dans $\mathscr{O}$. Nous pouvons alors fournir une définition plus précise de la métastabilité : l'évènement de sortie est métastable si le temps de sortie du domaine est bien plus grand que le temps d'atteinte de la DQS, qui est typiquement de l'ordre de $1/\alpha$.

Finalement, démarrant de la DQS du domaine $\mathscr{O}$, l'événement de sortie du domaine $\mathscr{O}$, i.e. le couple (temps de sortie, point de sortie par $\partial\mathscr{O}$), satisfait certaines propriétés intéressantes cf. [55, Proposition 2.4].

Théorème 1.2.4 ([55])**.** *Supposons les hypothèses du théorème 1.2.3 satisfaites. Si $\overline{q}_0$ est initialement distribué suivant la DQS $\overline{\mu}$ alors, suivant les notations du théorème précédent,*

(i) $\overline{\tau}_\partial$ suit la loi exponentielle de paramètre $\overline{\lambda}$,

(ii) $\overline{q}_{\overline{\tau}_\partial}$ est indépendant de $\overline{\tau}_\partial$ et suit la loi $-\frac{\beta^{-1}}{\overline{\lambda}}\nabla\overline{\psi} \cdot n\mathrm{d}\sigma_{\partial\mathscr{O}}$,

où $\mathrm{d}\sigma_{\partial\mathscr{O}}$ est la mesure de Lebesgue sur $\partial\mathscr{O}$ et pour $q \in \partial\mathscr{O}$, $n(q)$ est le vecteur normal unitaire sortant de $\mathscr{O}$.

Remarque 1.2.5. *Le fait que $\overline{\tau}_\partial$ satisfait (i) et que $\overline{q}_{\overline{\tau}_\partial}$ est indépendant de $\overline{\tau}_\partial$ est une propriété générale des DQS [23, Théorème 2.6].*

Le corollaire suivant est un résultat important qui découle du théorème ci-dessus et qui sera très utile pour la méthode numérique Parallel Replica de la sous-section suivante.

Corollaire 1.2.6. *Supposons les hypothèses du théorème 1.2.4 satisfaites. Soit un entier $N \geq 1$, considérons pour $i \in [\![1, N]\!]$, N répliques indépendantes $(\overline{q}_t^{(i)})_{t\geq 0}$ initialement distribuées suivant la DQS sur $\mathscr{O}$. Soit $\overline{\tau}_\partial^{(i)}$ le premier temps de sortie de $\mathscr{O}$ de la i-ème réplique, et notons $i^* := \mathrm{argmin}_{1\leq i\leq N}\, \overline{\tau}_\partial^{(i)}$. Nous avons alors l'égalité suivante en loi*

$$\left(\overline{\tau}_\partial^{(1)}, \overline{q}^{(1)}_{\overline{\tau}_\partial^{(1)}}\right) \overset{\mathscr{L}}{=} \left(N\overline{\tau}_\partial^{(i^*)}, \overline{q}^{(i^*)}_{\overline{\tau}_\partial^{(i^*)}}\right).$$

1.2.3 Méthode de simulation numérique accélérée : Parallel Replica

Afin de pallier le phénomène de métastabilité dans les dynamiques moléculaires, plusieurs méthodes ont été pensées afin de simuler plus rapidement l'évènement de sortie $(\overline{\tau}_\partial, \overline{q}_{\overline{\tau}_\partial})$. Nous allons ici détailler la méthode Parallel Replica qui a été introduite par A. Voter en 1998 [77] et dont la justification mathématique s'appuie sur la notion de DQS et ses propriétés détaillées précédemment comme expliqué originellement dans [55]. Dans cette méthode, nous décomposons le domaine entier, par exemple $\mathbb{R}^d$, en une partition d'états (typiquement les états métastables mentionnés en début d'introduction). On associe alors à chaque état un entier naturel qui lui est propre et on définit une fonction d'état S associant à chaque point $q \in \mathbb{R}^d$ le numéro de l'état dans lequel se situe q,

$$S : q \in \mathbb{R}^d \mapsto S(q) \in \mathbb{N}.$$

Dans le cas d'états métastables énergétiques, on peut définir les états métastables comme les bassins d'attraction des minima locaux de V, qui peuvent être identifiés en pratique en itérant un algorithme de descente de gradient $\dot{q} = -\nabla V(q)$. Dans Parallel Replica, nous ne nous intéressons alors plus à la trajectoire complète du processus $(\overline{q}_t)_{t\geq 0}$ mais seulement à la trajectoire $(S(\overline{q}_t))_{t\geq 0}$. La motivation étant que les modifications macroscopiques du système sont caractérisées par ces transitions entre états métastables.

La méthode Parallel Replica se divise en trois étapes cycliques détaillées ci-dessous. Cette méthode peut s'appliquer sans distinction à une dynamique issue de (1.4) ou de (1.1), cependant la justification mathématique n'est donnée dans la littérature actuelle que dans le cas suramorti. L'extension au cas du processus de Langevin se fera dans la section suivante.

Etape de décorrelation : Nous commençons par considérer une trajectoire de référence suivant (1.4). Pour cela nous itérons un schéma numérique de pas de temps Δt sur la dynamique (1.4). A chaque itération de cette étape nous déterminons l'état dans lequel se situe la trajectoire de référence à l'aide de la fonction S. Cette étape se poursuit tant que le processus change d'état avant d'atteindre la DQS. Elle s'arrête lorsque la trajectoire reste piégée dans un état $\mathscr{O}$ durant un temps suffisamment long tel qu'avec une bonne approximation nous puissions supposer que la dynamique est distribuée suivant la DQS de $\mathscr{O}$. Ce temps long est appelé temps de corrélation τ_{corr}, et est typiquement de l'ordre de $1/\alpha$ suivant les notations du théorème 1.2.3. Notons à présent T_1 le temps de la trajectoire de référence lorsque l'étape de décorrelation a abouti à une situation où la particule a été piégée dans un état pendant ce temps de décorrélation τ_{corr}.

Etape de déphasage : La trajectoire de référence est arrêtée durant cette étape, le temps physique de cette trajectoire demeure donc au temps T_1 ici. L'objectif à présent est de construire N répliques distribuées suivant la DQS dans $\mathscr{O}$. Cela se fait par exemple à l'aide de la méthode de rejet : on lance des trajectoires indépendantes suivant (1.4) et on attend qu'elles restent durant un temps τ_{corr} dans le domaine $\mathscr{O}$. Si l'une de ces trajectoires sort alors elle est réinitialisée à partir de son point de départ.

Etape parallèle : Maintenant que nous avons N répliques indépendantes distribuées suivant la DQS du domaine, nous pouvons utiliser le résultat du corollaire 1.2.6. Nous faisons évoluer alors les N répliques précédentes suivant la dynamique (1.4) à partir d'un temps $t = 0$ jusqu'à ce que l'une d'entre elles sorte à un temps $t = t^*$ par un point x^*. Le résultat du corollaire 1.2.6 indique alors qu'un tirage de l'évènement de sortie correspond au temps $(T_1 + Nt^*, x^*)$. La méthode Parallel Replica est alors réinitialisée à partir du point de sortie x^*.

Remarque 1.2.7. *Nous renvoyons à [42] et [12] pour des évolutions récentes de l'algorithme Parallel Replica permettant notamment de considérer des états qui ne constituent pas une partition du domaine, et d'évaluer en direct le temps de décorrélation associé à un état et à une condition initiale spécifique dans cet état en utilisant un système particulaire de Fleming-Viot. Ce système particulaire permet également d'échantillonner la DQS par une méthode alternative à la méthode du rejet évoquée ci-dessus.*

D'autres méthodes ont été développées comme Hyperdynamics [76] qui s'appuie sur une modification du potentiel pour accélerer l'évènement de sortie, et Temperature Accelerated Dynamics [74] où la température du thermostat est augmentée. Ces méthodes peuvent également être analysées en utilisant le concept de DQS, mais nécessitent d'identifier plus précisément la loi de sortie (utilisation de formules d'Eyring-Kramers) [25].

1.3 Extension à la dynamique de Langevin

Un des objectifs de la thèse est de généraliser au processus de Langevin (1.1) les résultats énoncés précédemment pour le processus de Langevin suramorti (1.4). En particulier, l'existence d'une distribution quasi-stationnaire sur un domaine borné en position justifie l'utilisation de l'algorithme Parallel Replica présenté en Section 1.2.3 au processus de Langevin sur des états bornés en position.

Soient $\gamma \in \mathbb{R}$, $\sigma > 0$ et $F : \mathbb{R}^d \mapsto \mathbb{R}^d$. Dans cette section, nous appellerons processus de Langevin $(X_t = (q_t, p_t))_{t\geq 0}$, la solution de l'EDS suivante :

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sigma \mathrm{d}B_t. \end{cases} \tag{1.6}$$

La différence avec (1.1) est que M est ici la matrice identité et F ne s'écrit pas forcément sous forme gradient. De plus, σ peut être indépendant de γ avec γ étant potentiellement négatif. Son générateur infinitésimal $\mathscr{L}$, aussi appelé opérateur de Fokker-Planck cinétique, est donné pour $(q, p) \in \mathbb{R}^d \times \mathbb{R}^d$ par

$$\mathscr{L} := p \cdot \nabla_q + F(q) \cdot \nabla_p - \gamma p \cdot \nabla_p + \frac{\sigma^2}{2}\Delta_p. \tag{1.7}$$

Son adjoint $\mathscr{L}^*$ dans $\mathrm{L}^2(\mathrm{d}x)$ s'écrit :

$$\mathscr{L}^* = -p \cdot \nabla_q - F(q) \cdot \nabla_p + \gamma \mathrm{div}_p(p\cdot) + \frac{\sigma^2}{2}\Delta.$$

Nous commencerons cette section par évoquer certains résultats obtenus dans la littérature sur le processus de Langevin non absorbé. Puis dans la section 1.3.2, nous nous intéresserons aux résultats présentés dans le chapitre 2 sur le processus de Langevin absorbé au bord d'un domaine. Ces outils nous permettront alors d'obtenir les résultats des chapitres 3 et 4, liés notamment à l'étude des distributions quasi-stationnaires pour le processus de Langevin, et détaillés en section 1.3.3. Finalement, nous conclurons cette section en présentant les résultats obtenus sur la trace du processus de Langevin traversant une frontière et présentés en section 1.3.4.

1.3.1 Quelques résultats connus sur le procesus de Langevin

Nous faisons ici l'hypothèse suivante supplémentaire sur F :

Hypothèse (F2). *$F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ et F est borné et globalement lipschitzien sur $\mathbb{R}^d$.*

Sous l'hypothèse (F2), le coefficient de dérive $(q, p) \mapsto (p, F(q) - \gamma p)$ dans (1.6) est globalement lipschitzien. Il existe donc une unique solution forte à (1.6) définie globalement, que nous noterons $(X_t)_{t\geq 0}$.

Pour $t > 0$, $x \in \mathbb{R}^{2d}$, définissons le noyau de transition $\mathrm{P}_t(x, \cdot)$ associé au processus $(X_t)_{t\geq 0}$:

$$\forall t > 0, \quad \forall x \in \mathbb{R}^{2d}, \quad \forall A \in \mathscr{B}(\mathbb{R}^{2d}), \qquad \mathrm{P}_t(x, A) := \mathbb{P}_x(X_t \in A).$$

Ce noyau de transition admet une densité de transition strictement positive $(t, x, y) \mapsto \mathrm{p}_t(x, y)$ qui est dans $\mathscr{C}^\infty(\mathbb{R}_+^* \times \mathbb{R}^{2d} \times \mathbb{R}^{2d})$ cf. [71, Corollaire 7.2] et [44, Corollary 3.3]. Nous avons donc

$$\forall t > 0, \quad \forall x \in \mathbb{R}^{2d}, \quad \forall A \in \mathscr{B}(\mathbb{R}^{2d}), \qquad \mathrm{P}_t(x, A) = \int_A \mathrm{p}_t(x, y)\mathrm{d}y.$$

Remarque 1.3.1. *Un travail récent [52] a permis d'obtenir à partir de la méthode parametrix une majoration gaussienne de la densité de transition* $\mathrm{p}_t(x,y)$ *lorsque le coefficient de drift* $(q,p) \mapsto (p, F(q) - \gamma p)$ *est borné et globalement lipschitzien. Cela est le cas lorsque l'hypothèse (F2) est satisfaite et que* $\gamma = 0$. *Nous verrons par la suite que ce résultat peut être étendu dans notre cas quand* $\gamma \neq 0$ *en nous inspirant du schéma de preuve dans [52].*

Pour $f \in \mathscr{C}^b(\mathbb{R}^{2d})$, nous avons alors que

$$\forall t > 0, \quad \forall x \in \mathbb{R}^{2d}, \qquad \mathbb{E}_x\left[f(X_t)\right] = \int_{\mathbb{R}^{2d}} \mathrm{p}_t(x,y)\mathrm{d}y.$$

Définissons alors

$$u(t,x) = \begin{cases} \mathbb{E}_x\left[f(X_t)\right] & \text{si } t > 0, x \in \mathbb{R}^{2d}, \\ f(x) & \text{si } t = 0, x \in \mathbb{R}^{2d}. \end{cases}$$

Il découle de [75] que u est l'unique solution classique dans $\mathscr{C}^{1,2}(\mathbb{R}_+^* \times \mathbb{R}^{2d}) \cap \mathscr{C}^b(\mathbb{R}_+ \times \mathbb{R}^{2d})$ au problème de Cauchy suivant

$$\begin{cases} \partial_t u(t,x) = \mathscr{L} u(t,x), & t > 0, x \in \mathbb{R}^{2d}, \\ u(0,x) = f(x), & x \in \mathbb{R}^{2d}. \end{cases}$$

Concernant l'équation associée à l'opérateur de Fokker-Planck cinétique avec condition initiale et condition de bord, la littérature s'est principalement intéressée à des solutions faibles de ce problème : citons par exemple les travaux [65, 3, 15, 47]. Nous reviendrons en particulier sur la solution faible construite dans [47] dans la section 1.4. Dans ce travail de thèse nous avons étudié les solutions classiques de l'équation de Fokker-Planck cinétique avec condition initiale et condition de bord, que nous définirons et dont nous détaillerons les résultats dans les sous-sections suivantes.

1.3.2 Chapitre 2 : Semigroupe du processus de diffusion de Langevin absorbé

Nous considérons ici le processus de Langevin $(X_t = (q_t, p_t))_{t \geq 0}$ défini dans (1.6). Soit $\mathscr{O} \subset \mathbb{R}^d$ et D le sous ensemble suivant de $\mathbb{R}^{2d}$,

$$D := \mathscr{O} \times \mathbb{R}^d.$$

Notons $\tau_\partial := \inf\{t > 0, X_t \notin D\}$ et définissons le processus de Langevin absorbé comme suit.

Definition 1.3.2 (Processus de Langevin absorbé)**.** *Sous les hypothèses (F1) et (O1), on appelle processus de Langevin absorbé le processus* $(X_t)_{0 \leq t \leq \tau_\partial}$.

Remarque 1.3.3. *Nous n'avons besoin que de l'hypothèse (F1) pour la définition du processus de Langevin absorbé. En effet, supposons l'hypothèse (F1) satisfaite, alors le coefficient de dérive* $(q,p) \mapsto (p, F(q) - \gamma p)$ *dans (1.6) est localement lipschitzien dans* $\mathbb{R}^{2d}$. *Il existe donc une unique solution forte jusqu'à un temps d'explosion. De plus, le coefficient de dérive est globalement lipschitz sur* $\overline{\mathscr{O}} \times \mathbb{R}^d$ *donc le temps d'explosion du processus* $(X_t)_{t \geq 0}$ *est donc nécessairement supérieur presque sûrement au temps de sortie* τ_∂ *de* D. *La définition ci-dessus est donc bien posée.*

Notons $n(q) \in \mathbb{R}^d$ le vecteur unitaire sortant de $\mathscr{O}$ au point $q \in \partial \mathscr{O}$. Définissons la partition suivante de ∂D :

- $\Gamma^0 = \{(q,p) \in \partial \mathscr{O} \times \mathbb{R}^d : p \cdot n(q) = 0\}$,
- $\Gamma^+ = \{(q,p) \in \partial \mathscr{O} \times \mathbb{R}^d : p \cdot n(q) > 0\}$,
- $\Gamma^- = \{(q,p) \in \partial \mathscr{O} \times \mathbb{R}^d : p \cdot n(q) < 0\}$.

Nous énonçons dans cette sous-section certains résultats importants issus du chapitre 2 de la thèse. Commençons par considérer le problème Fokker-Planck cinétique avec conditions initiale et de bord. Contrairement au cas elliptique et l'équation (1.5), les conditions de bord ne s'appliquent ici qu'à la portion Γ^+ du bord ∂D.

Théorème 1.3.4 (Solution classique à l'équation Fokker-Planck cinétique sur D)**.** *Supposons les hypothèses (O1) et (F1) satisfaites. Soit $f \in \mathscr{C}^b(D \cup \Gamma^-)$ et $g \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$, on définit la fonction u sur $\mathbb{R}_+ \times \overline{D}$ par*

$$u : (t, x) \mapsto \mathbb{E}_x \left[\mathbb{1}_{\tau_\partial > t} f(X_t) + \mathbb{1}_{\tau_\partial \leq t} g(X_{\tau_\partial})\right], \tag{1.8}$$

alors u est l'unique solution classique dans $\mathscr{C}^{1,2}(\mathbb{R}_+^* \times D) \cap \mathscr{C}^b((\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+))$ au problème

$$\begin{cases} \partial_t u(t,x) = \mathscr{L} u(t,x), & t > 0, \quad x \in D, \\ u(0,x) = f(x), & x \in D, \\ u(t,x) = g(x), & t > 0, \quad x \in \Gamma^+. \end{cases} \tag{1.9}$$

Considérons maintenant le noyau de transition P_t^D associé au processus de Langevin absorbé :

$$\forall t \geq 0, \quad \forall x \in D, \quad \forall A \in \mathscr{B}(D), \qquad \mathrm{P}_t^D(x, A) := \mathbb{P}_x(X_t \in A, \tau_\partial > t).$$

Nous montrons dans ce travail que le noyau de transition P_t^D admet pour $t > 0$ une densité de transition régulière.

Théorème 1.3.5 (Densité de transition du processus absorbé)**.** *Sous les hypothèses (O1) et (F1), il existe une fonction*

$$(t, x, y) \mapsto \mathrm{p}_t^D(x, y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D \times D) \cap \mathscr{C}(\mathbb{R}_+^* \times \overline{D} \times \overline{D})$$

telle que pour tout $t > 0$, $x \in \overline{D}$ et $A \in \mathscr{B}(D)$,

$$\mathrm{P}_t^D(x, A) = \int_A \mathrm{p}_t^D(x, y) \mathrm{d}y.$$

De plus, cette densité de transition p_t^D satisfait les équations de Kolmogorov rétrograde et progressive :

- *$(t, x) \mapsto \mathrm{p}_t^D(x, y)$ satisfait $\partial_t \mathrm{p}^D = \mathscr{L}_x \mathrm{p}^D$ sur $\mathbb{R}_+^* \times D$,*
- *$(t, y) \mapsto \mathrm{p}_t^D(x, y)$ satisfait $\partial_t \mathrm{p}^D = \mathscr{L}_y^* \mathrm{p}^D$ sur $\mathbb{R}_+^* \times D$.*

Finalement, pour tout $t > 0$, $(x, y) \in \overline{D} \times \overline{D}$,

- *$\mathrm{p}_t^D(x, y) = 0$ si $x \in \Gamma^+ \cup \Gamma^0$ ou $y \in \Gamma^- \cup \Gamma^0$,*
- *sous l'hypothèse (O2), $\mathrm{p}_t^D(x, y) > 0$ si $x \notin \Gamma^+ \cup \Gamma^0$ et $y \notin \Gamma^- \cup \Gamma^0$.*

Nous obtenons également une majoration gaussienne de la densité de transition p_t^D.

Théorème 1.3.6 (Majoration gaussienne de p_t^D)**.** *Sous les hypothèses (O1) et (F1), la densité de transition $\mathrm{p}_t^D(x, y)$ est telle que pour tout $\alpha \in (0, 1)$, $T > 0$, il existe $C > 0$ tel que pour tout $t \in (0, T]$, pour tous $x, y \in \mathbb{R}^{2d}$,*

$$\mathrm{p}_t^D(x, y) \leq C \widehat{\mathrm{p}}_t^{(\alpha)}(x, y), \tag{1.10}$$

où $\widehat{\mathrm{p}}_t^{(\alpha)}(x, y)$ est la densité de transition du processus gaussien $\left(\alpha^{-1/2} \widehat{X}_t^{\sqrt{\alpha} x}\right)_{t \geq 0}$, où $\widehat{X}_t^x = (\widehat{q}_t^x, \widehat{p}_t^x)$ est solution de

$$\begin{cases} \mathrm{d}\widehat{q}_t^x = \widehat{p}_t^x \mathrm{d}t, \\ \mathrm{d}\widehat{p}_t^x = -\gamma \widehat{p}_t^x \mathrm{d}t + \sigma \mathrm{d}B_t, \\ (\widehat{q}_0^x, \widehat{p}_0^x) = x. \end{cases} \tag{1.11}$$

Remarque 1.3.7. *Cette majoration gaussienne est également valable pour la densité de transition* p_t *si* F *satisfait l'hypothèse (F2).*

Nous pouvons définir pour $t \geq 0$, l'opérateur P_t^D sur $\mathscr{C}^b(\overline{D})$ associé à la densité de transition p_t^D, de la manière suivante : pour tout $f \in \mathscr{C}^b(\overline{D})$, pour tout $x \in \overline{D}$,

(i) $P_0^D f(x) = f(x)$,

(ii) $\forall t > 0, \quad P_t^D f(x) = \int_D \mathrm{p}_t^D(x,y) f(y) \mathrm{d}y$.

La majoration gaussienne précédente permet alors d'obtenir le résultat de compacité suivant. Mentionnons qu'un précédent travail a été mené par F. Nier dans [65] où des propriétés de régularités de résolvantes, liées à la compacité du semigroupe du processus de Langevin absorbé, ont été obtenues par d'autres approches.

Théorème 1.3.8 (Compacité de $(P_t^D)_{t>0}$). *Sous les hypothèses (O1) et (F1), la famille d'opérateurs* $(P_t^D)_{t\geq 0}$ *est un semigroupe compact sur* $\mathscr{C}^b(\overline{D})$ *et sur* $\mathrm{L}^p(D)$ *pour tout* $p \geq 1$.

En parallèle de ce résultat, nous avons étendu au processus de Langevin (1.6) deux propriétés bien connues pour les problèmes paraboliques, que sont le principe du maximum et l'inégalité de Harnack.

Théorème 1.3.9 (Principe du maximum). *Supposons les hypothèses (F1), (O1) et (O2) satisfaites. Soit* $u \in \mathscr{C}^{1,2}(\mathbb{R}_+^* \times D)$ *telle que* $\partial_t u - \mathscr{L} u \leq 0$ *sur* $\mathbb{R}_+^* \times D$.

(i) Supposons que $u \in \mathscr{C}^b((\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+))$*, alors*

$$\sup_{\mathbb{R}_+^* \times D} u(t,x) = \sup_{(\{t=0\}\times D)\cup(\mathbb{R}_+^* \times \Gamma^+)} u(t,x). \tag{1.12}$$

(ii) Supposons que u *atteigne son maximum en un point* $(t_0, x_0) \in \mathbb{R}_+^* \times D$*, alors*

$$\forall t \leq t_0, \quad \forall x \in D, \qquad u(t,x) = u(t_0, x_0).$$

L'inégalité de Harnack suivante étend une inégalité d'Harnack dans des boules petites prouvée dans [35] en utilisant le concept de chaine d'Harnack développé dans [2].

Théorème 1.3.10 (Inégalité d'Harnack). *Supposons les hypothèses (F1), (O1) et (O2) satisfaites. Pour tout ensemble compact* $K \subset D$, $\epsilon > 0$ *et* $T > 0$*, il existe une constante* $C_{K,\epsilon,T} > 0$ *telle que pour toute fonction* u *positive et solution au sens des distributions de* $\partial_t u = \mathscr{L} u$ *sur* $\mathbb{R}_+^* \times D$*, pour tout* $t \geq \epsilon$,

$$\sup_{x \in K} u(t,x) \leq C_{K,\epsilon,T} \inf_{x\in K} u(t+T, x). \tag{1.13}$$

1.3.3 Chapitres 3 et 4 : distribution quasi-stationnaire du processus de Langevin sur D

Dans cette sous-section nous énonçons les principaux résultats des chapitres 3 et 4 portant sur l'étude de la DQS du processus de Langevin sur le domaine D. Le premier résultat porte sur le rayon spectral de l'opérateur P_t^D dans $\mathscr{C}^b(\overline{D})$ pour $t > 0$. Rappelons la définition du rayon spectral d'un opérateur borné sur l'espace de Banach $\mathscr{C}^b(\overline{D})$, cf. [70, p. 192].

Definition 1.3.11. *Soit* T *un opérateur réel borné sur* $\mathscr{C}^b(\overline{D})$ *et soit* $\sigma(T)$ *son spectre. Le rayon spectral* $r(T)$ *de* T *est défini comme :*

$$r(T) := \sup_{\lambda \in \sigma(T)} |\lambda|.$$

Dans le chapitre 3 nous obtenons une dépendance explicite du rayon spectral de l'opérateur P_t^D en la variable t. De plus nous montrons qu'il est associé à un espace propre de dimension 1 du semigroupe P_t^D.

Théorème 1.3.12 (Rayon spectral)**.** *Sous les hypothèses (F1), (O1) et (O2), il existe $\lambda_0 > 0$ tel que pour tout $t > 0$,*

$$r(P_t^D) = \mathrm{e}^{-\lambda_0 t}.$$

De plus, il existe une unique fonction, à constante multiplicative près, $\phi \in \mathscr{C}^b(\overline{D})$ telle que pour tout $t > 0$,

$$P_t^D \phi = \mathrm{e}^{-\lambda_0 t}\phi.$$

Par ailleurs, $\phi \in \mathrm{L}^1(D) \cap \mathscr{C}^\infty(D)$. De plus, $\phi > 0$ sur $D \cup \Gamma^-$, $\phi = 0$ sur $\Gamma^+ \cup \Gamma^0$ et $\mathscr{L}\phi = -\lambda_0\phi$ sur D.

La preuve de ce theorème repose sur l'application du théorème de Krein-Rutman [72, p. 313] à l'opérateur P_t^D compact dans $\mathscr{C}^b(\overline{D})$, ainsi qu'à l'opérateur que nous appelons $\widetilde{P}_t^D$ dont le noyau $\widetilde{\mathrm{p}}_t^D(x,y)$ s'écrit $\mathrm{e}^{-d\gamma t}\mathrm{p}_t^D(y,x)$ et qui est également compact dans $\mathscr{C}^b(\overline{D})$. Remarquons que les variables x et y ont été permutées dans $\widetilde{\mathrm{p}}_t^D$ par rapport à la définition de P_t^D. La famille d'opérateurs $(\widetilde{P}_t^D)_{t\geq 0}$ ainsi définie correspond alors au semigroupe absorbé au bord de D du processus $(\widetilde{q}_t, \widetilde{p}_t)_{t\geq 0}$ défini par l'EDS suivante :

$$\begin{cases} \mathrm{d}\widetilde{q}_t = -\widetilde{p}_t \mathrm{d}t, \\ \mathrm{d}\widetilde{p}_t = F(\widetilde{q}_t)\mathrm{d}t + \gamma\widetilde{p}_t\mathrm{d}t + \sigma\mathrm{d}B_t. \end{cases} \tag{1.14}$$

L'étude jointe des semigroupes $(P_t^D)_{t\geq 0}$ et $(\widetilde{P}_t^D)_{t\geq 0}$ sera d'ailleurs très utile dans le chapitre 3. A partir du théorème 1.3.12, nous sommes alors capables de déduire l'existence d'une unique DQS sur D pour le processus $(X_t)_{t\geq 0}$. En particulier, cette DQS admet l'interprétation spectrale suivante.

Théorème 1.3.13 (Existence, unicité et interprétation spectrale de la DQS)**.** *Supposons les hypothèses (F1), (O1) et (O2) satisfaites, alors il existe une unique DQS μ sur D du processus de Langevin (1.6). De plus,*

- *il existe une fonction $\psi \in \mathscr{C}^\infty(D) \cap \mathscr{C}^b(\overline{D})$ telle que $\mu(\mathrm{d}x) = \psi(x)\mathrm{d}x$, où $\mathrm{d}x$ est la mesure de Lebesgue sur D,*
- *il existe un unique couple (λ, η), à normalisation près de η, tel que η est une solution positive classique dans $\mathscr{C}^2(D) \cap \mathscr{C}^b(\overline{D})$ du problème aux valeurs propres suivant*

$$\begin{cases} \mathscr{L}^*\eta(x) = -\lambda\,\eta(x) & \forall x \in D, \\ \eta(x) = 0 & \forall x \in \Gamma^-. \end{cases}$$

De plus $\frac{\eta}{\int_D \eta} = \psi$ et $\lambda = \lambda_0$.

Nous obtenons également le comportement suivant en temps long de l'opérateur P_t^D.

Théorème 1.3.14 (Convergence en temps long de P_t^D)**.** *Supposons les hypothèses (F1), (O1) et (O2) satisfaites. Soit α^* défini par*

$$\mathrm{e}^{-(\lambda_0+\alpha^*)} := \sup_{z\in\sigma(P_1^D)\setminus\{\mathrm{e}^{-\lambda_0}\}} |z|. \tag{1.15}$$

Alors $\alpha^* > 0$, et pour tout $\alpha \in [0, \alpha^*)$, il existe $C_\alpha > 0$ tel que pour tout $t \geq 0$,

$$\left|\!\left|\!\left| P_t^D - \mathrm{e}^{-\lambda_0 t}\frac{\phi\otimes\psi}{\int_D \phi\psi} \right|\!\right|\!\right|_{\mathscr{C}^b(\overline{D})} \leq C_\alpha \mathrm{e}^{-(\lambda_0+\alpha)t}, \tag{1.16}$$

où $|\!|\!|\cdot|\!|\!|_{\mathscr{C}^b(\overline{D})}$ est la norme triple sur l'espace $\mathscr{C}^b(\overline{D})$ et pour $f \in \mathscr{C}^b(\overline{D})$, $\phi\otimes\psi(f) = \left(\int_D \psi f\right)\phi$.

Remarque 1.3.15. *Pour le processus de Langevin non absorbé, la convergence exponentielle en temps du semigroupe est une propriété bien connue dans la littérature. Diverses méthodes ont été développées pour le prouver comme les techniques de Lyapunov [71, 80], estimées sous-elliptiques [43], l'hypocoercivité [41, 58, 11] ou des méthodes de couplage [29].*

Nous sommes alors en mesure d'en déduire la convergence suivante du semigroupe du processus de Langevin conditionné à rester dans D, vers sa DQS sur D.

Théorème 1.3.16 (Convergence en variation totale vers la DQS)**.** *Sous les hypothèses (F1), (O1) et (O2), pour tout $\alpha \in [0, \alpha^*)$, il existe $C'_\alpha > 0$ tel que, pour tout $t \geq 0$, pour toute mesure de probabilité θ sur D, $\mathbb{P}_\theta(\tau_\partial > t) > 0$, et*

$$\|\mathbb{P}_\theta\left(X_t \in \cdot | \tau_\partial > t\right) - \mu\|_{TV} \leq \frac{C'_\alpha}{\int_D \phi \mathrm{d}\theta} \mathrm{e}^{-\alpha t}, \tag{1.17}$$

où $\| \cdot \|_{TV}$ correspond à la norme en variation totale sur l'espace des mesures signées bornées sur $\mathbb{R}^{2d}$.

Remarque 1.3.17. *Notons qu'ici, contrairement au cas elliptique du Théorème 1.2.3, le préfacteur s'écrit $\frac{C}{\int_D \phi \mathrm{d}\theta}$ et dépend donc de la distribution initiale θ sur D. De plus, il tend vers l'infini lorsque θ se concentre proche du bord Γ^+ (où $\phi = 0$).*

Dans un deuxième temps, nous considérons dans le chapitre 3 le cas $\gamma > 0$ avec $\sigma = \sqrt{2\beta^{-1}\gamma}$ dans (1.6), où $\beta > 0$ est une constante fixée indépendant de γ. L'objectif étant d'étudier la limite suramortie, c'est à dire lorsque γ tend vers l'infini, de la DQS sur D du processus de Langevin (1.6). La motivation derrière ce travail est le résultat bien connu, (cf. par exemple [56, Proposition 2.15]) de convergence faible de la loi de la position du processus de Langevin $(q_{\gamma t})_{t\in[0,T]}$ pour $T > 0$ vers la loi du processus de Langevin suramorti $(\overline{q}_t)_{t\in[0,T]}$ quand $\gamma \to \infty$. Notre objectif est alors d'obtenir un résultat de convergence de la marginale en position de la DQS sur D du processus de Langevin (1.6) vers la DQS sur $\mathscr{O}$ du processus de Langevin suramorti (1.4). Nous prouvons en fait le théorème 1.3.19 plus général de la convergence faible de la DQS sur D vers une mesure de probabilité explicite sur D. Nous en déduisons alors aisément ce résultat de convergence faible de sa marginale. Le résultat de convergence faible repose en grande partie sur le théorème suivant.

Théorème 1.3.18 (Limite suramortie du processus de Langevin)**.** *Supposons l'hypothèse (F2) satisfaite. Soit $T > 0$ et $x = (q,p) \in \mathbb{R}^{2d}$. Soit $Z \sim \mathscr{N}_d\left(0, \beta^{-1} I_d\right)$ un vecteur gaussien indépendent du processus $(\overline{q}_t)_{t\in[0,T]}$. La loi du couple $((q_{\gamma t})_{t\in[0,T]}, p_{\gamma T})$ sous $\mathbb{P}_x$, converge étroitement vers la loi de $((\overline{q}_t)_{t\in[0,T]}, Z)$ sous $\mathbb{P}_q$, lorsque $\gamma \to \infty$.*

De cette convergence nous déduisons le résultat suivant.

Theorem 1.3.19 (Limite suramortie de la DQS)**.** *Supposons les hypothèses (F1), (O1) et (O2) satisfaites. La DQS $\mu^{(\gamma)}$ sur D du processus de Langevin converge étroitement, lorsque $\gamma \to \infty$, vers la mesure de probabilité $\mu^{(\infty)}$ sur D définie par :*

$$\mu^{(\infty)}(\mathrm{d}q\mathrm{d}p) := \overline{\psi}(q) \frac{\mathrm{e}^{-\beta \frac{|p|^2}{2}}}{(2\pi\beta^{-1})^{\frac{d}{2}}} \mathrm{d}q\mathrm{d}p.$$

De plus, la plus petite valeur propre $\lambda_0^{(\gamma)}$ de $-\mathscr{L}$ et $-\mathscr{L}^*$ satisfait

$$\lambda_0^{(\gamma)} \underset{\gamma\to\infty}{\sim} \frac{\overline{\lambda}}{\gamma},$$

où $\overline{\lambda}$ et $\overline{\psi}$ sont définies dans le théorème 1.2.3.

Dans le chapitre 4 nous obtenons les résultats d'existence, d'unicité et de convergence associés à la DQS sur D du Langevin (1.6) en utilisant l'approche récente de N. Champagnat et N. Villemonais dans [20, Theorem 3.5]. Nous montrons que les outils développés dans le chapitre 2, en particulier l'inégalité d'Harnack du théorème 1.3.10, permettent de satisfaire les hypothèses de [20, Theorem 3.5]. Contrairement à l'étude menée au chapitre 3, cette approche ne fait pas du tout appel à des résultats de compacité ou d'estimées gaussiennes.

Théorème 1.3.20. *Supposons les hypothèses (F1), (O1) et (O2) satisfaites. Le processus* $(X_t)_{t\geq 0}$ *admet une unique DQS* μ *sur* D. *De plus, il existe* $C, \beta > 0$, *une fonction* $\psi_2 > 0$ *sur* D, *tels que pour toute mesure de probabilité* θ *sur* D,

$$\forall t \geq 0, \qquad \|\mathbb{P}_\theta(X_t \in \cdot | \tau_\partial > t) - \mu(\cdot)\|_{TV} \leq \frac{Ce^{-\beta t}}{\int_D \psi_2 \mathrm{d}\theta}. \tag{1.18}$$

Il existe de plus $\lambda_0 \geq 0$ *tel que*

$$\forall t \geq 0, \qquad \mathbb{P}_\mu(\tau_\partial > t) = e^{-\lambda_0 t}.$$

Par ailleurs, il existe une fonction ϕ *bornée positive sur* D *telle que*

$$\mathrm{e}^{\lambda_0 t}\mathbb{P}_x(\tau_\partial > t) \underset{t\to\infty}{\longrightarrow} \phi(x), \tag{1.19}$$

où la convergence est uniforme sur D, *qui satisfait également pour tout* $t \geq 0$, $x \in D$, $\mathbb{E}_x[\phi(X_t)\mathbb{1}_{\tau_\partial > t}] = \mathrm{e}^{-\lambda_0 t}\phi(x)$.

Remarque 1.3.21. *Nous remarquons que malgré l'approche très différente, les théorèmes 1.3.16 et 1.3.20 font tous les deux intervenir un préfacteur qui dépend très similairement de la condition initiale.*

1.3.4 Chapitre 5 : Distribution stationnaire du processus de Langevin traversant une frontière

Considérons ici le processus de Langevin $(X_t = (q_t, p_t))_{t\geq 0}$ satisfaisant (1.6). La motivation du chapitre 5 fait suite aux travaux [8, 62] où un des objectifs est de simuler le temps moyen de réaction T_{AB} entre deux états A et B de $\mathbb{R}^d$ où A est typiquement un état métastable et le temps d'atteinte de B à partir de A est relativement long. Ce temps est défini de la manière suivante :

$$T_{AB} = \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N}(\tau_n^B - \tau_n^A),$$

où $\tau_{n+1}^A = \inf\{t > \tau_n^B,\ q_t \in A\}$ et $\tau_{n+1}^B = \inf\{t > \tau_{n+1}^A,\ q_t \in B\}$. La question qui se pose alors est comment simuler en pratique ce temps moyen de réaction.

Définissons les temps d'arrêt suivants $\tau_{n+1}^E = \inf\{t > \tau_n^E, X_t \in \Gamma_A^- \cup \Gamma_B^-\}$, $\tau_0^E = \inf\{t \geq 0, X_t \in \Gamma_A^- \cup \Gamma_B^-\}$ avec $\Gamma_A^- = \{(q,p) \in \partial A \times \mathbb{R}^d,\ p \cdot n_A(q) < 0\}$ et $\Gamma_B^- = \{(q,p) \in \partial B \times \mathbb{R}^d,\ p \cdot n_B(q) < 0\}$. Les vecteurs unitaires n_A et n_B dénotent la normale unitaire sortante à A et B respectivement. Soit la chaîne de Markov $(Y_n)_{n\geq 1}$ suivante pour $n \geq 1$,

$$Y_n = X_{\tau_n^E}.$$

Il a été montré [8, Section 4.2] que, sous certaines conditions de régularité sur le processus considéré [8, Hypothèse (A)] (ces hypothèses restent à prouver pour le processus de Langevin (1.6)), le temps T_{AB} pouvait également s'écrire comme :

$$T_{AB} = \frac{\mathbb{E}_{\overline{\mu}_{|\Gamma_A^-}}\left(\tau_1^E\right)}{\mathbb{P}_{\overline{\mu}_{|\Gamma_A^-}}(Y_1 \in \Gamma_B^-)}, \tag{1.20}$$

où $\overline{\mu}_{|\Gamma_A^-}$ est la distribution d'équilibre de $(Y_n)_{n\geq 0}$ conditionnée sur Γ_A^-. Dans le chapitre 5 nous donnons pour le processus de Langevin $(X_t)_{t\geq 0}$ (1.6) une expression pour la mesure $\overline{\mu}$ en fonction de la distribution d'équilibre du procesus de Langevin (1.6). En particulier, cette mesure est totalement explicite dans le cas $F = -\nabla V$, ce qui permet d'échantillonner directement des conditions initiales (cf. Remarque 1.3.24) pour estimer ensuite le numérateur et le dénominateur dans (1.20) par des méthodes de simulation d'évènements rares de type Adaptative Multilevel Splitting [17, 18] ou Forward Flux Sampling [1] par exemple. Ceci explique l'importance d'avoir une expression explicite pour la mesure d'équilibre de $(Y_n)_{n\geq 0}$ sur Γ_A^-. Nous renvoyons par exemple à [8] pour plus de détails.

Considérons $\gamma \in \mathbb{R}$, $\sigma > 0$ et une fonction $F : \mathbb{R}^d \mapsto \mathbb{R}^d$ satisfaisant (F1). Nous ajouterons des hypothèses ci-dessous. Comme le coefficient de dérive $(q,p) \mapsto (p, F(q) - \gamma p)$ de la dynamique (1.6) est localement lipschitzien, il existe donc une unique solution forte jusqu'à un temps d'explosion τ_∞ [48, Theorem IV.3.1] et nous supposerons que :

(A1) $\tau_\infty = \infty$ presque sûrement,

(A2) le processus $(q_t, p_t)_{t\geq 0}$ est ergodique par rapport à une unique distribution stationnaire $\mu(\mathrm{d}q\mathrm{d}p)$, qui admet une densité positive et régulière $\rho(q,p)$ par rapport à la mesure de Lebesgue sur $\mathbb{R}^d \times \mathbb{R}^d$;

(A3) la densité $\rho(q,p)$ satisfait

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} \left(|p \cdot \nabla_q \rho| + |\nabla_p \cdot (F(q)\rho)| + |\gamma \nabla_p (p\rho)| + \frac{\sigma^2}{2} |\Delta_p \rho| \right) \mathrm{d}q\mathrm{d}p < +\infty.$$

Remarque 1.3.22. *Les hypothèses ci-dessus sont en particulier satisfaites si* $\gamma > 0$, $\sigma = \sqrt{2\gamma\beta^{-1}}$ *pour un certain* $\beta > 0$, *et* $F = -\nabla V$ *avec* $V : \mathbb{R}^d \to \mathbb{R}$ *une fonction régulière telle que*

$$\int_{\mathbb{R}^d} (1 + |\nabla V(q)|) \mathrm{e}^{-\beta V(q)} \mathrm{d}q < +\infty,$$

auquel cas nous avons

$$\rho(q,p) = \frac{1}{Z_\beta} \mathrm{e}^{-\beta H(q,p)},$$

avec

$$H(q,p) := V(q) + \frac{|p|^2}{2}, \qquad Z_\beta := \int_{\mathbb{R}^d\times\mathbb{R}^d} \mathrm{e}^{-\beta H(q,p)} \mathrm{d}q\mathrm{d}p.$$

Considérons maintenant un ensemble $A \subset \mathbb{R}^d$ pouvant être non borné, de frontière Σ et satisfaisant les hypothèses suivantes :

(B1) L'ensemble A est un ouvert $\mathscr{C}^2$ de $\mathbb{R}^d$ et connexe.

(B2) Les ensembles A et $\mathbb{R}^d \setminus A$ ont une mesure de Lebesgue positive.

(C) la fonction $(q,p) \in \Sigma \times \mathbb{R}^d \mapsto |p \cdot n(q)| \rho(q,p)$ est dans $L^1(\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p)$,

où $n(q)$ est la normale unitaire sortante au point $q \in \partial A$ et $\sigma_\Sigma(q)$ est la mesure de Lebesgue sur la frontière Σ.

De plus, notons

$$\Gamma_A^+ = \{(q,p) \in \partial A \times \mathbb{R}^d : p \cdot n(q) > 0\},$$
$$\Gamma_A^- = \{(q,p) \in \partial A \times \mathbb{R}^d : p \cdot n(q) < 0\}.$$

Nous étudions ici les évènements successifs d'entrée dans A et sorties de A du processus $(X_t)_{t\geq 0}$. A chacune de ces entrées/sorties le processus traverse la frontière $\Gamma_A^+ \cup \Gamma_A^-$. On peut dès lors construire une chaine de Markov $(\overline{Y}_n)_{n\geq 0}$ sur le bord $\Gamma_A^+ \cup \Gamma_A^-$ définie de la manière suivante :

$$\forall n \geq 0, \qquad \overline{Y}_n := X_{\tau_n},$$

où $\tau_{n+1} := \inf\{t > 0 : X_t \in \Gamma_A^+ \cup \Gamma_A^-\}$, $\tau_0 := \inf\{t \geq 0 : X_t \in \Gamma_A^+ \cup \Gamma_A^-\}$.

Notons

$$z_\Sigma^\pm := \int_{\Gamma^\pm} |p \cdot n(q)| \rho(q,p) \mathrm{d}\sigma_\Sigma(q) \mathrm{d}p.$$

Théorème 1.3.23 (Distribution stationnaire de $(\overline{Y}_n)_{n\geq 0}$)**.** *Sous les hypothèses (A1-A2-A3), (B1-B2) et (C), la mesure de probabilité*

$$\overline{\mu}_\Sigma := \left(\frac{1}{2z_\Sigma^+}\mathbb{1}_{\{(q,p)\in\Gamma^+\}} + \frac{1}{2z_\Sigma^-}\mathbb{1}_{\{(q,p)\in\Gamma^-\}}\right)|p\cdot n(q)|\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p$$

est l'unique distribution stationnaire de la chaîne de Markov $(\overline{Y}_n)_{n\geq 0}$.

Remarque 1.3.24. *Nous décrivons ici brièvement comment échantillonner suivant la mesure stationnaire $\overline{\mu}_\Sigma$ lorsque $F = -\nabla V$. Dans ce cas, la densité ρ s'écrit sous la forme produit*

$$\rho(q,p) \propto \mathrm{e}^{-\beta V(q)}\mathrm{e}^{-\beta|p|^2/2}.$$

Considérons par exemple le premier terme dans l'expression de $\overline{\mu}_\Sigma$

$$\mathrm{e}^{-\beta V(q)}\mathrm{d}\sigma_\Sigma(q)\mathbb{1}_{(q,p)\in\Gamma^+}|p\cdot n(q)|\mathrm{e}^{-\beta|p|^2/2}\mathrm{d}p.$$

D'un point de vue numérique, on peut échantillonner cette mesure en suivant la procédure détaillée ci-dessous :

1. *échantillonner q suivant la mesure de probabilité avec densité proportionnelle à $\mathrm{e}^{-\beta V(q)}$ par rapport à la mesure surfacique $\mathrm{d}\sigma_\Sigma(q)$;*
2. *conditionnellement à $n(q)$, échantillonner p suivant la mesure de densité proportionnelle à $\mathbb{1}_{p\cdot n(q)>0}|p\cdot n(q)|\mathrm{e}^{-\beta|p|^2/2}$ par rapport à la mesure de Lebesgue sur $\mathbb{R}^d$.*

Pour l'étape 1 nous renvoyons aux méthodes développées par exemple dans [26, 57]. Pour l'étape 2 par exemple, il suffit de simuler $d+1$ variables aléatoires $Z_1, Z_1', Z_2, \ldots, Z_d$, indépendantes normales centrées réduites, i.e. de loi $\mathscr{N}(0,1)$, et de choisir

$$p = \frac{1}{\sqrt{\beta}}\left(\sqrt{Z_1^2 + Z_1'^2}n(q) + Z_2 e_2 + \cdots + Z_d e_d\right),$$

où $(e_2, \ldots, e_d)$ est une base orthonormale de l'hyperplan $n(q)^\perp$. Il est alors facile de vérifier que, conditionnellement à q, p suit bien la loi attendue.

1.4 Perspectives

Ce travail de thèse a permis d'étendre certains résultats bien connus pour des diffusions elliptiques absorbées et les équations aux dérivées partielles paraboliques associées, aux processus de Langevin, et aux équations aux dérivées partielles hypoelliptiques associées. Nous donnons ici quelques exemples de questions qui se posent naturellement sur les objets introduits dans ce manuscrit, et qui pourraient faire l'objet d'études ultérieures.

Régularité au bord. Considérons la fonction u définie dans (1.8). D'après le théorème 1.3.4, la fonction u est l'unique solution classique au problème (1.9). En particulier, cette solution classique vérifie que pour tout $t > 0$,

$$x \in \overline{D} \mapsto u(t,x) \in \mathscr{C}^b(\overline{D}).$$

Dans le cas $d = 1$, $\mathscr{O} = (0,1)$, pour une solution faible v au sens de [47, Definition 1.1] du problème (1.9) avec $F = 0$, $\gamma = 0$, $\sigma = \sqrt{2}$ dans (1.7), les auteurs ont montré que la solution est $\mathscr{C}^\infty$ sur le bord $\Gamma^+ \cup \Gamma^-$ avec une perte de régularité au bord Γ^0 où la régularité maximale attendue est hölderienne. Cette propriété a ensuite été généralisée dans [46] aux cas $d = 2$ et $d = 3$ sur $D = \mathscr{O} \times \mathbb{R}^d$ pour $\mathscr{O}$ un ouvert $\mathscr{C}^3$ de $\mathbb{R}^d$. Est il possible dès lors d'étendre ces résultats de régularité à notre solution classique u définie dans (1.8) en dimension quelconque ?

Unicité de la DQS dans un domaine non borné. Le théorème 1.3.13 donne l'existence d'une unique DQS du processus de Langevin (1.6) sur le domaine $\mathscr{O} \times \mathbb{R}^d$ lorsque $\mathscr{O}$ est un ouvert $\mathscr{C}^2$ borné de $\mathbb{R}^d$. La question qui se pose alors est que se passe-t-il si $\mathscr{O}$ n'est pas borné ? Par analogie avec le cas elliptique, on sait que la diffusion suivante

$$\mathrm{d}Y_t = -Y_t \mathrm{d}t + \mathrm{d}B_t,$$

admet une infinité de DQS sur $\mathbb{R}_+$ cf.[61]. Est ce que l'unicité de la DQS tombe en défaut lorsque l'on considère des domaines $\mathscr{O}$ non bornés pour le processus de Langevin ? C'est probable, et il serait intéressant d'avoir une caractérisation de la famille de DQS, même pour un cas simple d'une force linéaire.

Ergodicité conditionnelle uniforme. La dernière piste potentielle d'amélioration concerne le résultat de convergence obtenu dans les théorèmes 1.3.16 et 1.3.20. Si la distribution initiale est θ, le préfacteur intervenant dans la majoration s'écrit $C/\int_D \phi \mathrm{d}\theta$ et dépend donc de la condition initiale. De plus, il explose lorsque la distribution se concentre sur des points proches du bord étant donné que ϕ est continue sur $\overline{D}$ et s'annule sur Γ^+. Peut on obtenir un résultat similaire au cadre elliptique où le préfacteur est indépendant de la condition initiale ? Une des conditions suffisantes pour obtenir cela est de montrer [20, Proposition 3.8] l'existence d'un ensemble compact $K \subset D$ ainsi qu'un $t > 0$ tel que

$$\inf_{x \in D} \mathbb{P}_x(X_t \in K | \tau_\partial > t) > 0.$$

D'autres estimées permettent d'obtenir ce résultat comme les estimées bilatérales, i.e. l'existence de fonctions $\widetilde{\phi}, \widetilde{\psi} : D \mapsto \mathbb{R}_+$ telles que pour tout $t > 0$ il existe $c_t > 0$ tel que

$$\forall x, y \in D, \quad c_t^{-1} \widetilde{\phi}(x) \widetilde{\psi}(y) \leq \mathrm{p}_t^D(x, y) \leq c_t \widetilde{\phi}(x) \widetilde{\psi}(y).$$

Une preuve expliquant comment obtenir une convergence uniforme en la condition initiale à partir des estimées bilatérales est détaillée par exemple dans [8, Appendix C].

Temps de réaction, point de sortie. Le chapitre 5 a permis d'obtenir une expression analytique de la distribution des points de sortie d'un domaine en position pour le processus de Langevin. Comme expliqué ci-dessus, ceci doit permettre de mettre en oeuvre des méthodes d'estimation des temps de transition en utilisant la relation de Hill. Il reste cependant à prouver que la relation de Hill est bien valable pour l'équation de Langevin, i.e. à généraliser les résultats de [8] (qui s'appliquent typiquement à une diffusion elliptique) à l'équation de Langevin.

Part I

Probabilistic study of the kinetic Fokker-Planck

CHAPTER 2

A PROBABILISTIC STUDY OF THE KINETIC FOKKER-PLANCK EQUATION IN CYLINDRICAL DOMAINS

The following work focuses on some important properties of the solutions of the kinetic Fokker-Planck equations. It provides us with important tools which are used in the next chapters of this thesis.

Abstract: We consider classical solutions of the kinetic Fokker-Planck equation on a bounded domain $\mathscr{O} \subset \mathbb{R}^d$ in position, and we obtain a probabilistic representation of the solutions using the Langevin diffusion process with absorbing boundary conditions on the boundary of the phase-space cylindrical domain $D = \mathscr{O} \times \mathbb{R}^d$. Furthermore, a Harnack inequality, as well as a maximum principle, is provided on D for solutions to this kinetic Fokker-Planck equation, as well as the existence of a smooth transition density for the associated absorbed Langevin dynamics. The continuity of this transition density at the boundary of D is studied as well as the compactness, in various functional spaces, of the associated semigroup.

2.1 Introduction and motivation

In statistical physics, the evolution of a molecular system at a given temperature is typically modeled by the Langevin dynamics:

$$\begin{cases} \mathrm{d}q_t = M^{-1}p_t\mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma M^{-1}p_t\mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}B_t, \end{cases} \tag{2.1}$$

where $d = 3N$ for a number N of particles, $(q_t, p_t) \in \mathbb{R}^d \times \mathbb{R}^d$ denotes the respective vectors of positions and momenta of the particles, $M \in \mathbb{R}^{d\times d}$ is the mass matrix, $F : \mathbb{R}^d \to \mathbb{R}^d$ is the force acting on the particles, $\gamma > 0$ is the friction parameter, and $\beta^{-1} = k_B T$ with k_B the Boltzmann constant and T the temperature of the system. Such dynamics are used in particular to compute thermodynamic and dynamic quantities, with numerous applications in biology, chemistry and materials science. In practice, the system remains trapped for very long times in subsets of the phase space, called metastable states, see for example [58, Sections 6.3 and 6.4]. Typically, these states are defined in terms of positions only, and are thus cylinders of the form $D = \mathscr{O} \times \mathbb{R}^d$ with positions living in an open set $\mathscr{O}$ of $\mathbb{R}^d$, and momenta in $\mathbb{R}^d$.

In order to understand the behavior of the stochastic process in such a metastable state, it is important to study the Langevin diffusion with absorbing boundary conditions when leaving D. This is for example useful to define the quasi-stationary distribution which can be seen as a "local stationary distribution" within the metastable state, which is done in Chapters 3 and 4. This distribution is the cornerstone of so-called accelerated dynamics algorithms to sample metastable processes over long times, see for example [67]. Studying this process is also important to identify the stationary distribution of the entry and exit points of the process in D, see Chapter 5, which can then be employed to build unbiased estimators of the mean transition time between metastable states [8].

The objective of this work is to provide an ensemble of crucial properties on the absorbed Langevin process. In particular, we will obtain:

(i) a Feynman-Kac type formula to represent probabilistically the classical solution to a partial differential equation associated with the Langevin dynamics on a cylindrical domain, which is usually called the kinetic Fokker-Planck equation in the partial differential equation literature;

(ii) a Harnack inequality as well as a maximum principle for this partial differential equation;

(iii) the existence of a smooth transition density for the absorbed process, as well as Gaussian upper bounds, from which one can deduce the compactness of the transition kernel in appropriate functional spaces.

As will be explained below, such results are standard for elliptic diffusions (overdamped Langevin dynamics), but were not proven for the Langevin dynamics (which is not elliptic but only hypoelliptic) in the general setting of (2.1), at least to the best of our knowledge. The non-ellipticity requires in particular a careful treatment of the boundary conditions (determining precisely the set of exit points). The proofs rely on a combination of tools from stochastic analysis (in particular [32, 33] and extensions of [52]) and analysis of partial differential equations (in particular generalizations of [35, 2]).

Outline of the chapter. In Section 2.2, we give the main results, which are then proven in the subsequent sections. More precisely, Section 2.3 is devoted to the proof of the existence of a classical solution to the kinetic Fokker-Planck equation, as well as its probabilistic representation. Section 2.4 gives the proof of the Harnack inequality and the maximum principle. In Section 2.5, we provide the proofs of the existence of a smooth density of the absorbed Langevin process as well as Gaussian upper bounds on the latter. Finally, we prove in Section 2.6 the compactness of the semigroup associated with the absorbed Langevin process.

Notation. Let us conclude this introductory section with some notation that will be used in the following. We denote by $x = (q, p)$ generic elements of $\mathbb{R}^{2d}$. The Euclidean norm is denoted by $|\cdot|$, indifferently on $\mathbb{R}^d$ and on $\mathbb{R}^{2d}$, and the scalar product between vectors u and v of $\mathbb{R}^d$ or $\mathbb{R}^{2d}$ is denoted by $u \cdot v$. The open ball of $\mathbb{R}^{2d}$ centered at x with radius ρ is denoted by $\mathrm{B}(x, \rho)$. The distance between a point u and a subset A of $\mathbb{R}^d$ or $\mathbb{R}^{2d}$ is denoted, and defined, by $\mathrm{d}(u, A) := \inf_{v \in A} |u - v|$.

For a subset A of $\mathbb{R}^d$ or $\mathbb{R}^{2d}$, we denote by:

(i) $\overline{A}$ the closure of A, ∂A its boundary and A^c its complement,

(ii) $\mathscr{B}(A)$ the Borel σ-algebra on A,

(iii) $|A|$ the Lebesgue measure of A (if A is measurable),

For a subset A of $\mathbb{R}^d$, $\mathbb{R}^{2d}$, $\mathbb{R}_+^* \times \mathbb{R}^{2d}$ or $\mathbb{R}_+^* \times \mathbb{R}^{2d} \times \mathbb{R}^{2d}$, we denote by:

(i) for $1 \leq p \leq \infty$, $\mathrm{L}^p(A)$ the set of L^p scalar-valued functions on A and $\|\cdot\|_{\mathrm{L}^p(A)}$ the associated norm,

(ii) $\mathscr{C}(A)$ (resp. $\mathscr{C}^b(A)$) the set of scalar-valued continuous (resp. continuous and bounded) functions on A,

(iii) for $1 \leq k \leq \infty$, $\mathscr{C}^k(A)$ (resp. $\mathscr{C}^k_c(A)$) the set of scalar-valued $\mathscr{C}^k$ (resp. $\mathscr{C}^k$ with compact support) functions on A,

(iv) if $A \subset \mathbb{R}^d$ or $\mathbb{R}^{2d}$, $\mathscr{C}^{1,2}(\mathbb{R}_+^* \times A)$ the set of scalar-valued functions $u(t, x)$ on $\mathbb{R}_+^* \times A$ such that u, $\partial_t u$, $\nabla_x u$ and $\nabla_x^2 u$ exist and are continuous on $\mathbb{R}_+^* \times A$.

When we work with vector-valued functions, we use such notations as $\mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ or $\mathscr{C}([0,T], \mathbb{R}^{2d})$. For bounded functions ϕ, we shall also use the notation $\|\phi\|_\infty$ as a shorthand for the L^∞ norm.

For $a, b \in \mathbb{R}$, we use the notation $a \wedge b = \min(a,b)$ and $a \vee b = \max(a,b)$. We write $\mathbb{N} = \{0, 1, 2, \dots\}$ and $\mathbb{N}^* = \{1, 2, \dots\}$. Integer intervals are denoted by $[\![a, b]\!]$.

2.2 Main results

This section presents the main results we obtained. As a motivation, we first recall in Section 2.2.1 some well-known results for parabolic equations and overdamped Langevin dynamics, which we then extend to our hypoelliptic and degenerate framework: the existence of a classical solution to the kinetic Fokker-Planck equation, as well as its probabilistic representation using the Langevin dynamics in Section 2.2.2; the existence of a transition density and Gaussian upper bounds for the Langevin process in Section 2.2.3; the existence of a transition density, Gaussian upper bounds and compactness for the absorbed Langevin process in Section 2.2.4.

2.2.1 Parabolic equations and the overdamped Langevin process

As an introduction to our results, we briefly review standard material on the probabilistic interpretation, and a few properties of the associated diffusion process, of Initial-Boundary Value Problems for parabolic equations on bounded domains. The prototypical example of such a problem writes

$$\begin{cases} \partial_t \overline{u}(t,q) = \overline{\mathscr{L}}\,\overline{u}(t,q), & t>0, \quad q \in \mathscr{O}, \\ \overline{u}(0,q) = \overline{f}(q), & q \in \mathscr{O}, \\ \overline{u}(t,q) = \overline{g}(q), & t>0, \quad q \in \partial\mathscr{O}, \end{cases} \tag{2.2}$$

where $\overline{\mathscr{L}}$ is the second-order differential operator

$$\overline{\mathscr{L}} = F \cdot \nabla + \frac{\sigma^2}{2}\Delta \tag{2.3}$$

for some vector field $F : \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma > 0$; $\mathscr{O}$ is an open, regular and bounded subset of $\mathbb{R}^d$; $\overline{f} : \mathscr{O} \to \mathbb{R}$, $\overline{g} : \partial\mathscr{O} \to \mathbb{R}$ are given initial and boundary conditions. Under suitable assumptions on the data,

1. weak solutions $\overline{u}$ can be constructed by variational approach;
2. parabolic regularization implies that weak solutions are actually smooth;
3. the smoothness of $\overline{u}$ allows to apply the Ito formula to obtain the probabilistic representation

$$\overline{u}(t,q) = \mathbb{E}\left[\mathbb{1}_{\overline{\tau}^q_\partial > t}\overline{f}(\overline{q}^q_t) + \mathbb{1}_{\overline{\tau}^q_\partial \le t}\overline{g}(\overline{q}^q_{\overline{\tau}^q_\partial})\right], \tag{2.4}$$

   where $(\overline{q}^q_t)_{t\ge 0}$ is the so-called overdamped Langevin process, defined by the stochastic differential equation

$$\begin{cases} \mathrm{d}\overline{q}^q_t = F(\overline{q}^q_t)\mathrm{d}t + \sigma \mathrm{d}B_t, \\ \overline{q}^q_0 = q, \end{cases} \tag{2.5}$$

   and

$$\overline{\tau}^q_\partial := \inf\{t > 0 : \overline{q}^q_t \notin \mathscr{O}\}.$$

   This representation implies in particular the uniqueness of classical solutions to (2.2).

We refer to Evans [30, Section 7.1] for the first two steps, and Friedman [32, 33, 31] for the last step. These references also present a Harnack inequality and a maximum principle for (2.2).

The following facts are closely related with the probabilistic representation formula (2.4):

(i) for any $q \in \mathscr{O}$, the nonnegative measure $\overline{\mathrm{P}}_t^{\mathscr{O}}(q,\cdot) := \mathbb{P}(\overline{q}_t^q \in \cdot, \overline{\tau}_\partial^q > t)$ has a smooth density $\overline{\mathrm{p}}_t^{\mathscr{O}}(q,q')$ with respect to the Lebesgue measure on $\mathscr{O}$;

(ii) this transition density satisfies the backward and forward Kolmogorov equations

$$\partial_t \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q') = \mathscr{L}_q \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q'), \qquad \partial_t \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q') = \mathscr{L}_{q'}^* \overline{\mathrm{p}}_t^{\mathscr{O}}(q,q'),$$

where $\mathscr{L}^*$ is the formal $\mathrm{L}^2(\mathrm{d}x)$ adjoint of $\mathscr{L}$ and the subscripts q, q' in the notation $\mathscr{L}_q$, $\mathscr{L}_{q'}^*$ indicate the variable on which the operator acts;

(iii) for all $t > 0$, the function $\overline{\mathrm{p}}_t^{\mathscr{O}}$ is positive on $\mathscr{O} \times \mathscr{O}$ and has a continuous extension to $\overline{\mathscr{O}} \times \overline{\mathscr{O}}$ which vanishes on $\partial(\mathscr{O} \times \mathscr{O})$;

(iv) the semigroup $(\overline{P}_t^{\mathscr{O}})_{t\geq 0}$ defined by $\overline{P}_t^{\mathscr{O}}\eta(q) = \mathbb{E}[\eta(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q > t}]$ is compact on certain functional spaces.

We refer to the work of [36] for the last property where the the authors proved such compactness, using in particular, sharp estimates of the Green function of $\overline{\mathscr{L}}$ obtained in [38].

In the next sections, we shall address the extension of both the probabilistic representation of the solution to the Initial-Boundary Value Problem (2.2) and the study of the transition density $\overline{\mathrm{p}}_t^{\mathscr{O}}$ associated with the Langevin process (2.1) rather than the overdamped Langevin process (2.5). A technical tool on which several of our results crucially rely is the fact that the transition density of the Langevin process is bounded from above by an explicit Gaussian mesure (see Theorem 2.2.19 below). This fact is a natural extension of Baldi's results [6, Théorème 4.2] for the overdamped Langevin process, based on the so-called parametrix method.

2.2.2 Kinetic Fokker-Planck equation and Langevin process

2.2.2.1 The kinetic Fokker-Planck equation

From now on, we fix $\gamma \in \mathbb{R}$ and $\sigma > 0$, and let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a vector field satisfying the following

Assumption (F1). $F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$.

The kinetic Fokker-Planck operator $\mathscr{L}_{F,\gamma,\sigma}$, simply denoted by $\mathscr{L}$ when there is no ambiguity, writes for $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$,

$$\mathscr{L} = \mathscr{L}_{F,\gamma,\sigma} = p \cdot \nabla_q + F(q) \cdot \nabla_p - \gamma p \cdot \nabla_p + \frac{\sigma^2}{2}\Delta_p. \tag{2.6}$$

The operator $\mathscr{L}$ is the infinitesimal generator of the Langevin dynamics (2.1), in which we consider the mass to be identity without loss of generality (see the change of variables in [56, Equation (.117)]). As explained in the introduction, in the case $\gamma > 0$ and $\sigma^2 = 2\gamma\beta^{-1}$ with $\beta^{-1} = k_B T$ this process is used to describe the behavior of particles moving in a thermal bath at temperature T and a rate γ and subject to the force field F. Let us emphasize that in the following, we consider the general case $\gamma \in \mathbb{R}$ and $\sigma > 0$ not necessarily related to γ.

Remark 2.2.1. *In the case when $F = -\nabla V$ and $\sigma^2 = 2\gamma\beta^{-1}$, the density h of the process solution to (2.1) with respect to the equibrium measure $\exp[-\beta(V(q) + |p|^2/2)]\mathrm{d}q\mathrm{d}p$ satisfies $\partial_t h = \mathscr{L}h$, which justifies the denomination kinetic Fokker-Planck operator for $\mathscr{L}$.*

Let $\mathscr{O} \subset \mathbb{R}^d$ satisfy

Assumption (O1). *$\mathscr{O}$ is open, $\mathscr{C}^2$ and bounded,* and consider the following cylindrical domain of $\mathbb{R}^{2d}$:

$$D := \mathscr{O} \times \mathbb{R}^d.$$

This is the natural phase space domain of the Langevin process absorbed when leaving the set of positions in $\mathscr{O}$. For $q \in \partial\mathscr{O}$, let $n(q) \in \mathbb{R}^d$ be the unitary outward normal vector to $\mathscr{O}$ at $q \in \partial\mathscr{O}$. Let us introduce the following partition of ∂D :

$$\Gamma^0 = \{(q,p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) = 0\},$$
$$\Gamma^+ = \{(q,p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) > 0\},$$
$$\Gamma^- = \{(q,p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) < 0\}.$$

The kinetic Fokker-Planck equation on the domain D with initial condition f and boundary condition g is the Initial-Boundary Value Problem

$$\begin{cases} \partial_t u(t,x) = \mathscr{L}u(t,x) & t > 0, \quad x \in D, \\ u(0,x) = f(x) & x \in D, \\ u(t,x) = g(x) & t > 0, \quad x \in \Gamma^+. \end{cases} \tag{2.7}$$

Notice that, in contrast with the Initial-Boundary Value Problem (2.2) associated with the overdamped Langevin dynamics (2.5), the boundary condition only applies on the subset Γ^+ of the boundary ∂D. We refer the reader to [33, Chapter 11] for a general study of boundary conditions for degenerate diffusions.

Let us make precise the notions of solutions we will need in the following.

Definition 2.2.2 (Classical solutions). *A function u is a classical solution to (2.7) if $u \in \mathscr{C}^{1,2}(\mathbb{R}_+^* \times D) \cap \mathscr{C}((\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+))$ and u satisfies (2.7).*

Notice that the regularity on u in this definition is required in order to make sense of the boundary value and initial condition in (2.7) in a classical sense. We will also use the notion of distributional solutions to

$$\partial_t u = \mathscr{L}u \qquad \text{on } \mathbb{R}_+^* \times D, \tag{2.8}$$

without initial condition or boundary value.

Definition 2.2.3 (Distributional solutions). *A distribution u on $\mathbb{R}_+^* \times D$ is a distributional solution of (2.8) if for all $\Phi \in \mathscr{C}_c^\infty(\mathbb{R}_+^* \times D)$,*

$$\iint_{\mathbb{R}_+^* \times D} u(t,x) \left(\partial_t \Phi(t,x) + \mathscr{L}^* \Phi(t,x)\right) \mathrm{d}t \, \mathrm{d}x = 0,$$

where $\mathscr{L}^*$ is the formal adjoint of $\mathscr{L}$ in $\mathrm{L}^2(\mathrm{d}x)$, i.e.

$$\mathscr{L}^* = -p \cdot \nabla_q - F(q) \cdot \nabla_p + \gamma \mathrm{div}_p(p \cdot) + \frac{\sigma^2}{2} \Delta_p. \tag{2.9}$$

A distributional solution to (2.8) differs from a classical solution to (2.7) in two ways: interior regularity, and boundary regularity (required to define boundary and initial conditions in (2.7)). On the one hand, additional regularity is necessary to properly define the initial and boundary values of distributional solutions, see for example the works [65, 3, 15, 47]. On the other hand, concerning interior regularity, it is actually known that distributional solutions of (2.8) are $\mathscr{C}^\infty(\mathbb{R}_+^* \times D)$ by hypoellipticity. Let us recall these standard results, see [45].

Definition 2.2.4 (Hypoellipticity). *A differential operator $\mathscr{G}$ is said to be hypoelliptic on an open set $A \subset \mathbb{R}^d$, $\mathbb{R}^{2d}$ or $\mathbb{R}_+^* \times \mathbb{R}^{2d}$ if for all $f \in \mathscr{C}^\infty(A)$ and u a distributional solution to $\mathscr{G}u = f$ on A then $u \in \mathscr{C}^\infty(A)$.*

It is well known that under Assumption (F1) the operators $\mathscr{L}$ and $\mathscr{L}^*$ (resp. $\partial_t - \mathscr{L}$ and $\partial_t - \mathscr{L}^*$) are hypoelliptic on D (resp. on $\mathbb{R}_+^* \times D$), see for example [58, Section 2.3.1] and references therein.

2.2.2.2 Probabilistic representation of classical solution

In this work, we are interested in the well-posedness of classical solutions of (2.7), see Theorem 2.2.10 below. Besides we will show that this solution admits a probabilistic representation in terms of the Langevin process $(X_t^x = (q_t^x, p_t^x))_{t\geq 0}$, described by its position q_t^x and velocity p_t^x at time t and defined by the following SDE:

$$\begin{cases} \mathrm{d}q_t^x = p_t^x \mathrm{d}t, \\ \mathrm{d}p_t^x = F(q_t^x)\mathrm{d}t - \gamma p_t^x \mathrm{d}t + \sigma \mathrm{d}B_t, \\ (q_0^x, p_0^x) = x. \end{cases} \tag{2.10}$$

Let τ_∂^x be the first exit time from D of the process $(X_t^x)_{t\geq 0}$, i.e.

$$\tau_\partial^x = \inf\{t > 0 : X_t^x \notin D\} = \inf\{t > 0 : q_t^x \notin \mathscr{O}\}.$$

Under Assumption (F1), the drift coefficient $(q, p) \mapsto (p, F(q) - \gamma p)$ in (2.10) is locally Lipschitz continuous on $\mathbb{R}^{2d}$, therefore (2.10) admits a unique strong solution $(X_t^x)_{t\geq 0}$, which is *a priori* only defined up to some explosion time τ_∞^x by [48, Theorem IV.3.1]. Under the additional Assumption (O1), this drift coefficient is globally Lipschitz continuous on D, and thus the process exits the set D before the explosion time almost surely, so that the solution $(X_t^x)_{t\geq 0}$ is at least well-defined until τ_∂^x. Since observing the process only up to the time τ_∂^x amounts to imposing an absorbing boundary condition on ∂D, this justifies the following definition.

Definition 2.2.5 (Absorbed Langevin process)**.** *Under Assumptions (F1) and (O1), the process $(X_t^x)_{0\leq t\leq \tau_\partial^x}$ is called the absorbed Langevin process.*

Since $(X_t^x)_{0\leq t\leq \tau_\partial^x}$ is a solution to the SDE (2.10), it is a continuous-time Markov process with almost surely continuous sample paths. Besides, since the coefficients in (2.10) are locally bounded on $\mathbb{R}^{2d}$, then $(X_t^x)_{0\leq t\leq \tau_\partial^x}$ satisfies the strong Markov property, see [49, Theorem 4.20 p. 322].

Remark 2.2.6. *Friedman's uniqueness result [32, Theorem 5.2.1.] ensures that the trajectories $(X_t^x)_{0\leq t\leq \tau_\partial^x}$ do not depend on the values of F outside of $\mathscr{O}$. Therefore, whenever we are interested in quantities which only depend on the absorbed Langevin process, there is no loss of generality in modifying F outside of $\mathscr{O}$ so that it satisfies the following strengthening of Assumption (F1):*

Assumption (F2). *$F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ and F is bounded and globally Lipschitz continuous on $\mathbb{R}^d$.*

Under Assumption (F2), the drift coefficient $(q, p) \mapsto (p, F(q)-\gamma p)$ in (2.10) is globally Lipschitz continuous, with a Lipschitz constant which we shall denote by C_{Lip}, and therefore the strong solution $(X_t^x)_{t\geq 0}$ (without absorbing boundary condition) is defined globally.

In order to describe the probabilistic representation of the classical solution to (2.7), we first state a trajectorial result on the solution $(q_t^x, p_t^x)_{t\geq 0}$ of (2.10) for $x \in \mathbb{R}^{2d} \setminus \Gamma^0$. We prove that, almost surely, the process $(q_t^x, p_t^x)_{t\geq 0}$ does not reach the set Γ^0 in finite time. In other words, the set Γ^0 is non attainable in the sense of [33, Chapter 11.1].

Proposition 2.2.7 (Non-attainability of Γ^0)**.** *Under Assumptions (O1) and (F2), for all $x \in \mathbb{R}^{2d} \setminus \Gamma^0$,*

$$\mathbb{P}\left(\exists t > 0 : X_t^x \in \Gamma^0\right) = 0.$$

Using this non-attainability result we are able to characterize more precisely the exit event from D in the following proposition.

Proposition 2.2.8 (Attainability of the boundary)**.** *Let Assumptions (O1) and (F1) hold.*

(i) If $x \in \Gamma^+ \cup \Gamma^0$, then for all $\epsilon > 0$, $(q_t^x, p_t^x)_{t\geq 0}$ visits $\overline{D}^c$ almost surely on $[0,\epsilon]$, i.e.

$$\mathbb{P}\left(\exists t \in [0,\epsilon] : q_t^x \in \overline{\mathscr{O}}^c\right) = 1. \tag{2.11}$$

In particular, $\tau_\partial^x = 0$ almost surely.

(ii) If $x \in D \cup \Gamma^-$, then $\tau_\partial^x > 0$ almost surely and one has

$$\mathbb{P}\left(p_{\tau_\partial^x}^x \cdot n(q_{\tau_\partial^x}^x) \leq 0, \tau_\partial^x < \infty\right) = 0. \tag{2.12}$$

Remark 2.2.9. *One can actually prove (see Section 3.2.3 in Chapter 3 that for all $x \in D \cup \Gamma^-$, $\tau_\partial^x < \infty$ almost surely). Therefore, the equality (2.12) writes equivalently: for all $x \in D \cup \Gamma^-$, $\mathbb{P}(X_{\tau_\partial^x}^x \in \Gamma^-) = 1$.*

Proposition 2.2.8 implies that for all $t \geq 0$, almost surely, if $\tau_\partial^x > t$ then $X_t^x \in D \cup \Gamma^-$, and if $\tau_\partial^x \leq t$ then $X_{\tau_\partial^x}^x \in \Gamma^+ \cup \Gamma^0$. This ensures that the definition of the function u in Equation (2.13) below is legitimate.

We are now in position to state the main result of this section, namely the existence of a unique classical solution to the kinetic Fokker-Planck equation (2.7), and its probabilistic representation.

Theorem 2.2.10 (Classical solution and probabilistic representation for the kinetic Fokker-Planck equation (2.7))**.** *Under Assumptions (O1) and (F1), let $f \in \mathscr{C}^b(D \cup \Gamma^-)$ and $g \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$, and define the function u on $\mathbb{R}_+ \times \overline{D}$ by*

$$u : (t,x) \mapsto \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t} f(X_t^x) + \mathbb{1}_{\tau_\partial^x \leq t} g(X_{\tau_\partial^x}^x)\right]. \tag{2.13}$$

Then we have the following results:

(i) *Initial and boundary values: the function u satisfies*

$$u(0,x) = \begin{cases} f(x) & \text{if } x \in D \cup \Gamma^-, \\ g(x) & \text{if } x \in \Gamma^+ \cup \Gamma^0, \end{cases}$$

and

$$\forall t > 0, \quad \forall x \in \Gamma^+ \cup \Gamma^0, \qquad u(t,x) = g(x).$$

(ii) *Continuity: $u \in \mathscr{C}^b((\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^+ \cup \Gamma^0)))$, and if f and g satisfy the compatibility condition*

$$x \in \overline{D} \mapsto \mathbb{1}_{x \in D \cup \Gamma^-} f(x) + \mathbb{1}_{x \in \Gamma^+ \cup \Gamma^0} g(x) \in \mathscr{C}^b(\overline{D}), \tag{2.14}$$

then $u \in \mathscr{C}^b(\mathbb{R}_+ \times \overline{D})$.

(iii) *Interior regularity: $u \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D)$ and, for all $t > 0$, $x \in D$,*

$$\partial_t u(t,x) = \mathscr{L} u(t,x). \tag{2.15}$$

Conditions (i), (ii) and (iii) show that u is a classical solution to (2.7) in the sense of Definition 2.2.2. We also have the following uniqueness result for (2.7):

(iv) *Let v be a classical solution to (2.7) in the sense of Definition 2.2.2. If, for all $T > 0$, v is bounded on the set $[0,T] \times D$, then $v(t,x) = u(t,x)$ for all $(t,x) \in (\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+)$.*

Proposition 2.2.8 and Theorem 2.2.10 are proved in Section 2.3. The proof essentially follows the same three-step structure as for the probabilistic representation formula (2.4) of solutions to the Initial-Boundary Value Problem (2.2): we construct weak (actually, distributional) solutions to (2.15) by parabolic approximation, use the hypoellipticity of $\partial_t - \mathscr{L}$ to obtain the smoothness of such solutions and apply the Itô formula to identify the solution with u defined by (2.13). We mention here that, regarding the first step, a variational approach to (2.7), closer to the spirit of the proof outlined in Section 2.2.1 than our parabolic approximation argument, was recently developed by Armstrong and Mourrat [3].

Remark 2.2.11 (Extension to bounded and measurable functions)**.** *Let $f : D \cup \Gamma^- \to \mathbb{R}$ be measurable and bounded, and take $g \equiv 0$. Using an elementary regularization argument, which can be rigorously justified with the help of Theorem 2.2.20 and Corollary 2.2.21 stated below, it is easy to check that the function u defined by (2.13) remains a distributional solution of (2.15) on $\mathbb{R}_+^* \times D$ and therefore, by hypoellipticity, still satisfies Assertion (iii).*

Remark 2.2.12. *It is easy to check that, using the same proofs, these results also hold for a time-dependent boundary condition $g(t,x) \in \mathscr{C}^b(\mathbb{R}_+ \times (\Gamma^+ \cup \Gamma^0))$, replacing (2.13) by $u(t,x) = \mathbb{E}[\mathbb{1}_{\tau_\partial^x > t} f(X_t^x) + \mathbb{1}_{\tau_\partial^x \leq t} g(t - \tau_\partial^x, X_{\tau_\partial^x}^x)]$. We stick to a time-homogeneous boundary conditions for the ease of notation.*

Remark 2.2.13. *Note that the compatibility condition (2.14) is necessary to ensure the continuity of the solution at $\{0\} \times \overline{D}$. Furthermore, the continuity result at the boundary ∂D is sharp as it has been shown in the one-dimensional case ($d = 1$) that the solution is only expected to be Hölder-continuous close to the singular set $\Gamma^0 = \{(q,p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) = 0\}$, and not differentiable, see [47].*

2.2.2.3 Maximum principle and Harnack inequality

As an immediate consequence of Theorem 2.2.10, under Assumptions (O1) and (F1), if $f \geq 0$ on D and $g \geq 0$ on Γ^+ then it follows that any solution v of (2.7) which satisfies the conditions of (iv) is such that $v \geq 0$ on $\mathbb{R}_+ \times \overline{D}$. We now state stronger forms of this maximum principle, as well as a Harnack inequality, under the following supplementary assumption on the domain $\mathscr{O}$.

Assumption (O2). *The set $\mathscr{O}$ is connected.*

Theorem 2.2.14 (Maximum principle)**.** *Let Assumptions (F1), (O1) and (O2) hold. Let $u \in \mathscr{C}^{1,2}(\mathbb{R}_+^* \times D)$ such that $\partial_t u - \mathscr{L} u \leq 0$ on $\mathbb{R}_+^* \times D$.*

(i) Assume that $u \in \mathscr{C}^b((\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+))$, then

$$\sup_{\mathbb{R}_+^* \times D} u(t,x) = \sup_{(\{t=0\} \times D) \cup (\mathbb{R}_+^* \times \Gamma^+)} u(t,x). \tag{2.16}$$

(ii) Assume that u reaches a maximum at a point $(t_0, x_0) \in \mathbb{R}_+^* \times D$, then

$$\forall t \leq t_0, \quad \forall x \in D, \qquad u(t,x) = u(t_0, x_0).$$

Theorem 2.2.14 is proven in Section 2.4.2. Let us conclude this section by stating a Harnack inequality. In the literature, a variant of the Harnack inequality was obtained in the stationary case for hypoelliptic operators, see [13]. In [35], the authors prove a local Harnack inequality satisfied by distributional solutions to $\partial_t u = \mathscr{L} u$. Here, we extend their result on a compact set of D in the following theorem. The proof uses in particular the concept of Harnack chains from [2].

Theorem 2.2.15 (Harnack inequality)**.** *Let Assumptions (F1), (O1) and (O2) hold. For any compact set $K \subset D$, $\epsilon > 0$ and $T > 0$, there exists a constant $C_{K,\epsilon,T} > 0$ such that for any non-negative distributional solution u of $\partial_t u = \mathscr{L} u$ on $\mathbb{R}_+^* \times D$ (in the sense of Defintion 2.2.3), for all $t \geq \epsilon$,*

$$\sup_{x \in K} u(t,x) \leq C_{K,\epsilon,T} \inf_{x \in K} u(t+T, x). \tag{2.17}$$

Theorem 2.2.15 is proven in Section 2.4.1.

Remark 2.2.16. *For a given compact set K, one can find an open set $\mathscr{O}$ satisfying Assumptions (O1) and (O2) such that $K \subset \mathscr{O} \times \mathbb{R}^d$. Therefore, Theorem 2.2.15 remains valid for any non-negative distributional solution u of $\partial_t u = \mathscr{L} u$ on $\mathbb{R}_+^* \times \mathbb{R}^{2d}$.*

2.2.3 Kolmogorov equations and Gaussian bounds for the Langevin process

In this section, we consider the Langevin process (2.10) without absorbing boundary condition. We recall that under Assumption (F2), for all $x \in \mathbb{R}^{2d}$ the equation (2.10) admits a unique strong global solution $(X_t^x)_{t\geq 0}$ on $\mathbb{R}^{2d}$. Let us introduce the associated transition kernel P_t:

$$\forall t > 0, \quad \forall x \in \mathbb{R}^{2d}, \quad \forall A \in \mathscr{B}(\mathbb{R}^{2d}), \qquad \mathrm{P}_t(x, A) := \mathbb{P}(X_t^x \in A).$$

The following properties of $\mathrm{P}_t(x, \cdot)$ are proven in [71, Corollary 7.2] and [44, Corollary 3.3].

Proposition 2.2.17 (Kolmogorov equations for the Langevin process)**.** *Under Assumption (F2), there exists a function*

$$(t, x, y) \mapsto \mathrm{p}_t(x, y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times \mathbb{R}^{2d} \times \mathbb{R}^{2d}) \tag{2.18}$$

such that for all $t > 0$, $x \in \mathbb{R}^{2d}$ and $A \in \mathscr{B}(\mathbb{R}^{2d})$,

$$\mathrm{P}_t(x, A) = \int_A \mathrm{p}_t(x, y)\mathrm{d}y.$$

Moreover, this transition density is positive on $\mathbb{R}_+^* \times \mathbb{R}^{2d}$ and satisfies the backward and forward Kolmogorov equations:

(i) $(t, x) \mapsto \mathrm{p}_t(x, y)$ *satisfies* $\partial_t \mathrm{p} = \mathscr{L}_x \mathrm{p}$ *on* $\mathbb{R}_+^* \times \mathbb{R}^{2d}$*,*

(ii) $(t, y) \mapsto \mathrm{p}_t(x, y)$ *satisfies* $\partial_t \mathrm{p} = \mathscr{L}_y^* \mathrm{p}$ *on* $\mathbb{R}_+^* \times \mathbb{R}^{2d}$*.*

The subscript in $\mathscr{L}_x$ and $\mathscr{L}_y$ indicates on which variable the differential operator $\mathscr{L}$ applies. We will also need the following immediate corollary of Proposition 2.2.17.

Corollary 2.2.18 (Atoms of τ_∂^x)**.** *Under the assumptions of Proposition 2.2.17, for all $x \in \overline{D}$, for all $t > 0$,*

$$\mathbb{P}(\tau_\partial^x = t) \leq \mathbb{P}(q_t^x \in \partial\mathscr{O}) = 0.$$

Theorem 2.2.19 below states that the transition density $\mathrm{p}_t(x, y)$ admits an explicit Gaussian upper bound. This has already been proven in [52] in the case $\gamma = 0$, using the parametrix method, if Assumption (F2) holds. In this case, the drift coefficient $(q, p) \mapsto F(q)$ for the velocity-related SDE in (2.10) is indeed globally Lipschitz continuous and bounded, and thus satisfies the hypothesis required in [52]. If $\gamma \neq 0$ the drift coefficient $(q, p) \mapsto F(q) - \gamma p$ is not bounded in $\mathbb{R}^{2d}$, but we adapt the idea of the parametrix method to obtain a Gaussian upper bound in this case, see Section 2.5.1.

Theorem 2.2.19 (Gaussian upper bound on p_t)**.** *Under Assumption (F2), the transition density $\mathrm{p}_t(x, y)$ of the Langevin process $(X_t^x)_{t\geq 0}$ satisfying (2.10) is such that for all $\alpha \in (0, 1)$, there exists $c_\alpha > 0$, depending only on α, such that for all $T > 0$ and $t \in (0, T]$, for all $x, y \in \mathbb{R}^{2d}$,*

$$\mathrm{p}_t(x, y) \leq \frac{1}{\alpha^d} \sum_{j=0}^{\infty} \frac{\left(\|F\|_\infty c_\alpha (1 + \sqrt{\gamma_- T})\sqrt{\pi t}\right)^j}{\sigma^j \Gamma\left(\frac{j+1}{2}\right)} \widehat{\mathrm{p}}_t^{(\alpha)}(x, y), \tag{2.19}$$

where $\gamma_- = \max(-\gamma, 0)$ is the negative part of $\gamma \in \mathbb{R}$, Γ is the Gamma function and $\widehat{\mathrm{p}}_t^{(\alpha)}(x, y)$ is the transition density of the Gaussian process with infinitesimal generator $\mathscr{L}_{0,\gamma,\sigma/\sqrt{\alpha}}$ defined in (2.6), see also Equations (2.74)-(2.79) below for explicit formulas.

2.2.4 Kolmogorov equations and compactness properties for the absorbed Langevin process

Let us define the transition kernel P_t^D for the absorbed Langevin process $(X_t^x)_{0\leq t\leq \tau_\partial^x}$:

$$\forall t\geq 0,\quad \forall x\in D,\quad \forall A\in\mathscr{B}(D),\qquad \mathrm{P}_t^D(x,A):=\mathbb{P}(X_t^x\in A,\tau_\partial^x>t). \tag{2.20}$$

It is easy to see that for any $t\geq 0$, $x\in D$ and $A\in\mathscr{B}(D)$,

$$\mathrm{P}_t^D(x,A)\leq \mathrm{P}_t(x,A). \tag{2.21}$$

The next theorem is the equivalent of Proposition 2.2.17 for the transition kernel $\mathrm{P}_t^D(x,\cdot)$.

Theorem 2.2.20 (Kolmogorov equations for the absorbed Langevin process)**.** *Under Assumptions (O1) and (F1), there exists a function*

$$(t,x,y)\mapsto \mathrm{p}_t^D(x,y)\in\mathscr{C}^\infty(\mathbb{R}_+^*\times D\times D)\cap\mathscr{C}(\mathbb{R}_+^*\times\overline{D}\times\overline{D})$$

such that for all $t>0$, $x\in\overline{D}$ and $A\in\mathscr{B}(D)$,

$$\mathrm{P}_t^D(x,A)=\int_A \mathrm{p}_t^D(x,y)\mathrm{d}y.$$

Moreover, this transition density p_t^D satisfies the backward and forward Kolmogorov equations:

(i) $(t,x)\mapsto \mathrm{p}_t^D(x,y)$ *satisfies* $\partial_t\mathrm{p}^D=\mathscr{L}_x\mathrm{p}^D$ *on* $\mathbb{R}_+^*\times D$,

(ii) $(t,y)\mapsto \mathrm{p}_t^D(x,y)$ *satisfies* $\partial_t\mathrm{p}^D=\mathscr{L}_y^*\mathrm{p}^D$ *on* $\mathbb{R}_+^*\times D$.

Finally, for all $t>0$, $(x,y)\in\overline{D}\times\overline{D}$,

(i) $\mathrm{p}_t^D(x,y)=0$ *if* $x\in\Gamma^+\cup\Gamma^0$ *or* $y\in\Gamma^-\cup\Gamma^0$,

(ii) under Assumption (O2), $\mathrm{p}_t^D(x,y)>0$ *if* $x\notin\Gamma^+\cup\Gamma^0$ *and* $y\notin\Gamma^-\cup\Gamma^0$.

The proof of the existence of a transition density $\mathrm{p}_t^D(x,y)$ which is smooth on $\mathbb{R}_+^*\times D\times D$ and satisfies the backward and forward Kolmogorov equations will be done in Propositions 2.5.4 and 2.5.5, in Section 2.5.2. The results on the continuity at the boundary as well as on the positivity of p_t^D are stated in Theorem 2.6.3. They crucially rely on the introduction and study of a so-called adjoint process to (2.10), which is carried out in Section 2.6.

An immediate useful corollary of Theorem 2.2.20, the inequality (2.21) and Theorem 2.2.19 is the following.

Corollary 2.2.21 (Gaussian upper bound on p_t^D)**.** *Under Assumptions (O1) and (F1), the transition density p_t^D only depends on the values of F inside $\mathscr{O}$, see Remark 2.2.6. Therefore, up to a modification of F outside of $\mathscr{O}$ so that F satisfies (F2), $\mathrm{p}_t^D(x,y)$ satisfies the Gaussian upper bound of Theorem 2.2.19.*

It is an easy consequence of Corollary 2.2.21 and the explicit expression of $\widehat{\mathrm{p}}_t^{(\alpha)}$ that, for any $t>0$ and $x\in\overline{D}$, $\mathrm{p}_t^D(x,\cdot)\in\mathrm{L}^1(D)\cap\mathrm{L}^\infty(D)$. By Theorem 2.2.20, this remark allows us to define, for any $t\geq 0$, $p\in[1,+\infty]$ and $f\in\mathrm{L}^p(D)$,

$$P_t^D f: x\in\overline{D}\mapsto \int_D \mathrm{P}_t^D(x,\mathrm{d}y)f(y).$$

The Gaussian estimate of Corollary 2.2.21 then implies the following results, which are proved in Section 2.6.2.

Theorem 2.2.22 (Compactness of the semigroup $(P_t^D)_{t\geq 0}$)**.** *Let Assumptions (O1) and (F1) hold, and let $p, q \in [1, +\infty]$.*

(i) *The family of operators $(P_t^D)_{t\geq 0}$ is a semigroup on $\mathrm{L}^p(D)$ and on $\mathscr{C}^b(\overline{D})$.*

(ii) *For any $t > 0$, the operator P_t^D maps $L^p(D)$ into $L^q(D)$ continuously.*

(iii) *For any $t > 0$, the operator P_t^D is compact from $\mathrm{L}^p(D)$ to $\mathrm{L}^p(D)$, and from $\mathscr{C}^b(\overline{D})$ to $\mathscr{C}^b(\overline{D})$.*

As an alternative to our probabilistic approach, we expect that a similar statement might also be deduced from the subelliptic estimates on the kinetic Fokker-Planck operator recently obtained by Nier [65] in a very general framework (both on the geometry of the underlying phase space and on the boundary conditions).

2.3 The Initial-Boundary Value problem

This section is devoted to the proof of Theorem 2.2.10. In this theorem, Assertion (i) is an immediate consequence of Proposition 2.2.8 which is proven in Section 2.3.4. Assertions (iv), (ii) and (iii) are respectively proven in Sections 2.3.1, 2.3.2 and 2.3.3. Finally, the preliminary Proposition 2.2.8 is proved in Section 2.3.4.

All the results in this section are proved under Assumptions (O1) and (F2). Since the final statement of Theorem 2.2.10 only depends on the values of F in $\mathscr{O}$ (see Remark 2.2.6), this statement remains valid if Assumption (F2) is replaced by Assumption (F1).

Before proceeding, we introduce some notation which will be used throughout the sequel of the paper. Let d_∂ be the Euclidean distance function to the boundary $\partial\mathscr{O}$ from a point in $\mathscr{O}$, i.e.

$$\mathrm{d}_\partial : q \in \mathbb{R}^d \mapsto \begin{cases} \mathrm{d}(q, \partial\mathscr{O}) & \text{if } q \in \mathscr{O}, \\ 0 & \text{if } q \notin \mathscr{O}. \end{cases} \tag{2.22}$$

In addition, we denote by $\overline{\mathrm{d}}_\partial$ the signed Euclidean distance to the boundary $\partial\mathscr{O}$, i.e.

$$\overline{\mathrm{d}}_\partial : q \in \mathbb{R}^d \mapsto \begin{cases} \mathrm{d}(q, \partial\mathscr{O}) & \text{if } q \in \mathscr{O}, \\ -\mathrm{d}(q, \partial\mathscr{O}) & \text{if } q \notin \mathscr{O}, \end{cases}$$

so that d_∂ is the positive part of $\overline{\mathrm{d}}_\partial$. Last, $\mathrm{d}_{\overline{\mathscr{O}}}$ is the Euclidean distance to the compact $\overline{\mathscr{O}}$,

$$\mathrm{d}_{\overline{\mathscr{O}}} : q \in \mathbb{R}^d \mapsto \mathrm{d}(q, \overline{\mathscr{O}}). \tag{2.23}$$

All these distance functions are 1-Lipschitz continuous.

2.3.1 Uniqueness: proof of Assertion (iv) in Theorem 2.2.10

Assertion (iv) in Theorem 2.2.10 follows from the application of the Itô formula. Although the general argument is well-known, we detail its application here in order to emphasize two specificities of our framework: the fact that the domain D is unbounded, and the fact that the kinetic nature of the Langevin process $(X_t^x)_{t\geq 0}$ makes boundary conditions on v only necessary on the subset Γ^+ of ∂D.

Proof of Assertion (iv) in Theorem 2.2.10. Let $g \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$ and $f \in \mathscr{C}^b(D \cup \Gamma^-)$. Let v be a solution of (2.7), satisfying the conditions of Assertion (iv) in Theorem 2.2.10.

Let $x \in D$. Let $(X_t^x = (q_t^x, p_t^x))_{t\geq 0}$ be the strong solution of (2.10) on $\mathbb{R}^{2d}$. For $k > 0$, let V_k be the following open and bounded subset of D

$$V_k := \left\{ (q,p) \in D : |p| < k, \mathrm{d}_\partial(q) > \frac{1}{k} \right\}. \tag{2.24}$$

Let us choose k large enough so that $x \in V_k$. Let $\tau^x_{V_k^c}$ be the following stopping time:

$$\tau^x_{V_k^c} = \inf\{t > 0 : X^x_t \notin V_k\}.$$

Let $t > 0$ and $s \in [0,t)$. Since $v \in \mathscr{C}^{1,2}(\mathbb{R}^*_+ \times D)$, Itô's formula applied to the process $(v(t-r, X^x_r))_{0\leq r\leq s}$ between 0 and $s \wedge \tau^x_{V_k^c}$ yields: almost surely, for $s \in [0,t)$

$$v(t - s \wedge \tau^x_{V_k^c}, X^x_{s\wedge\tau^x_{V_k^c}}) = v(t,x) + \sigma \int_0^{s\wedge\tau^x_{V_k^c}} \nabla_p v(t-r, X^x_r)\cdot \mathrm{d}B_r,$$

since $\partial_t v - \mathscr{L} v = 0$ on $\mathbb{R}^*_+ \times D$. Besides, since $\nabla_p v$ is continuous on the compact set $[t-s,t] \times \overline{V_k}$, hence bounded on $(t-s,t) \times V_k$, the stochastic integral in the right-hand side is a martingale and its expectation vanishes. Therefore

$$\begin{aligned} v(t,x) &= \mathbb{E}\left[v(t - s\wedge\tau^x_{V_k^c}, X^x_{s\wedge\tau^x_{V_k^c}})\right] \\ &= \mathbb{E}\left[\mathbb{1}_{\tau^x_{V_k^c}>s} v(t-s, X^x_s) + \mathbb{1}_{\tau^x_{V_k^c}\leq s} v(t-\tau^x_{V_k^c}, X^x_{\tau^x_{V_k^c}})\right]. \end{aligned} \tag{2.25}$$

Now we would like to let $k \to \infty$ and then $s \to t$ in (2.25).

First let us prove the following limit

$$\lim_{k\to\infty} \tau^x_{V_k^c} = \tau^x_\partial \quad \text{almost surely.}$$

The sequence $(\tau^x_{V_k^c})_{k\geq 1}$ is an increasing sequence of random variables, therefore it converges almost surely to $\sup_{k\geq 1}\tau^x_{V_k^c}$. Besides, using the continuity of the trajectories of $(X^x_t)_{t\geq 0}$, one gets, for all $r > 0$,

$$\begin{aligned} \left\{\sup_{k\geq 1}\tau^x_{V_k^c} > r\right\} &= \left\{\exists k \geq 1 : \tau^x_{V_k^c} > r\right\} \\ &= \left\{\exists k\geq 1 : \sup_{u\in[0,r]}|p^x_u| < k, \inf_{u\in[0,r]} \mathrm{d}_\partial(q^x_u) > \frac{1}{k}\right\} \\ &= \left\{\sup_{u\in[0,r]}|p^x_u| < \infty, \inf_{u\in[0,r]} \mathrm{d}_\partial(q^x_u) > 0\right\} \\ &= \left\{\sup_{u\in[0,r]}|p^x_u| < \infty, \tau^x_\partial > r\right\}. \end{aligned}$$

For all $r > 0$, we have that, almost surely, $\sup_{u\in[0,r]}|p^x_u| < \infty$. Therefore, $\sup_{k\geq 1}\tau^x_{V_k^c} > r$ if and only if $\tau^x_\partial > r$, that is to say $\sup_{k\geq 1}\tau^x_{V_k^c} = \tau^x_\partial$ almost surely. As a result, one gets $\lim_{k\to\infty}\tau^x_{V_k^c} = \tau^x_\partial$ almost surely. Consequently, since $k \mapsto \tau^x_{V_k^c}$ is increasing and $t \mapsto \mathbb{1}_{t>s}$ is left-continuous, one has almost surely that for all $s > 0$,

$$\mathbb{1}_{\tau^x_{V_k^c}>s} \underset{k\to\infty}{\longrightarrow} \mathbb{1}_{\tau^x_\partial > s}. \tag{2.26}$$

Second, notice that $X^x_{\tau^x_\partial} \in \Gamma^+$ almost surely on the event $\{\tau^x_\partial \leq s\}$ by Proposition 2.2.8 since $x \in D$. Consequently, since $v \in \mathscr{C}(\mathbb{R}^*_+ \times (D\cup\Gamma^+))$ and $v = g$ on $\mathbb{R}^*_+ \times \Gamma^+$

$$\mathbb{1}_{\tau^x_{V_k^c}\leq s} v(t-\tau^x_{V_k^c}, X^x_{\tau^x_{V_k^c}}) \underset{k\to\infty}{\longrightarrow} \mathbb{1}_{\tau^x_\partial\leq s} g(X^x_{\tau^x_\partial}) \quad \text{almost surely.} \tag{2.27}$$

We now use (2.26), (2.27) to apply the dominated convergence theorem to (2.25) when k goes to infinity, using the fact that v is assumed to be bounded on $[0,t] \times D$. Therefore, one gets for $x \in D$ and $s \in [0,t)$,

$$v(t,x) = \mathbb{E}\left[\mathbb{1}_{\tau^x_\partial > s} v(t-s, X^x_s)\right] + \mathbb{E}\left[\mathbb{1}_{\tau^x_\partial\leq s} g(X^x_{\tau^x_\partial})\right]. \tag{2.28}$$

Finally, let us consider the limit $s \to t$ in (2.28). Notice that

$$\mathbb{1}_{\tau_\partial^x > s} \underset{s \to t}{\longrightarrow} \mathbb{1}_{\tau_\partial^x > t} \quad \text{almost surely,}$$

using Corollary 2.2.18 (which follows from Proposition 2.2.17, which holds independently from the results proven in this section). Therefore, the second term in the right-hand side of the equality (2.28) satisfies by dominated convergence,

$$\mathbb{E}\left[\mathbb{1}_{\tau_\partial^x \le s} g(X^x_{\tau_\partial^x})\right] \underset{s \to t}{\longrightarrow} \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x \le t} g(X^x_{\tau_\partial^x})\right].$$

Moreover the continuity of the trajectories of $(X^x_s)_{s\ge 0}$ and the continuity of v on $\mathbb{R}_+ \times D$ ensure that

$$\mathbb{1}_{\tau_\partial^x > s} v(t-s, X^x_s) \underset{s \to t}{\longrightarrow} \mathbb{1}_{\tau_\partial^x > t} v(0, X^x_t) = \mathbb{1}_{\tau_\partial^x > t} f(X^x_t) \quad \text{almost surely.}$$

Finally, taking the limit $s \to t$ in (2.28), the dominated convergence theorem ensures that

$$v(t,x) = \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t} f(X^x_t) + \mathbb{1}_{\tau_\partial^x \le t} g(X^x_{\tau_\partial^x})\right]$$

for all $t > 0$, $x \in D$. This concludes the proof of Assertion (iv) in Theorem 2.2.10 using the continuity of v in $(\mathbb{R}_+ \times (D \cup \Gamma^+)) \setminus (\{0\} \times \Gamma^+)$. □

2.3.2 Continuity: proof of Assertion (ii) in Theorem 2.2.10

The proof of Assertion (ii) in Theorem 2.2.10 relies on the the following lemmata. We recall that under Assumption (F2), we denote by C_{Lip} the Lipschitz constant of the drift of (2.10).

Lemma 2.3.1 (Gronwall Lemma). *Under Assumption (F2), for all $t \ge 0$, for all $x, y \in \mathbb{R}^{2d}$, one has*

$$\sup_{s\in[0,t]} |X^x_s - X^y_s| \le |x-y| \mathrm{e}^{C_{\mathrm{Lip}} t} \quad \textit{almost surely.} \tag{2.29}$$

Besides, for $(t_0, x_0) \in \mathbb{R}_+ \times \mathbb{R}^{2d}$ we have

$$X^x_t \underset{(t,x)\to(t_0,x_0)}{\longrightarrow} X^{x_0}_{t_0} \quad \textit{almost surely.} \tag{2.30}$$

The estimate (2.29) follows from a standard application of the Gronwall Lemma which we do not detail here. The joint continuity statement (2.30) is then a straightforward consequence of the continuity of the trajectories of $(X^x_t)_{t\ge 0}$.

Lemma 2.3.2 (Continuity of the exit event indicator). *Under Assumptions (O1) and (F2), let $(t,x) \in (\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^+ \cup \Gamma^0))$. Let $(t_n, x_n)_{n\ge 1}$ be a sequence of $\mathbb{R}_+ \times \overline{D}$ converging towards (t,x). Then one has*

$$\mathbb{1}_{\tau_\partial^{x_n} > t_n} \underset{n\to\infty}{\longrightarrow} \mathbb{1}_{\tau_\partial^x > t} \quad \textit{almost surely.} \tag{2.31}$$

Proof. We prove the convergence (2.31) on the events $\{\tau_\partial^x < t\}$, $\{\tau_\partial^x = t\}$ and $\{\tau_\partial^x > t\}$, separately.

Step 1. Let us start by proving (2.31) on the event $\{\tau_\partial^x < t\}$ (necessarily $t > 0$). Let $\epsilon \in (0, t - \tau_\partial^x)$. If $x \in \Gamma^+ \cup \Gamma^0$, then by Proposition 2.2.8, $\tau_\partial^x = 0$ and there exists $s \in (0, \epsilon]$ such that $\mathrm{d}_{\overline{\mathcal{O}}}(q^x_s) > 0$. If $x \in D \cup \Gamma^-$, then $X^x_{\tau_\partial^x} \in \Gamma^+$ almost surely by Proposition 2.2.8. By the strong Markov property and Proposition 2.2.8, there exists again $s \in (\tau_\partial^x, \tau_\partial^x + \epsilon]$ such that $\mathrm{d}_{\overline{\mathcal{O}}}(q^x_s) > 0$.

Since $x_n \underset{n\to\infty}{\longrightarrow} x$, there exists $N_1 \ge 1$ such that for all $n \ge N_1$, $|x_n - x| \le \frac{\mathrm{d}_{\overline{\mathcal{O}}}(q^x_s)}{2} \mathrm{e}^{-C_{\mathrm{Lip}}(\tau_\partial^x + \epsilon)}$. As a result using Lemma 2.3.1 along with the fact that the distance function $\mathrm{d}_{\overline{\mathcal{O}}}$ is 1-Lipschitz continuous, it follows that for all $n \ge N_1$

$$\mathrm{d}_{\overline{\mathcal{O}}}(q^{x_n}_s) \ge \frac{\mathrm{d}_{\overline{\mathcal{O}}}(q^x_s)}{2} > 0.$$

Therefore, we have $\tau_\partial^{x_n} < s \leq \tau_\partial^x + \epsilon$. In addition, the convergence $t_n \underset{n\longrightarrow\infty}{\longrightarrow} t$ implies that there exists $N_2 \geq 1$ such that for all $n \geq N_2$, one has $t_n \geq \tau_\partial^x + \epsilon$, since $\tau_\partial^x + \epsilon < t$. As a result for $n \geq \max(N_1, N_2)$,

$$\tau_\partial^{x_n} < \tau_\partial^x + \epsilon \leq t_n.$$

Hence the convergence (2.31) on the event $\{\tau_\partial^x < t\}$.

Step 2. Let us consider the event $\{\tau_\partial^x = t\}$. For $t = 0$ and $x \in D \cup \Gamma^-$, $\mathbb{P}(\tau_\partial^x = 0) = 0$ by Proposition 2.2.8. Moreover for $t > 0$, $\mathbb{P}(\tau_\partial^x = t) = 0$ by Corollary 2.2.18. As a result, it is not necessary to prove the convergence (2.31) on the event $\{\tau_\partial^x = t\}$ as the latter is negligible.

Step 3. Finally, it only remains to prove the convergence (2.31) on the event $\{\tau_\partial^x > t\}$. Let $t^{'} := \frac{1}{2}(\tau_\partial^x + t)$. Since $t_n \underset{n\longrightarrow\infty}{\longrightarrow} t$, there exists $N_1 \geq 1$ such that for $n \geq N_1$, $t_n \leq t^{'}$.

On the one hand, if $x \in D$, then by the continuity of the trajectories of $(q_s^x)_{s\in[0,t']}$, one has $\inf_{s\in[0,t']} \mathrm{d}_\partial(q_s^x) > 0$. By Lemma 2.3.1 and the fact that the distance function d_∂ is 1-Lipschitz continuous, there exists $N_2 \geq 1$ such that for $n \geq N_2$,

$$\inf_{s\in[0,t']} \mathrm{d}_\partial(q_s^{x_n}) > 0,$$

which yields $\tau_\partial^{x_n} > t^{'}$. As a result, for $n \geq \max(N_1, N_2)$,

$$\tau_\partial^{x_n} > t^{'} \geq t_n.$$

On the other hand, if $x \in \partial D$, then necessarily $x \in \Gamma^-$, otherwise $\tau_\partial^x = 0$ by Proposition 2.2.8. Then for all $k \geq 1$,

$$\inf_{s\in\left[\frac{1}{k},t'\right]} \mathrm{d}_\partial(q_s^x) > 0.$$

Using Lemma 2.3.1 again, we get that there exists $M_k \geq 1$ such that for $n \geq M_k$, $\tau_\partial^{x_n} > t^{'}$ or $\tau_\partial^{x_n} \leq \frac{1}{k}$. Assume that there exists an unbounded sequence $(n_k)_{k\geq 1}$ such that $\tau_\partial^{x_{n_k}} \leq \frac{1}{k}$. Then $x \in \Gamma^+ \cup \Gamma^0$ since $X_{\tau_\partial^{x_{n_k}}}^{x_{n_k}} \in \Gamma^+$ and $X_{\tau_\partial^{x_{n_k}}}^{x_{n_k}} \underset{n\longrightarrow\infty}{\longrightarrow} x$ by Lemma 2.3.1, which is in contradiction with the fact that $x \in \Gamma^-$. As a result there exists $N_2 \geq 1$ such that for all $n \geq N_2$, $\tau_\partial^{x_n} > t^{'}$. Hence, for $n \geq \max(N_1, N_2)$, $\tau_\partial^{x_n} > t_n$. This concludes the proof of the convergence (2.31) on the event $\{\tau_\partial^x > t\}$. □

Remark 2.3.3. *Notice that the convergence (2.31) cannot be satisfied for* $(t, x) \in \{0\} \times (\Gamma^+ \cup \Gamma^0)$. *Indeed, if* $x \in \Gamma^+ \cup \Gamma^0$ *and* $(x_n)_{n\geq 1}$ *is a sequence of elements of* D *which converges towards* x, *then by Proposition 2.2.8 we have* $\mathbb{1}_{\tau_\partial^{x_n}>0} = 1$ *almost surely while* $\mathbb{1}_{\tau_\partial^x>0} = 0$ *almost surely.*

Remark 2.3.4. *Let us take* $t_n = t > 0$ *for all* $n \geq 1$ *in Lemma 2.3.2. Then we get that for any sequence* $(x_n)_{n\geq 1}$ *of elements of* $\overline{D}$ *converging to some* $x \in \overline{D}$, $\mathbb{1}_{\tau_\partial^{x_n}>t}$ *converges almost surely to* $\mathbb{1}_{\tau_\partial^x>t}$. *Using the monotonicity of the functions* $t \mapsto \mathbb{1}_{\tau_\partial^{x_n}>t}$ *and* $t \mapsto \mathbb{1}_{\tau_\partial^x>t}$, *we deduce that almost surely, for any* $t > 0$ *such that* $t \neq \tau_\partial^x$, $\mathbb{1}_{\tau_\partial^{x_n}>t}$ *converges almost surely to* $\mathbb{1}_{\tau_\partial^x>t}$. *Integrating in time, we conclude that* $\tau_\partial^{x_n}$ *converges almost surely to* τ_∂^x.

We are now in position to prove Assertion (ii) in Theorem 2.2.10.

Proof of Assertion (ii) in Theorem 2.2.10. The proof is divided into two steps. In the first step we show that u is continuous on $(\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^+ \cup \Gamma^0))$, and in the second step we show that if f and g satisfy the compatibility condition (2.14) then u is continuous on $\mathbb{R}_+ \times \overline{D}$.

Step 1. Let $(t, x) \in (\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^+ \cup \Gamma^0))$. Let $(t_n, x_n)_{n\geq 1}$ be a sequence in $\mathbb{R}_+ \times \overline{D}$ converging to (t, x). Let us prove that

$$u(t_n, x_n) \underset{n\longrightarrow\infty}{\longrightarrow} u(t, x). \tag{2.32}$$

To this aim, let us study the difference $|u(t_n, x_n) - u(t, x)|$. It follows from the expression (2.13) of u and the triangle inequality that

$$|u(t_n, x_n) - u(t, x)| \leq \mathbb{E}\left[\left|f(X_{t_n}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} > t_n} - f(X_t^x)\mathbb{1}_{\tau_\partial^x > t}\right|\right] + \mathbb{E}\left[\left|g(X_{\tau_\partial^{x_n}}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} \leq t_n} - g(X_{\tau_\partial^x}^x)\mathbb{1}_{\tau_\partial^x \leq t}\right|\right]. \tag{2.33}$$

Let us start with the first term in the right-hand side of the inequality above. We have that

$$\begin{aligned}
&\left|f(X_{t_n}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} > t_n} - f(X_t^x)\mathbb{1}_{\tau_\partial^x > t}\right| \\
&= \left|\mathbb{1}_{\tau_\partial^{x_n} > t_n, \tau_\partial^x > t}\left[f(X_{t_n}^{x_n}) - f(X_t^x)\right] + f(X_{t_n}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} > t_n, \tau_\partial^x \leq t} - f(X_t^x)\mathbb{1}_{\tau_\partial^x > t, \tau_\partial^{x_n} \leq t_n}\right| \\
&\leq \mathbb{1}_{\tau_\partial^{x_n} > t_n, \tau_\partial^x > t}\left|f(X_{t_n}^{x_n}) - f(X_t^x)\right| + \|f\|_\infty \left|\mathbb{1}_{\tau_\partial^{x_n} > t_n} - \mathbb{1}_{\tau_\partial^x > t}\right|,
\end{aligned}$$

since $\mathbb{1}_{\tau_\partial^{x_n} > t_n, \tau_\partial^x \leq t} + \mathbb{1}_{\tau_\partial^x > t, \tau_\partial^{x_n} \leq t_n} = |\mathbb{1}_{\tau_\partial^{x_n} > t_n} - \mathbb{1}_{\tau_\partial^x > t}|$. By Lemmata 2.3.1 and 2.3.2, since $f \in \mathscr{C}^b(D \cup \Gamma^-)$, it follows by the dominated convergence theorem that $\mathbb{E}[\left|f(X_{t_n}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} > t_n} - f(X_t^x)\mathbb{1}_{\tau_\partial^x > t}\right|] \underset{n\to\infty}{\longrightarrow} 0$.

Let us now consider the second term in the right-hand side of the inequality (2.33). We have that

$$\begin{aligned}
&\left|g(X_{\tau_\partial^{x_n}}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} \leq t_n} - g(X_{\tau_\partial^x}^x)\mathbb{1}_{\tau_\partial^x \leq t}\right| \\
&= \left|\mathbb{1}_{\tau_\partial^{x_n} \leq t_n, \tau_\partial^x \leq t}\left[g(X_{\tau_\partial^{x_n}}^{x_n}) - g(X_{\tau_\partial^x}^x)\right] + g(X_{\tau_\partial^{x_n}}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} \leq t_n, \tau_\partial^x > t} - g(X_{\tau_\partial^x}^x)\mathbb{1}_{\tau_\partial^{x_n} > t_n, \tau_\partial^x \leq t}\right| \\
&\leq \mathbb{1}_{\tau_\partial^{x_n} \leq t_n, \tau_\partial^x \leq t}\left|g(X_{\tau_\partial^{x_n}}^{x_n}) - g(X_{\tau_\partial^x}^x)\right| + \|g\|_\infty \left|\mathbb{1}_{\tau_\partial^{x_n} > t_n} - \mathbb{1}_{\tau_\partial^x > t}\right|,
\end{aligned}$$

so that we deduce again from Lemmata 2.3.1 and 2.3.2 along with Remark 2.3.4 and the dominated convergence theorem, since $g \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$, that

$$\mathbb{E}\left[\left|g(X_{\tau_\partial^{x_n}}^{x_n})\mathbb{1}_{\tau_\partial^{x_n} \leq t_n} - g(X_{\tau_\partial^x}^x)\mathbb{1}_{\tau_\partial^x \leq t}\right|\right] \underset{n\to\infty}{\longrightarrow} 0,$$

which completes the proof of (2.32).

Step 2. Assume now that f and g satisfy the compatibility condition (2.14). Let $x \in \Gamma^+ \cup \Gamma^0$ and $(t_n, x_n)_{n\geq 1}$ be a sequence in $\mathbb{R}_+ \times \overline{D}$ converging to $(0, x)$. Let us prove that

$$u(t_n, x_n) \underset{n\longrightarrow\infty}{\longrightarrow} u(0, x) = g(x).$$

We have that

$$\begin{aligned}
|u(t_n, x_n) - g(x)| &= \left|\mathbb{E}\left[\left(f(X_{t_n}^{x_n}) - g(x)\right)\mathbb{1}_{\tau_\partial^{x_n} > t_n}\right] + \mathbb{E}\left[\left(g(X_{\tau_\partial^{x_n}}^{x_n}) - g(x)\right)\mathbb{1}_{\tau_\partial^{x_n} \leq t_n}\right]\right| \\
&\leq \mathbb{E}\left[\left|f(X_{t_n}^{x_n}) - g(x)\right|\mathbb{1}_{\tau_\partial^{x_n} > t_n}\right] + \mathbb{E}\left[\left|g(X_{\tau_\partial^{x_n}}^{x_n}) - g(x)\right|\mathbb{1}_{\tau_\partial^{x_n} \leq t_n}\right].
\end{aligned}$$

It follows from the compatibility condition (2.14) and Lemma 2.3.1 that, $\mathbb{1}_{\tau_\partial^{x_n} > t_n}\left|f(X_{t_n}^{x_n}) - g(x)\right| \underset{n\to\infty}{\longrightarrow} 0$ almost surely. Therefore, using the dominated convergence theorem, the first term in the right-hand side of the inequality above converges to 0. Furthermore, on the event $\{\tau_\partial^{x_n} \leq t_n\}$, it follows by Lemma 2.3.1 that

$$\begin{aligned}
\left|X_{\tau_\partial^{x_n}}^{x_n} - x\right| &\leq \left|X_{\tau_\partial^{x_n}}^{x_n} - X_{\tau_\partial^{x_n}}^x\right| + \left|X_{\tau_\partial^{x_n}}^x - x\right| \\
&\leq \underbrace{|x_n - x|\mathrm{e}^{C_{\mathrm{Lip}} t_n}}_{\underset{n\to\infty}{\longrightarrow} 0} + \underbrace{\left|X_{\tau_\partial^{x_n}}^x - x\right|}_{\underset{n\to\infty}{\longrightarrow} 0 \text{ a.s.}},
\end{aligned}$$

since $\tau_\partial^{x_n} \leq t_n \underset{n\to\infty}{\longrightarrow} 0$. As a result, $\mathbb{E}\left[\left|g(X_{\tau_\partial^{x_n}}^{x_n}) - g(x)\right|\mathbb{1}_{\tau_\partial^{x_n} \leq t_n}\right] \underset{n\to\infty}{\longrightarrow} 0$ since $g \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$. Hence $u(t_n, x_n) \underset{n\longrightarrow\infty}{\longrightarrow} g(x)$. This concludes the proof of Assertion (ii) in Theorem 2.2.10. □

2.3.3 Interior regularity: proof of Assertion (iii) in Theorem 2.2.10

The link between functions of the form of u defined by (2.13) and parabolic problems of the form (2.15) is standard for uniformly elliptic operators in bounded domains with compatible initial and boundary conditions, see for instance [32, Chapter 6]. In order to extend this link to the degenerate operator $\mathscr{L}$, we proceed by approximating (2.15) by the uniformly elliptic problem

$$\partial_t u_\epsilon = \mathscr{L} u_\epsilon + \epsilon \Delta_q u_\epsilon. \tag{2.34}$$

Let $\epsilon > 0$ and $(\widetilde{B}_t)_{t\geq 0}$ be a $d-$dimensional Brownian motion independent of $(B_t)_{t\geq 0}$. Under Assumption (F2), for all $x \in D$ we denote by $(X_t^{x,\epsilon} = (q_t^{x,\epsilon}, p_t^{x,\epsilon}))_{t\geq 0}$ the strong solution of

$$\begin{cases} \mathrm{d}q_t^{x,\epsilon} = p_t^{x,\epsilon}\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}\widetilde{B}_t, \\ \mathrm{d}p_t^{x,\epsilon} = F(q_t^{x,\epsilon})\mathrm{d}t - \gamma p_t^{x,\epsilon}\mathrm{d}t + \sigma \mathrm{d}B_t, \\ (q_0^{x,\epsilon}, p_0^{x,\epsilon}) = x. \end{cases} \tag{2.35}$$

Let $\tau_\partial^{x,\epsilon} = \inf\{t > 0 : X_t^{x,\epsilon} \notin D\}$ be the first exit time from D of the process $(X_t^{x,\epsilon})_{t\geq 0}$.

We first assume that the functions f and g satisfy the compatibility condition (2.14), define the function $h \in \mathscr{C}^b(\overline{D})$ by

$$h(x) = \mathbb{1}_{x\in D\cup\Gamma^-} f(x) + \mathbb{1}_{\Gamma^+\cup\Gamma^0} g(x), \tag{2.36}$$

and state the following two lemmata.

Lemma 2.3.5 (Perturbed problem)**.** *Under Assumptions (O1) and (F2), let $\epsilon > 0$ and let $f \in \mathscr{C}^b(D\cup \Gamma^-)$, $g \in \mathscr{C}^b(\Gamma^+\cup\Gamma^0)$ satisfy (2.14). Let $h \in \mathscr{C}^b(\overline{D})$ be defined by (2.36). The function u_ϵ on $\mathbb{R}_+^* \times D$ defined by*

$$u_\epsilon : (t, x) \mapsto \mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x,\epsilon} > t} h_{|D}(X_t^{x,\epsilon}) + \mathbb{1}_{\tau_\partial^{x,\epsilon} \leq t} h_{|\partial D}\left(X^{x,\epsilon}_{\tau_\partial^{x,\epsilon}}\right)\right]. \tag{2.37}$$

satisfies (2.34) in the sense of distributions on $\mathbb{R}_+^* \times D$.

Lemma 2.3.6 (Convergence)**.** *Under the assumptions of Lemma 2.3.5, for all $t > 0$ and $x \in D$,*

$$u_\epsilon(t, x) \underset{\epsilon\to 0}{\longrightarrow} u(t, x).$$

Before proving Lemmata 2.3.5 and 2.3.6, let us conclude the proof of Assertion (iii) in Theorem 2.2.10 using these results. Under the assumption that f and g satisfy the compatibility condition (2.14), it is immediate, using the result of Lemma 2.3.6, to obtain that u solves (2.15) in the sense of distributions, by passing to the limit $\epsilon \to 0$ in the weak formulation of the partial differential equation and using the fact that $\|u_\epsilon\|_{L^\infty(\overline{D})} \leq \|h\|_{L^\infty(\overline{D})}$.

If f and g do not satisfy the compatibility condition (2.14), one can use the following approximation argument to conclude. First, we note that since g is continuous on the closed set $\Gamma^+ \cup \Gamma^0$, there exists a function $\widetilde{g} \in \mathscr{C}^b(\overline{D})$ which coincides with g on $\Gamma^+ \cup \Gamma^0$ by Tietze-Urysohn's extension theorem [27, Theorem 4.5.1]. For any $k \geq 1$ and $x \in D \cup \Gamma^-$, let us now set

$$\widetilde{f}_k(x) = (1 - \psi_k(x))f(x) + \psi_k(x)\widetilde{g}(x),$$

where $\psi_k : \overline{D} \to [0, 1]$ is a continuous function such that

$$\psi_k(x) = \begin{cases} 1 & \text{if } x \in \Gamma^+ \cup \Gamma^0, \\ 0 & \text{if } \mathrm{d}(x, \Gamma^+ \cup \Gamma^0) \geq 1/k. \end{cases}$$

Then $\widetilde{f}_k$ and g satisfy the compatibility condition (2.14), so that the argument above shows that the function $\widetilde{u}_k$ defined by

$$\widetilde{u}_k(t, x) := \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t} \widetilde{f}_k(X_t^x) + \mathbb{1}_{\tau_\partial^x \leq t} g(X^x_{\tau_\partial^x})\right]$$

solves (2.15) in the distributional sense. On the other hand, $\widetilde{f}_k(x)$ converges to $f(x)$ for all $x \in D \cup \Gamma^-$ when $k \to +\infty$, which by the dominated convergence theorem implies that $\widetilde{u}_k(t,x)$ converges to $u(t,x)$ and therefore shows that u is a distributional solution to (2.15), also in the case when f and g do not satisfy the compatibility condition (2.14).

It finally follows from the hypoellipticity of the operator $\partial_t - \mathscr{L}$ that u is actually in $\mathscr{C}^\infty(\mathbb{R}_+^* \times D)$, which completes the proof of Assertion (iii) in Theorem 2.2.10.

Let us now conclude this section by proving the two Lemmata 2.3.5 and 2.3.6.

Proof of Lemma 2.3.5. The result is standard for bounded domains, but D is not bounded. We thus use an approximation argument. Let $(\widetilde{V}_k)_{k\geq 1}$ be a sequence of $\mathscr{C}^2$ bounded open subsets of D such that:

(i) for all $k \geq 1$, $\widetilde{V}_k \subset D \cap \{(q,p) \in \mathbb{R}^{2d} : |p| \leq k\}$,

(ii) for all $k \geq 1$, $\widetilde{V}_k \subset \widetilde{V}_{k+1}$,

(iii) $\bigcup_{k\geq 1} \widetilde{V}_k = D$.

For $\epsilon > 0$, let $\tau^{x,\epsilon}_{\widetilde{V}_k^c}$ be the following stopping time :

$$\tau^{x,\epsilon}_{\widetilde{V}_k^c} = \inf\{t > 0 : X_t^{x,\epsilon} \notin \widetilde{V}_k\}.$$

Let $T > 0$. Consider the following Initial-Boundary Value Problem,

$$\begin{cases} \partial_t v_{k,\epsilon}(t,x) = \mathscr{L} v_{k,\epsilon}(t,x) + \epsilon \Delta_q v_{k,\epsilon}(t,x), & t \in (0,T], \quad x \in \widetilde{V}_k, \\ v_{k,\epsilon}(0,x) = h_{|\widetilde{V}_k}(x), & x \in \widetilde{V}_k, \\ v_{k,\epsilon}(t,x) = h_{|\partial\widetilde{V}_k}(x), & t \in (0,T], \quad x \in \partial\widetilde{V}_k. \end{cases} \tag{2.38}$$

By [32, Chapter 6, Theorem 5.2] there exists a unique classical solution $v_{k,\epsilon}$ in $\mathscr{C}^2((0,T] \times \widetilde{V}_k) \cap \mathscr{C}^b([0,T] \times \overline{\widetilde{V}_k})$ of (2.38). Furthermore, the solution writes as follows: for all $t > 0$ and $x \in D$

$$v_{k,\epsilon}(t,x) = \mathbb{E}\left[\mathbb{1}_{\tau^{x,\epsilon}_{\widetilde{V}_k^c} > t} h_{|\widetilde{V}_k}(X_t^{x,\epsilon}) + \mathbb{1}_{\tau^{x,\epsilon}_{\widetilde{V}_k^c} \leq t} h_{|\partial\widetilde{V}_k}\left(X^{x,\epsilon}_{\tau^{x,\epsilon}_{\widetilde{V}_k^c}}\right)\right].$$

Moreover when k goes to infinity one has (following the proof of Assertion (iv) in Theorem 2.2.10, see Section 2.3.1):

$$v_{k,\epsilon}(t,x) \underset{k\longrightarrow\infty}{\longrightarrow} u_\epsilon(t,x). \tag{2.39}$$

Therefore, since $v_{k,\epsilon}$ is a classical solution of (2.38) it is also a solution in the sense of distributions of $\partial_t v_{k,\epsilon} = \mathscr{L} v_{k,\epsilon} + \epsilon\Delta_q v_{k,\epsilon}$ on $(0,T) \times \widetilde{V}_k$. But then, since T is arbitrary, u_ϵ is also a solution in the sense of distributions of $\partial_t u_\epsilon = \mathscr{L} u_\epsilon$ on $\mathbb{R}_+^* \times D$. Indeed, for $\Phi \in \mathscr{C}_c^\infty(\mathbb{R}_+^* \times D)$, there exists $k_0 > 0$ and $T_0 > 0$ such that $\mathrm{supp}(\Phi) \subset (0,T_0] \times \widetilde{V}_{k_0}$. As a result, for all $k > k_0$ and $T > T_0$,

$$\iint_{\mathbb{R}_+^* \times D} v_{k,\epsilon}(t,x)\left(\partial_t \Phi(t,x) + \mathscr{L}^*\Phi(t,x) + \epsilon\Delta_q\Phi(t,x)\right) \mathrm{d}t\mathrm{d}x = 0.$$

The proof is then easily completed, using (2.39) and the dominated convergence theorem. □

Proof of Lemma 2.3.6. An application of Gronwall's Lemma, as in the proof of Lemma 2.3.1, shows that, almost surely,

$$\sup_{s\in[0,t]} |X_s^{x,\epsilon} - X_s^x| \leq \sqrt{2\epsilon} \sup_{s\in[0,t]} |\widetilde{B}_s| \mathrm{e}^{C_{\mathrm{Lip}} t} \tag{2.40}$$

where C_{Lip} is the Lipschitz constant of the drift of (2.10). In particular, for all $t \geq 0$, $X_t^{x,\epsilon} \underset{\epsilon\longrightarrow 0}{\longrightarrow} X_t^x$ almost surely.

Let us now consider the difference between $u_\epsilon(t,x)$ and $u(t,x)$ for $t>0$, $x\in D$. Using the same triangle inequality as in the proof of Assertion (ii) of Theorem 2.2.10 (see Section 2.3.2), one has

$$\begin{aligned}|u_\epsilon(t,x)-u(t,x)| \leq \mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x,\epsilon}>t,\tau_\partial^x>t}\left|h_{|D}(X_t^{x,\epsilon})-h_{|D}(X_t^x)\right|\right]+2\|h\|_\infty\mathbb{E}\left[\left|\mathbb{1}_{\tau_\partial^{x,\epsilon}>t}-\mathbb{1}_{\tau_\partial^x>t}\right|\right]\\ +\mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x,\epsilon}\leq t,\tau_\partial^x\leq t}\left|h_{|\partial D}(X^{x,\epsilon}_{\tau_\partial^{x,\epsilon}})-h_{|\partial D}(X^x_{\tau_\partial^x})\right|\right].\end{aligned}$$

Using (2.40) and the fact that $h_{|D}\in\mathscr{C}^b(D)$, it follows from the dominated convergence theorem that the first term in the right-hand side of the inequality converges to 0 as ϵ goes to 0. Besides, remember that $\mathbb{P}(\tau_\partial^x=t)=0$ for $x\in D$ and $t>0$ by Corollary 2.2.18. As a result if one can prove that for all $x\in D$, $t>0$,

$$\mathbb{1}_{\tau_\partial^{x,\epsilon}>t}\underset{\epsilon\to0}{\longrightarrow}\mathbb{1}_{\tau_\partial^x>t}\quad\text{almost surely on the events }\{\tau_\partial^x<t\}\text{ and }\{\tau_\partial^x>t\},\tag{2.41}$$

and

$$\tau_\partial^{x,\epsilon}\underset{\epsilon\longrightarrow0}{\longrightarrow}\tau_\partial^x\quad\text{almost surely on the event }\{\tau_\partial^x<t\},\tag{2.42}$$

then using (2.40), the fact that $h_{|\partial D}\in\mathscr{C}^b(\Gamma^+\cup\Gamma^0)$ and the continuity of the trajectories of $(X_t^x)_{t\geq0}$, the convergence of $u_\epsilon(t,x)$ towards $u(t,x)$ follows from the dominated convergence theorem, and the proof is complete.

Let us now prove the two convergences (2.41) and (2.42).

Step 1. Consider first the convergence (2.41) on the event $\{\tau_\partial^x>t\}$. By the continuity of the trajectories of $(q_s^x)_{s\geq0}$,

$$\epsilon_0:=\inf_{0\leq s\leq t}\mathrm{d}_\partial(q_s^x)>0.$$

Let $S_t:=\sup_{0\leq s\leq t}|\widetilde{B}_s|$. For $\epsilon\leq\frac{\epsilon_0^2}{8S_t^2}\mathrm{e}^{-2C_{\mathrm{Lip}}t}$ (which is positive since $S_t<\infty$ almost surely), one has by (2.40):

$$\sup_{0\leq s\leq t}|q_s^{x,\epsilon}-q_s^x|\leq\sup_{0\leq s\leq t}|X_s^{x,\epsilon}-X_s^x|\leq\frac{\epsilon_0}{2}.$$

Hence, since d_∂ is 1-Lipschitz continuous, for $\epsilon\leq\frac{\epsilon_0^2}{8S_t^2}\mathrm{e}^{-2C_{\mathrm{Lip}}t}$

$$\inf_{0\leq s\leq t}\mathrm{d}_\partial(q_s^{x,\epsilon})\geq\frac{\epsilon_0}{2}>0,$$

which implies $\mathbb{1}_{\tau_\partial^{x,\epsilon}>t}=1$ and (2.41) thus holds on the event $\{\tau_\partial^x>t\}$.

Step 2. Let us now prove the convergences (2.41) and (2.42) on the event $\{\tau_\partial^x<t\}$. Since $x\in D$, by Proposition 2.2.8 one has $(q^x_{\tau_\partial^x},p^x_{\tau_\partial^x})\in\Gamma^+$ almost surely. Let $0<\eta<(t-\tau_\partial^x)\wedge\tau_\partial^x$. The strong Markov property along with Proposition 2.2.8 ensure that there exists almost surely $t_0\in(\tau_\partial^x,\tau_\partial^x+\eta)$ such that

$$\epsilon_1:=\mathrm{d}_{\overline{\mathcal{O}}}(q_{t_0}^x)>0.$$

Besides, the continuity of the trajectories of $(q_s^x)_{s\geq0}$ ensures that

$$\epsilon_2:=\inf_{0\leq s\leq\tau_\partial^x-\eta}\mathrm{d}_\partial(q_s^x)>0.$$

As a result, for $\epsilon\leq\frac{\epsilon_1^2\wedge\epsilon_2^2}{8S_t^2}\mathrm{e}^{-2C_{\mathrm{Lip}}t}$,

$$\sup_{0\leq s\leq t}|q_s^{x,\epsilon}-q_s^x|\leq\sup_{0\leq s\leq t}|X_s^{x,\epsilon}-X_s^x|\leq\frac{\epsilon_1\wedge\epsilon_2}{2}.$$

Hence, since $\mathrm{d}_{\overline{\mathscr{O}}}$ is 1-Lipschitz continuous,

$$\mathrm{d}_{\overline{\mathscr{O}}}(q_{t_0}^{x,\epsilon}) \geq \frac{\epsilon_1}{2} > 0,$$

and since d_∂ is 1-Lipschitz continuous as well, one has

$$\inf_{0 \leq s \leq \tau_\partial^x - \eta} \mathrm{d}_\partial(q_s^{x,\epsilon}) \geq \frac{\epsilon_2}{2} > 0.$$

Therefore, for ϵ small enough,

$$|\tau_\partial^{x,\epsilon} - \tau_\partial^x| \leq \eta \quad \text{and in particular} \quad \tau_\partial^{x,\epsilon} \leq \tau_\partial^x + \eta < t.$$

Consequently, the convergences (2.41) and (2.42) hold on the event $\{\tau_\partial^x < t\}$. □

2.3.4 Proof of Propositions 2.2.7 and 2.2.8

We conclude Section 2.3 with the proof of Propositions 2.2.7 and 2.2.8, which are the cornerstones of all the previous results. It is shown here that Assertion (ii) in Proposition 2.2.8 actually follows immediately from Proposition 2.2.7, it remains then to prove Assertion (i) in Proposition 2.2.8 along with Proposition 2.2.7.

2.3.4.1 Preliminary results

2.3.4.1.1 Interior and exterior sphere conditions. It is easy to check that under Assumption (O1), the set $\mathscr{O}$ satisfies the so-called *uniform interior and exterior sphere conditions*, which means that there exists $\rho > 0$ such that for any $q \in \partial\mathscr{O}$, there exist two points $q_{\mathrm{int}} \in \mathscr{O}$ and $q_{\mathrm{ext}} \in \overline{\mathscr{O}}^c$ such that the open Euclidean balls $\mathrm{B}(q_{\mathrm{int}}, \rho)$ and $\mathrm{B}(q_{\mathrm{ext}}, \rho)$ satisfy

$$\mathrm{B}(q_{\mathrm{int}}, \rho) \subset \mathscr{O}, \qquad \mathrm{B}(q_{\mathrm{ext}}, \rho) \subset \overline{\mathscr{O}}^c, \qquad \overline{\mathrm{B}(q_{\mathrm{int}}, \rho)} \cap \mathscr{O}^c = \overline{\mathrm{B}(q_{\mathrm{ext}}, \rho)} \cap \overline{\mathscr{O}} = \{q\}.$$

This property combined with the differentiability of the trajectory of the process $(q_t^x)_{t \geq 0}$, already allow us to prove some parts of Proposition 2.2.8. Indeed, let us check (2.11) for $x = (q,p) \in \Gamma^+$. Let $q_{\mathrm{ext}} \in \overline{\mathscr{O}}^c$ be given by the exterior sphere condition. Notice that necessarily, the vectors $q_{\mathrm{ext}} - q$ and $n(q)$ are colinear. On the other hand, for $t \to 0$, $(q_t^x - q) \cdot n(q) \sim tp \cdot n(q) > 0$, which then implies that $|q_t^x - q_{\mathrm{ext}}|^2 = \rho^2 - 2\rho tp \cdot n(q) + o(t)$ so that $q_t^x \in \mathrm{B}(q_{\mathrm{ext}}, \rho) \subset \overline{\mathscr{O}}^c$ for t small enough.

With similar arguments, the interior sphere condition shows that if $x \in \Gamma^-$, then $\tau_\partial^x > 0$ almost surely. Moreover, it is obvious that if $x \in D$, then $\tau_\partial^x > 0$ almost surely. Finally, if $x \in D \cup \Gamma^-$, then on the event $\tau_\partial^x \leq T$ one necessarily has $X_{\tau_\partial^x}^x \in \Gamma^+ \cup \Gamma^0$ almost surely, which rewrites:

$$\forall T > 0, \quad \forall x \in D \cup \Gamma^-, \qquad \mathbb{P}\left(p_{\tau_\partial^x}^x \cdot n(q_{\tau_\partial^x}^x) < 0, \tau_\partial^x \leq T\right) = 0. \tag{2.43}$$

Therefore, taking Proposition 2.2.7 for granted, we obtain Assertion (ii) in Proposition 2.2.8.

In the sequel of this section, we prove the remaining part of Proposition 2.2.8, namely that (2.11) holds for $x \in \Gamma^0$, and Proposition 2.2.7. Both proofs use the reduction to a Gaussian process, thanks to the Girsanov theorem, which we first detail.

2.3.4.1.2 Reduction to a Gaussian process. Proposition 2.2.7 and Assertion (i) in Proposition 2.2.8 rely on the following preliminary result.

Lemma 2.3.7 (Girsanov Theorem)**.** *Let Assumption (F2) hold. Let $x \in \mathbb{R}^{2d}$ and let $(\breve{q}_t^x, \breve{p}_t^x)_{t \geq 0}$ be the strong solution on $\mathbb{R}^{2d}$ of*

$$\begin{cases} \mathrm{d}\breve{q}_t^x = \breve{p}_t^x \mathrm{d}t, \\ \mathrm{d}\breve{p}_t^x = \sigma \mathrm{d}B_t, \\ (\breve{q}_0^x, \breve{p}_0^x) = x. \end{cases} \tag{2.44}$$

For $T \geq 0$, the laws of $(\check{q}_t^x, \check{p}_t^x)_{t\in[0,T]}$ and $(q_t^x, p_t^x)_{t\in[0,T]}$ are equivalent in the space of sample paths $\mathscr{C}([0,T], \mathbb{R}^{2d})$, i.e. for all Borel sets A of $\mathscr{C}([0,T], \mathbb{R}^{2d})$,

$$\mathbb{P}((\check{q}_t^x, \check{p}_t^x)_{t\in[0,T]} \in A) = 0 \quad \text{if and only if} \quad \mathbb{P}((q_t^x, p_t^x)_{t\in[0,T]} \in A) = 0.$$

Proof. Let $x = (q,p) \in \mathbb{R}^{2d}$. The equation (2.44) admits a unique global strong solution $(\check{q}_t^x, \check{p}_t^x)_{t\geq 0}$ on $\mathbb{R}^{2d}$ since its coefficients are globally Lipschitz continuous. For $T \geq 0$, let us define,

$$\mathscr{Z}_T^x = F(\check{q}_T^x) - \gamma \check{p}_T^x,$$

and

$$\mathscr{E}_T^x = \exp\left(\int_0^T \mathscr{Z}_s^x \cdot \mathrm{d}B_s - \frac{1}{2}\int_0^T |\mathscr{Z}_s^x|^2 \mathrm{d}s\right).$$

It is clear that $\mathscr{E}_T^x$ is $\mathscr{F}_T$-measurable. Let us show that for all $T \geq 0$, $\mathbb{E}[\mathscr{E}_T^x] = 1$. According to [32, Theorem 1.1 p. 152], this equality is satisfied if there exists $\mu > 0$ such that

$$\sup_{s\in[0,T]} \mathbb{E}[\exp(\mu|\mathscr{Z}_s^x|^2)] < \infty,$$

which we now prove. Since F satisfies Assumption (F2), it follows that for $s \in [0,T]$,

$$|\mathscr{Z}_s^x|^2 = |F(\check{q}_s^x) - \gamma \check{p}_s^x|^2 \leq 2\|F\|_\infty^2 + 2\gamma^2 |\check{p}_s^x|^2.$$

In addition, $\check{p}_s^x \sim \mathscr{N}_d(p, \sigma^2 s I_d)$. Let $G \sim \mathscr{N}_d(0, I_d)$, we get for $s \in [0,T]$,

$$\begin{aligned}\mathbb{E}[\exp(\mu|\mathscr{Z}_s^x|^2)] &\leq \exp(2\mu\|F\|_\infty^2)\mathbb{E}(\exp(2\mu\gamma^2|\check{p}_s^x|^2))\\ &= \exp(2\mu\|F\|_\infty^2)\mathbb{E}(\exp(2\mu\gamma^2|p + \sigma\sqrt{s}G|^2))\\ &\leq \exp(2\mu\|F\|_\infty^2 + 4\mu\gamma^2|p|^2)\mathbb{E}(\exp(4\mu\gamma^2\sigma^2 T|G|^2)).\end{aligned}$$

Moreover, $\mathbb{E}(\exp(4\mu\gamma^2\sigma^2 T|G|^2) < \infty$ for sufficiently small μ.

This result allows us to define the probability measure $\mathbb{Q}_T$ on $\mathscr{F}_T$ by $\mathrm{d}\mathbb{Q}_T = \mathscr{E}_T^x \mathrm{d}\mathbb{P}|_{\mathscr{F}_T}$. Since $\mathscr{E}_T^x > 0$, $\mathbb{P}|_{\mathscr{F}_T}$-a.s., the measures $\mathbb{P}|_{\mathscr{F}_T}$ and $\mathbb{Q}_T$ are equivalent. Besides, by the Girsanov Theorem [32, Theorem 1.1 p. 152] the process

$$\left(\check{B}_s := B_s - \int_0^s \mathscr{Z}_r^x \mathrm{d}r\right)_{0\leq s\leq T}$$

is a $(\mathscr{F}_s)_{s\in[0,T]}$-Brownian motion under the probability $\mathbb{Q}_T$. As a result, the process $(\check{X}_s^x, \check{B}_s)_{s\in[0,T]}$ satisfies (2.10) on the probability space $(\Omega, \mathscr{F}, (\mathscr{F}_s)_{s\in[0,T]}, \mathbb{Q}_T)$. On the other hand, the pathwise uniqueness for (2.10) implies the uniqueness in distribution by Yamada Watanabe's theorem, so that the law of $(\check{q}_s^x, \check{p}_s^x)_{s\in[0,T]}$ under $\mathbb{Q}_T$ is the law of $(q_s^x, p_s^x)_{s\in[0,T]}$ under $\mathbb{P}$, whence the final result. □

We are now in position to complete the proof of Proposition 2.2.8 and to detail the proof of Proposition 2.2.7. By Lemma 2.3.7 it is sufficient to prove both statements for the process $(\check{X}_t^x)_{t\geq 0}$ defined in (2.44), and for which we introduce the notation $\check{\tau}_\partial^x := \inf\{t > 0 : \check{X}_t^x \notin D\}$.

2.3.4.2 Proof of Assertion (i) of Proposition 2.2.8

Proof of Assertion (i) in Proposition 2.2.8. If $x \in \Gamma^+$, then (2.11) follows from the exterior sphere condition, see Section 2.3.4.1. It remains now to prove (2.11) for $x = (q,p) \in \Gamma^0$. One has from (2.44) that for all $t \geq 0$,

$$\check{p}_t^x = p + \sigma B_t \text{ and thus } \check{q}_t^x = q + pt + \sigma \int_0^t B_s \, \mathrm{d}s.$$

The idea of the proof it to go back to the case of a flat boundary by a change of variable, and then to use known results for 1-d integrated Brownian motion, see [53].

Let $(e_1, \dots, e_d)$ be the canonical basis of $\mathbb{R}^d$. Since $\mathscr{O}$ is a bounded $\mathscr{C}^2$ set of $\mathbb{R}^d$, by [10, Thm 2.1.2.] there exists an open neighborhood U of q and a $\mathscr{C}^2$-diffeomorphism $\phi : (-1,1)^d \to U$ satisfying $\phi(0) = q$ and

$$\mathscr{O} \cap U = \phi(\{y \in (-1,1)^d : y \cdot e_d < 0\}) \quad \text{and} \quad \partial\mathscr{O} \cap U = \phi(\{y \in (-1,1)^d : y \cdot e_d = 0\}).$$

Moreover, $n(q) \in \mathbb{R}^d$ is the unique vector such that

$$n(q) \in \operatorname{Span}(d_0\phi(e_1), \dots, d_0\phi(e_{d-1}))^{\perp}, |n(q)| = 1, \text{ and } d_0\phi(e_d) \cdot n(q) > 0, \tag{2.45}$$

where $d_0\phi$ is the differential at $0 \in \mathbb{R}^d$ of ϕ.

Now let K be a compact set included in U such that $q \in \mathring{K}$. Let $\breve{\tau}^x_{K^c} := \inf\{t > 0 : \breve{q}^x_t \notin K\}$ be the first exit time of K for $(\breve{q}^x_t)_{t\geq 0}$, then $\breve{\tau}^x_{K^c} > 0$ almost surely by continuity of the trajectories of $(\breve{q}^x_t)_{t\geq 0}$.

For $t \leq \breve{\tau}^x_{K^c}$ we have

$$\phi^{-1}(\breve{q}^x_t) = \underbrace{\phi^{-1}(q)}_{=0} + \int_0^t d_{\breve{q}^x_s}(\phi^{-1})\,(p + \sigma B_s)\,\mathrm{d}s. \tag{2.46}$$

Since ϕ^{-1} is a $\mathscr{C}^2$-diffeomorphism from U to $(-1,1)^d$, then $y \in K \subset U \mapsto d_y(\phi^{-1})$ is $\mathscr{C}^1$ on the compact set K. In particular it is Lipschitz continuous with some Lipschitz constant k. As a result, since for $t \geq 0$, $\breve{q}^x_t = q + \int_0^t \breve{p}^x_s \mathrm{d}s$, then for all $t \in [0, \breve{\tau}^x_{K^c}]$ and $z \in \mathbb{R}^d$,

$$\begin{aligned}\left|d_{\breve{q}^x_t}(\phi^{-1})(z) - d_q(\phi^{-1})(z)\right| &\leq k|\breve{q}^x_t - q||z| = k\left|tp + \sigma \int_0^t B_s \mathrm{d}s\right| |z| \\ &\leq kt\left(|p| + \sigma \sup_{s\in[0,t]} |B_s|\right)|z|.\end{aligned} \tag{2.47}$$

Hence we have from (2.46) and (2.47)

$$\left|\phi^{-1}(\breve{q}^x_t) - \int_0^t d_q(\phi^{-1})(p + \sigma B_s)\mathrm{d}s\right| \leq kt^2\left(|p| + \sigma \sup_{s\in[0,t]}|B_s|\right)^2.$$

Therefore

$$\left|\phi^{-1}(\breve{q}^x_t)\cdot e_d - td_q(\phi^{-1})(p)\cdot e_d - \sigma d_q(\phi^{-1})\left(\int_0^t B_s\mathrm{d}s\right)\cdot e_d\right| \leq kt^2\left(|p| + \sigma \sup_{s\in[0,t]}|B_s|\right)^2. \tag{2.48}$$

Let us now prove that, since $x \in \Gamma^0$,

$$d_q(\phi^{-1})(p) \cdot e_d = 0. \tag{2.49}$$

Since ϕ is a $\mathscr{C}^1$-diffeomorphism from $(-1,1)^d$ to U with U a neighborhood of q and $\phi(0) = q$, then $d_0(\phi)$ is invertible with inverse satisfying

$$(d_0(\phi))^{-1} = d_q(\phi^{-1})$$

In particular, the family $(d_0(\phi)(e_1), \dots, d_0(\phi)(e_d))$ is a basis of $\mathbb{R}^d$. Let us now decompose the vector p in this basis :

$$p = \sum_{j=1}^d p_j d_0(\phi)(e_j).$$

Using (2.45) and the fact that $p \cdot n(q) = 0$ since $x \in \Gamma^0$, we get $p_d = 0$. As a result,

$$d_q(\phi^{-1})(p) \cdot e_d = d_q(\phi^{-1}) \left(\sum_{j=1}^{d} p_j d_0(\phi)(e_j) \right) \cdot e_d$$
$$= \sum_{j=1}^{d} p_j (d_0(\phi))^{-1} d_0(\phi)(e_j) \cdot e_d = p_d = 0.$$

This concludes the proof of (2.49).

Now notice that

$$d_q(\phi^{-1}) \left(\int_0^t B_s \mathrm{d}s \right) \cdot e_d = \int_0^t B_s \cdot d_0(\phi)^{-T}(e_d) \mathrm{d}s, \tag{2.50}$$

where $d_0(\phi)^{-T}$ is the transpose matrix of $d_0(\phi)^{-1}$. Moreover, $|d_0(\phi)^{-T}(e_d)| > 0$, since $d_0(\phi)^{-T}$ is also invertible. Using (2.49) and (2.50) in (2.48), one gets

$$\left| \phi^{-1}(\check{q}_t^x) \cdot e_d - \sigma \int_0^t B_s \cdot d_0(\phi)^{-T}(e_d) \mathrm{d}s \right| \leq kt^2 \left(|p| + \sigma \sup_{s \in [0,t]} |B_s| \right)^2. \tag{2.51}$$

Let us define the process $(\widehat{B}_s)_{s \in [0,t]}$ by

$$\forall s \in [0,t], \qquad \widehat{B}_s := B_s \cdot \frac{d_0(\phi)^{-T}(e_d)}{|d_0(\phi)^{-T}(e_d)|}.$$

It is clearly a one-dimensional Brownian motion on $[0, t]$. Then (2.51) rewrites

$$\left| \phi^{-1}(\check{q}_t^x) \cdot e_d - \sigma |d_0(\phi)^{-T}(e_d)| \int_0^t \widehat{B}_s \mathrm{d}s \right| \leq kt^2 \left(|p| + \sigma \sup_{s \in [0,t]} |B_s| \right)^2.$$

The law of the iterated logarithm for the integrated Brownian motion (see [53, Theorem 1]) provides us with the following asymptotic:

$$\limsup_{t \to 0} \frac{\int_0^t \widehat{B}_s \mathrm{d}s}{\sqrt{\frac{2}{3}} t^{\frac{3}{2}} \sqrt{\log \log(1/t)}} = 1 \quad \text{almost surely.}$$

For $t > 0$, let $\Psi(t) = \sqrt{\frac{2}{3}} t^{\frac{3}{2}} \sqrt{\log \log(1/t)}$, then

$$\left| \frac{\phi^{-1}(\check{q}_t^x) \cdot e_d}{\Psi(t)} - \sigma |d_0(\phi)^{-T}(e_d)| \frac{\int_0^t \widehat{B}_s \mathrm{d}s}{\Psi(t)} \right| \leq \underbrace{\frac{kt^2}{\Psi(t)}}_{\underset{t \to 0}{\longrightarrow} 0} \left(|p| + \sigma \sup_{s \in [0,t]} |B_s| \right)^2.$$

Therefore, almost surely,

$$\limsup_{t \to 0} \frac{\phi^{-1}(\check{q}_t^x) \cdot e_d}{\Psi(t)} = \sigma |d_0(\phi)^{-T}(e_d)| > 0.$$

As a result, the process $(\check{q}_t^x)_{t \geq 0}$ visits $U \cap \overline{\mathscr{O}}^c$ infinitely often for times close to 0. This implies in particular that $\check{\tau}_\partial^x = 0$ almost surely. $\square$

2.3.4.3 Proof of Proposition 2.2.7

We now address the proof of Proposition 2.2.7. For $x \in \mathbb{R}^{2d}$, let $\check{\tau}_0^x := \inf\{t > 0 : (\check{q}_t^x, \check{p}_t^x) \in \Gamma^0\}$ and let us show here that for all $x \in \mathbb{R}^{2d} \setminus \Gamma^0$,

$$\mathbb{P}(\check{\tau}_0^x < \infty) = 0,$$

which is equivalent to

$$\forall T > 0, \qquad \mathbb{P}(\check{\tau}_0^x \leq T) = 0. \tag{2.52}$$

The idea of the proof is the following. If one replaces the random time $\check{\tau}_0^x$ by a deterministic time $t \leq T$, and denote by $\check{n}$ some continuous extension of the normal vector n in a neighborhood of $\partial\mathscr{O}$, then using the fact that $\check{p}_t^x$ has a nondegenerate Gaussian conditional distribution given $\check{q}_t^x$ allows us to write

$$\mathbb{P}\left(\check{p}_t^x \cdot \check{n}(\check{q}_t^x) = 0\right) = \mathbb{E}\left[\mathbb{P}\left(\check{p}_t^x \cdot \check{n}(\check{q}_t^x) = 0 | \check{q}_t^x\right)\right] = 0.$$

Our proof therefore relies on the approximation of $\check{\tau}_0^x$ by a grid of deterministic times and exploits the fact that while assuming that such a time t is close to $\check{\tau}_0^x$ makes the distribution of $\check{q}_t^x$ quite singular, it leaves 'enough randomness' in the distribution of $\check{p}_t^x$ for quantities of the form $\mathbb{P}(\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \simeq t)$ to be sufficiently small.

Proof of Proposition 2.2.7. Let $x = (q,p) \in \mathbb{R}^{2d} \setminus \Gamma^0$. As explained above, the objective is to prove (2.52).

Let $\alpha \in (0, 1/2)$. Since $(\check{p}_t^x)_{0 \leq t \leq T}$ is a Brownian motion, one has that

$$\sup_{0 \leq t \leq T} |\check{p}_t^x| < \infty, \qquad \sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} < \infty \quad \text{almost surely.}$$

Let $\epsilon > 0$ and let us choose M large enough so that

$$\mathbb{P}\left(\sup_{0 \leq t \leq T} |\check{p}_t^x| > M\right) \leq \epsilon, \quad \mathbb{P}\left(\sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} > M\right) \leq \epsilon. \tag{2.53}$$

Therefore,

$$\begin{aligned}
&\mathbb{P}\left(\check{\tau}_0^x \leq T\right) \\
&= \mathbb{P}\left(\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \leq T\right) \\
&\leq \mathbb{P}\left(\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \leq T, \sup_{0 \leq t \leq T} |\check{p}_t^x| \leq M, \sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} \leq M\right) + 2\epsilon.
\end{aligned}$$

Let us now consider the first term in the right-hand side of the inequality above .

Step 1. Let $N \in \mathbb{N}^*$. We divide the interval $(0, T]$ into N intervals $(t_k, t_{k+1}]$ with $t_k := k\eta_N$ and $\eta_N := \frac{T}{N}$. As a result, since $\check{\tau}_0^x > 0$ almost surely, because x belongs to the open set $\mathbb{R}^{2d} \setminus \Gamma^0$,

$$\begin{aligned}
&\mathbb{P}\left(\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \leq T, \sup_{0 \leq t \leq T} |\check{p}_t^x| \leq M, \sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} \leq M\right) \\
&= \sum_{k=0}^{N-1} \mathbb{P}\left(\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \in (t_k, t_{k+1}], \sup_{0 \leq t \leq T} |\check{p}_t^x| \leq M, \sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} \leq M\right).
\end{aligned}$$

Recall that we denote by $\overline{\mathrm{d}}_\partial$ the signed Euclidean distance to $\partial\mathscr{O}$. On the event

$$\mathscr{A}_{k,M} := \left\{\check{p}_{\check{\tau}_0^x}^x \cdot n(\check{q}_{\check{\tau}_0^x}^x) = 0, \check{\tau}_0^x \in (t_k, t_{k+1}], \sup_{0 \leq t \leq T} |\check{p}_t^x| \leq M, \sup_{0 \leq s < t \leq T} \frac{|\check{p}_t^x - \check{p}_s^x|}{|t-s|^\alpha} \leq M\right\},$$

we have

$$\left|\breve{q}^x_{\breve{\tau}^x_0} - \breve{q}^x_{t_k}\right| = \left|\int_{t_k}^{\breve{\tau}^x_0} \breve{p}^x_u \mathrm{d}u\right| \leq M(\breve{\tau}^x_0 - t_k) \leq M\eta_N.$$

Thus,

$$|\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})| \leq \left|\breve{q}^x_{t_k} - \breve{q}^x_{\breve{\tau}^x_0}\right| \leq M\eta_N.$$

For $\mu > 0$, let

$$\overline{\mathscr{O}}_\mu := \{q \in \mathbb{R}^d : |\bar{\mathrm{d}}_\partial(q)| \leq \mu\}. \tag{2.54}$$

Since the bounded open set $\mathscr{O}$ is $\mathscr{C}^2$ there exists a constant $\mu > 0$ such that the signed distance $\bar{\mathrm{d}}_\partial(q)$ to $\partial\mathscr{O}$ is $\mathscr{C}^2$ on the set $\overline{\mathscr{O}}_\mu$ according to [34, Lemma 14.16]. Moreover $\bar{\mathrm{d}}_\partial(q)$ satisfies the following eikonal equation

$$\begin{cases} |\nabla\bar{\mathrm{d}}_\partial(q)| = 1 & \text{for } q \in \overline{\mathscr{O}}_\mu, \\ \nabla\bar{\mathrm{d}}_\partial(q) = -n(q) & \text{for } q \in \partial\mathscr{O}. \end{cases} \tag{2.55}$$

Let us now choose N large enough so that $M\eta_N = M\frac{T}{N} \leq \mu$. As a result, since $\breve{q}^x_{t_k} \in \overline{\mathscr{O}}_\mu$ on $\mathscr{A}_{k,M}$,

$$\begin{aligned}
|\breve{p}^x_{t_k} \cdot \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})| &\leq \left|\left(\breve{p}^x_{t_k} - \breve{p}^x_{\breve{\tau}^x_0}\right) \cdot \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})\right| + \left|\breve{p}^x_{\breve{\tau}^x_0} \cdot (\nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k}) - \nabla\bar{\mathrm{d}}_\partial(q^x_{\breve{\tau}^x_0}))\right| + \underbrace{\left|\breve{p}^x_{\breve{\tau}^x_0} \cdot \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{\breve{\tau}^x_0})\right|}_{=0 \text{ on } \mathscr{A}_{k,M} \text{ by } (2.55)} \\
&\leq \left|\breve{p}^x_{t_k} - \breve{p}^x_{\breve{\tau}^x_0}\right| + M\left|\nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k}) - \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{\breve{\tau}^x_0})\right| \\
&\leq M\eta_N^\alpha + M^2K\eta_N
\end{aligned}$$

with K the Lipschitz constant of $\nabla\bar{\mathrm{d}}_\partial$ on the compact set $\overline{\mathscr{O}}_\mu$ since $\bar{\mathrm{d}}_\partial$ is $\mathscr{C}^2$ on $\overline{\mathscr{O}}_\mu$. Defining $M_1 := M + M^2K$, one gets for N large enough so that $\eta_N \leq 1$

$$\left|\breve{p}^x_{t_k} \cdot \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})\right| \leq M_1\eta_N^\alpha.$$

This yields that

$$\begin{aligned}
&\mathbb{P}\left(\breve{p}^x_{\breve{\tau}^x_0} \cdot n(\breve{q}^x_{\breve{\tau}^x_0}) = 0, \breve{\tau}^x_0 \leq T, \sup_{0\leq t\leq T}|\breve{p}^x_t| \leq M, \sup_{0\leq s<t\leq T}\frac{|\breve{p}^x_t - \breve{p}^x_s|}{|t-s|^\alpha} \leq M\right) \\
&\leq \sum_{k=0}^{N-1}\mathbb{P}\left(\left|\breve{p}^x_{t_k} \cdot \nabla\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})\right| \leq M_1\eta_N^\alpha, |\bar{\mathrm{d}}_\partial(\breve{q}^x_{t_k})| \leq M\eta_N\right).
\end{aligned} \tag{2.56}$$

Let $k_0 := \lceil\frac{4M}{|p\cdot n(q)|}\rceil$. For $k \in ⟦0, k_0 - 1⟧$, the summand in (2.56) vanishes when N goes to infinity since $t_k = k\frac{T}{N} \leq (k_0 - 1)\frac{T}{N} \underset{N\to\infty}{\longrightarrow} 0$ and either $|\bar{\mathrm{d}}_\partial(q)| > 0$ (if $q \notin \partial\mathscr{O}$) or $|p \cdot \nabla\bar{\mathrm{d}}_\partial(q)| > 0$ (if $q \in \partial\mathscr{O}$, because $(q,p) \notin \Gamma^0$).

Step 2. Let us now prove that for $k \in ⟦k_0 + 1, N - 1⟧$, the summand in (2.56) is of order $\eta_N^{1+\alpha}$.

It is easy to check that $(\breve{q}^x_t, \breve{p}^x_t)$ is a Gaussian vector in $\mathbb{R}^{2d}$ with law

$$\begin{pmatrix}\breve{q}^x_t \\ \breve{p}^x_t\end{pmatrix} \sim \mathscr{N}_{2d}\left(\begin{pmatrix}q + tp \\ p\end{pmatrix}, \begin{pmatrix}\frac{\sigma^2t^3}{3}I_d & \frac{\sigma^2t^2}{2}I_d \\ \frac{\sigma^2t^2}{2}I_d & \sigma^2tI_d\end{pmatrix}\right). \tag{2.57}$$

In particular,

$$\breve{q}^x_t \sim \mathscr{N}_d\left(q + tp, \frac{\sigma^2t^3}{3}I_d\right)$$

with a density denoted by f_t for $t > 0$. We can also compute the conditional law of $\breve{p}^x_t$ knowing $\breve{q}^x_t$ using [28, Prop 3.13]. It is given by

$$\mathscr{N}_d\left(p + \frac{3}{2t}(\breve{q}^x_t - q - tp), \frac{\sigma^2t}{4}I_d\right),$$

with a density denoted by $h_t(\cdot|\check{q}_t^x)$. As a result, using the fact that $|\nabla \overline{\mathrm{d}}_\partial| = 1$ on $\overline{\mathscr{O}}_\mu$, (see (2.55)), the conditional law of $\check{p}_t^x \cdot \nabla \overline{\mathrm{d}}_\partial(\check{q}_t^x)$ knowing $\check{q}_t^x$, when $\check{q}_t^x \in \overline{\mathscr{O}}_\mu$, is given by

$$\mathscr{N}\left(\left(p + \frac{3}{2t}(\check{q}_t^x - q - tp)\right) \cdot \nabla \overline{\mathrm{d}}_\partial(\check{q}_t^x), \frac{\sigma^2 t}{4}\right)$$

with a density denoted by $g_t(\cdot|\check{q}_t^x)$.

As a consequence, for $k \in \llbracket k_0, N-1 \rrbracket$,

$$\begin{aligned}&\mathbb{P}\left(\left|\check{p}_{t_k}^x \cdot \nabla \overline{\mathrm{d}}_\partial(\check{q}_{t_k}^x)\right| \leq M_1 \eta_N^\alpha, |\overline{\mathrm{d}}_\partial(\check{q}_{t_k}^x)| \leq M \eta_N\right)\\ &= \int_{q' \in \mathbb{R}^d} \mathbb{1}_{|\overline{\mathrm{d}}_\partial(q')| \leq M\eta_N} f_{t_k}(q') \left(\int_{y \in \mathbb{R}} \mathbb{1}_{|y| \leq M_1 \eta_N^\alpha} g_{t_k}(y|q') \mathrm{d}y\right) \mathrm{d}q'.\end{aligned}$$

Let $m_k(q') := (p + \frac{3}{2t_k}(q' - q - t_k p)) \cdot \nabla \overline{\mathrm{d}}_\partial(q')$ then for $q' \in \overline{\mathscr{O}}_\mu$,

$$\int_{y \in \mathbb{R}} \mathbb{1}_{|y| \leq M_1 \eta_N^\alpha} g_{t_k}(y|q') \mathrm{d}y = \int_{y \in \mathbb{R}} \mathbb{1}_{|y| \leq M_1 \eta_N^\alpha} \underbrace{\frac{\mathrm{e}^{-2\frac{(y - m_k(q'))^2}{\sigma^2 t_k}}}{\sqrt{\frac{\pi \sigma^2 t_k}{2}}}}_{\leq \frac{1}{\sqrt{\frac{\pi\sigma^2 t_k}{2}}}} \mathrm{d}y \leq \frac{2\sqrt{2} M_1 \eta_N^\alpha}{\sqrt{\pi \sigma^2 t_k}}.$$

Hence

$$\begin{aligned}&\mathbb{P}\left(\left|\check{p}_{t_k}^x \cdot \nabla \overline{\mathrm{d}}_\partial(\check{q}_{t_k}^x)\right| \leq M_1 \eta_N^\alpha, |\overline{\mathrm{d}}_\partial(\check{q}_{t_k}^x)| \leq M \eta_N\right)\\ &\leq \int_{q' \in \mathbb{R}^d} \mathbb{1}_{|\overline{\mathrm{d}}_\partial(q')| \leq M\eta_N} \frac{2\sqrt{2} M_1 \eta_N^\alpha}{\sqrt{\pi \sigma^2 t_k}} \left(\frac{3}{2\pi\sigma^2 t_k^3}\right)^{\frac{d}{2}} \mathrm{e}^{-\frac{3|z - q - t_k p|^2}{2\sigma^2 t_k^3}} \mathrm{d}q'\\ &\leq \left(\frac{3}{2\pi\sigma^2}\right)^{\frac{d}{2}} \frac{2\sqrt{2} M_1 \eta_N^\alpha}{\sqrt{\pi\sigma^2}} \int_{\mathbb{R}^d} \frac{\mathrm{e}^{-\frac{3|q' - q - t_k p|^2}{2\sigma^2 t_k^3}}}{t_k^{\frac{3d+1}{2}}} \mathrm{d}q'.\end{aligned} \tag{2.58}$$

Let us now prove that the integrand is bounded by a constant independent of k.

Case a). Assume that $q \notin \partial \mathscr{O}$, then $|\overline{\mathrm{d}}_\partial(q)| > 0$ and there exists $\mu_1 > 0$ such that for any $q' \in \mathscr{O}_{\mu_1}$,

$$|q' - q| \geq \sqrt{\frac{2}{3}} |\overline{\mathrm{d}}_\partial(q)|.$$

Let us pick N large enough so that

$$M\eta_N \leq \min(\mu, \mu_1). \tag{2.59}$$

Let $C_2 := \sup_{q' \in \mathscr{O}} |q - q'|$. For $C_2 |p| t_k \leq \frac{\overline{\mathrm{d}}_\partial(q)^2}{6}$,

$$-|q' - q - t_k p|^2 = -|q' - q|^2 - t_k^2 |p|^2 + 2t_k (q' - q) \cdot p \leq -|q' - q|^2 + 2t_k C_2 |p| \leq -\frac{\overline{\mathrm{d}}_\partial(q)^2}{3}$$

and

$$\frac{\mathrm{e}^{-\frac{3|q' - q - t_k p|^2}{2\sigma^2 t_k^3}}}{t_k^{\frac{3d+1}{2}}} \leq \frac{\mathrm{e}^{-\frac{\overline{\mathrm{d}}_\partial(q)^2}{2\sigma^2 t_k^3}}}{t_k^{\frac{3d+1}{2}}}.$$

Moreover, if $C_2 |p| t_k > \frac{\overline{\mathrm{d}}_\partial(q)^2}{6}$ (necessarily $|p| \neq 0$),

$$\frac{\mathrm{e}^{-\frac{3|z - q - t_k p|^2}{2\sigma^2 t_k^3}}}{t_k^{\frac{3d+1}{2}}} \leq \frac{1}{\left(\frac{\overline{\mathrm{d}}_\partial(q)^2}{6C_2|p|}\right)^{\frac{3d+1}{2}}}. \tag{2.60}$$

Besides, the function $t > 0 \mapsto \frac{e^{-\frac{\overline{d}_\partial(q)^2}{2\sigma^2 t^3}}}{t^{\frac{3d+1}{2}}} + \frac{1}{(\frac{\overline{d}_\partial(q)^2}{6C_2|p|})^{\frac{3d+1}{2}}}$ is bounded by a constant C_3 which depends only on q, p and d.

Case b). Assume that $q \in \partial\mathscr{O}$, then necessarily $|p \cdot n(q)| > 0$ since $(q, p) \notin \Gamma^0$. By the right continuity in 0 of $s \mapsto p \cdot \nabla\overline{d}_\partial(q+sp)$, there exists $\beta > 0$ such that for all $s \in [0, \beta]$, $|p \cdot \nabla\overline{d}_\partial(q+sp)| \geq \frac{|p \cdot n(q)|}{2}$ (and $p \cdot \nabla\overline{d}_\partial(q+sp)$ has constant sign on $[0, \beta]$).

Assume that $t_k \leq \beta$. One has that

$$\overline{d}_\partial(q + t_k p) = \int_0^{t_k} p \cdot \nabla\overline{d}_\partial(q + sp)\mathrm{d}s.$$

Therefore, since the integrand $p \cdot \nabla\overline{d}_\partial(q + sp)$ has constant sign on $[0, t_k]$,

$$|\overline{d}_\partial(q + t_k p)| \geq t_k \frac{|p \cdot n(q)|}{2}.$$

As a result, for $q' \in \mathscr{O}_{M\eta_N}$ since $\overline{d}_\partial$ is $1-$Lipschitz continuous,

$$\begin{aligned}|q' - q - t_k p| &\geq |\overline{d}_\partial(q + t_k p) - \overline{d}_\partial(q')| \\ &\geq t_k \frac{|p \cdot \nabla\overline{d}_\partial(q)|}{2} - M\eta_N \\ &= t_k \frac{|p \cdot \nabla\overline{d}_\partial(q)|}{2}\left(1 - \frac{\eta_N}{t_k}\frac{2M}{|p \cdot \nabla\overline{d}_\partial(q)|}\right).\end{aligned}$$

Besides, since $k \geq k_0$,

$$\begin{aligned}\frac{\eta_N}{t_k}\frac{2M}{|p \cdot \nabla\overline{d}_\partial(q)|} &= \frac{1}{k}\frac{2M}{|p \cdot \nabla\overline{d}_\partial(q)|} &\quad (2.61)\\ &\leq \frac{1}{k_0}\frac{2M}{|p \cdot \nabla\overline{d}_\partial(q)|} \leq \frac{1}{2}, &\quad (2.62)\end{aligned}$$

by definition of k_0. Therefore, for $t_k \leq \beta$,

$$|q' - q - t_k p| \geq t_k \frac{|p \cdot \nabla\overline{d}_\partial(q)|}{4},$$

which ensures that the integrand in (2.58) is smaller than $\frac{e^{-\frac{3|p\cdot\nabla\overline{d}_\partial(q)|^2}{32\sigma^2 t_k}}}{t_k^{\frac{3d+1}{2}}}$ which is smaller than a constant $C_4 > 0$ only depending on q, p and d. On the other hand, if $t_k \geq \beta$, the integrand (2.58) also admits a constant upper-bound independent of k.

As a result, one gets that $q' \in \mathscr{O}_{M\eta_N} \mapsto \frac{e^{-\frac{3|q'-q-t_k p|^2}{2\sigma^2 t_k^3}}}{t_k^{\frac{3d+1}{2}}}$ is bounded by $C_5 := C_3 \wedge C_4$, which is independent of k.

Last, using Weyl's tube formula [79], one gets that there exists $C_6 > 0$ only depending on $\mathscr{O}$ such that

$$\int_{\mathscr{O}_{M\eta_N}} \mathrm{d}q' \leq C_6 M\eta_N.$$

As a consequence,

$$\mathbb{P}\left(\left|\check{p}^x_{t_k} \cdot \nabla\overline{d}_\partial(\check{q}^x_{t_k})\right| \leq M_1\eta_N^\alpha, |\overline{d}_\partial(\check{q}^x_{t_k})| \leq M\eta_N\right) \leq \left(\frac{3}{2\pi\sigma^2}\right)^{\frac{d}{2}} \frac{2\sqrt{2}M_1\eta_N^\alpha}{\sqrt{\pi\sigma^2}} C_5 C_6 M\eta_N \quad (2.63)$$

which is independent of k.

Step 3. Finally summing over all k one gets from (2.56) and (2.63), for N large enough:

$$\mathbb{P}\left(\check{p}^x_{\check{\tau}^x_0} \cdot n(\check{q}^x_{\check{\tau}^x_0}) = 0, \check{\tau}^x_0 \le T, \sup_{0\le t\le T} |\check{p}^x_t| \le M, \sup_{0\le s<t\le T} \frac{|\check{p}^x_t - \check{p}^x_s|}{|t-s|^\alpha} \le M\right)$$

$$\le \underbrace{\sum_{k=0}^{k_0-1} \mathbb{P}\left(|\check{p}^x_{t_k} \cdot \nabla \overline{\mathrm{d}}_\partial(\check{q}^x_{t_k})| \le M_1 \eta_N^\alpha, |\overline{\mathrm{d}}_\partial(\check{q}^x_{t_k})| \le M\eta_N\right)}_{\underset{N\to\infty}{\longrightarrow} 0} + \frac{N}{N-k_0} \underbrace{\left(\frac{3}{2\pi\sigma^2}\right)^{\frac{d}{2}} \frac{2\sqrt{2}M_1}{\sqrt{\pi\sigma^2}} C_5 C_6 M T}_{\text{not depending on } N} \eta_N^\alpha.$$

Letting $\eta_N \underset{N\to\infty}{\longrightarrow} 0$, we get

$$\mathbb{P}\left(\check{p}^x_{\check{\tau}^x_0} \cdot n(\check{q}^x_{\check{\tau}^x_0}) = 0, \check{\tau}^x_0 \le T, \sup_{0\le t\le T} |\check{p}^x_t| \le M, \sup_{0\le s<t\le T} \frac{|\check{p}^x_t - \check{p}^x_s|}{|t-s|^\alpha} \le M\right) = 0.$$

Thus, for all $\epsilon > 0$,

$$\mathbb{P}\left(\check{p}^x_{\check{\tau}^x_0} \cdot n(\check{q}^x_{\check{\tau}^x_0}) = 0, \check{\tau}^x_0 \le T\right) \le 2\epsilon$$

which concludes the proof of (2.52). □

2.4 Harnack inequality and Maximum principle

This section is devoted to the proof of the Harnack inequality stated in Theorem 2.2.15 and of the maximum principle of Theorem 2.2.14. The proofs are respectively detailed in Sections 2.4.1 and 2.4.2.

2.4.1 Proof of Theorem 2.2.15

A Harnack inequality for weak solutions of (2.15) was already proven in [35]. It says that for every point $(t_0, x_0) \in \mathbb{R}^*_+ \times D$ there exist $T > 0$, two small disjoint cylinders $Q^+, Q^- \subset D$ close to x_0 and a constant $C > 0$ such that for any non-negative distributional solution u of $\partial_t u = \mathscr{L}u$, we have for all $t_0 \ge 0$,

$$\sup_{x\in Q^-} u(t_0, x) \le C \inf_{x\in Q^+} u(t_0 + T, x).$$

Adapting a chaining argument from [2] with a suitable chaining function, we extend this inequality to any compact set K of D to obtain the result (2.17). In order to prepare the chaining argument, we first introduce some notation. For all $x, y \in D$ and $T, M, \delta > 0$, we denote by $\mathscr{H}_{T,x,y,M,\delta}$ the set of $\mathscr{C}^1$ and piecewise $\mathscr{C}^2$ paths $\phi : [0,T] \to \mathscr{O}$ such that

$$\left(\phi(0), \dot\phi(0)\right) = x, \quad \left(\phi(T), \dot\phi(T)\right) = y, \quad \sup_{s\in[0,T]} \left(\left|\dot\phi\right| + \left|\ddot\phi\right|\right)(s) \le M, \quad \inf_{s\in[0,T]} \mathrm{d}_\partial(\phi(s)) > \delta.$$

Lemma 2.4.1. *There exists a universal constant $C > 1$ such that for all $\Delta > 0$, $x = (q,p), y = (q',p') \in \mathbb{R}^{2d}$, there exists $\phi \in \mathscr{C}^2([0,\Delta], \mathbb{R}^d)$ such that*

(i) $\left(\phi(0), \dot\phi(0)\right) = x$ *and* $\left(\phi(\Delta), \dot\phi(\Delta)\right) = y$*,*

(ii) $\sup_{t\in[0,\Delta]} |\phi(t) - q| \le C(|q'-q| + \Delta|p'-p| + \Delta|p|)$*,*

(iii) $\sup_{t\in[0,\Delta]} |\dot\phi(t)| \le \frac{C}{\Delta}(|q'-q| + \Delta|p'-p| + \Delta|p|)$*,*

(iv) $\sup_{t\in[0,\Delta]} |\ddot\phi(t)| \le \frac{C}{\Delta^2}(|q'-q| + \Delta|p'-p| + \Delta|p|)$*.*

Proof. Let $\Delta > 0$. For all $t \in [0, \Delta]$, we define

$$\phi(t) := q + (q' - q)\left(3\frac{t^2}{\Delta^2} - 2\frac{t^3}{\Delta^3}\right) + \Delta(p' - p)\left(\frac{t^3}{\Delta^3} - \frac{t^2}{\Delta^2}\right) + \Delta p\left(\frac{t}{\Delta} + 2\frac{t^3}{\Delta^3} - 3\frac{t^2}{\Delta^2}\right).$$

It is easy to see that ϕ satisfies the conditions above. □

We recall that under Assumption (O1), the set $\mathscr{O}$ satisfies the uniform interior sphere condition and denote by $\rho > 0$ the associated radius (see Section 2.3.4.1).

In the next statement, we denote by $\mathrm{dist}(A, B) = \inf_{x\in A, y\in B} |x - y|$ the distance between two subsets $A, B \subset \mathbb{R}^d$.

Lemma 2.4.2 (Admissible paths)**.** *Under Assumptions (O1) and (O2), let $K \subset D$ be a compact set and $\delta_K := \mathrm{dist}(K, \partial D) \wedge \rho$. For all $T > 0$, there exists $M_{K,T} > 0$ such that for all $x, y \in K$ the set $\mathscr{H}_{T,x,y,M_{K,T},\delta_K/2}$ is nonempty.*

Proof. Let $K \subset D$ be a compact set and $\delta_K > 0$ be defined accordingly. Let $k := \sup_{(q,p)\in K} |p|$, $K' := \{(q, p) \in D : |p| \leq k, d_\partial(q) \geq \delta_K\}$ and $M_K := k + 1$. By the uniform interior sphere condition and Assumption (O2), K' is a connected compact subset of D, and $K \subset K'$.

Let $T > 0$ and $\epsilon := \delta_K/2$. Let $C > 1$ be the constant from Lemma 2.4.1. The compact set K' can be covered by $N \geq 1$ closed balls $\overline{\mathrm{B}}(z_1, \frac{\epsilon}{8C}), \dots, \overline{\mathrm{B}}(z_N, \frac{\epsilon}{8C})$ included in D with $z_i = (q_i, p_i) \in K'$ for all $i \in \llbracket 1, N \rrbracket$. We can take N large enough so that $\Delta := \frac{T}{N+1} \in (0, \frac{\epsilon}{2M_K C} \wedge 1)$. We can now build a graph $\mathscr{G}$ with N vertices corresponding to the points $(z_i)_{1\leq i\leq N}$, and for every $i, j \in \llbracket 1, N \rrbracket$, we link z_i to z_j if $|z_j - z_i| \leq \frac{\epsilon}{4C}$. Since the set K' is connected, then so is the graph $\mathscr{G}$.

Furthermore, for all $i, j \in \llbracket 1, N \rrbracket$ which are adjacent in $\mathscr{G}$, by Lemma 2.4.1, there exists a path $\phi_{i,j} \in \mathscr{C}^2([0, \Delta], \mathbb{R}^d)$ such that

(i) $\left(\phi_{i,j}(0), \dot{\phi}_{i,j}(0)\right) = z_i$ and $\left(\phi_{i,j}(\Delta), \dot{\phi}_{i,j}(\Delta)\right) = z_j$

(ii) $\sup_{t\in[0,\Delta]} |\phi_{i,j}(t) - q_i| \leq C(|z_j - z_i|(1 + \Delta) + \Delta|p_i|) \leq C\left(2\frac{\epsilon}{4C} + k\frac{\epsilon}{2M_K C}\right) < \epsilon$

(iii) $\sup_{t\in[0,\Delta]} \left(\left|\dot{\phi}_{i,j}\right| + \left|\ddot{\phi}_{i,j}\right|\right)(t) \leq C\left(\frac{1}{\Delta} + \frac{1}{\Delta^2}\right)(|z_j - z_i|(1+\Delta) + \Delta|p_i|) \leq \epsilon\left(\frac{1}{\Delta} + \frac{1}{\Delta^2}\right) \leq \frac{2\epsilon}{\Delta^2}$.

Since $z_i \in K'$, the second condition ensures that, for all $t \in [0, \Delta]$, $\phi_{i,j}(t)$ remains at a distance from $\partial\mathscr{O}$ strictly larger than $\delta_K - \epsilon \geq \delta_K/2$.

Now let $x, y \in K'$. By the previous cover, there exist $i_0, i_N \in \llbracket 1, N \rrbracket$ such that

$$|x - z_{i_0}| \leq \frac{\epsilon}{8C}, \quad |y - z_{i_N}| \leq \frac{\epsilon}{8C}.$$

Using Lemma 2.4.1 again, we construct $\psi_0, \psi_N : [0, \Delta] \to \mathscr{O}$ respectively joining x to z_{i_0} and z_{i_N} to y and such that $\sup_{t\in[0,\Delta]}(|\dot{\psi}_0| + |\ddot{\psi}_0|)(t) \leq \frac{\delta_K}{\Delta^2}$ and $\sup_{t\in[0,\Delta]}(|\dot{\psi}_N| + |\ddot{\psi}_N|)(t) \leq \frac{\delta_K}{\Delta^2}$. The connectedness of the graph $\mathscr{G}$ ensures the existence of $i_1, \dots, i_{N-1} \in \llbracket 1, N \rrbracket$ such that for all $j \in \llbracket 1, N \rrbracket$, $|z_{i_j} - z_{i_{j-1}}| \leq \frac{\epsilon}{4C}$. If the path obtained on the graph $\mathscr{G}$ is smaller than N then we can complete with loops around the same point. It is important here that this path in the graph have exactly $N - 1$ vertices, because in the end we aim at constructing a trajectory ϕ by piecing together trajectories $\phi_{i_j,i_{j+1}}$, $j = 0, \dots, N$, of length $\Delta = T/(N + 1)$ and we want the final trajectory ϕ to have exact length T. Let us now define the path function ϕ on $[0, T]$ as follows:

$$\phi(t) = \begin{cases} \psi_0(t) & \text{if } t \in [0, \Delta], \\ \phi_{i_j,i_{j+1}}(t - j\Delta) & \text{if } t \in [j\Delta, (j + 1)\Delta], \\ \psi_N(t - T + \Delta) & \text{if } t \in [T - \Delta, T], \end{cases}$$

then it is easy to see that $\phi \in \mathscr{H}_{T,x,y,\frac{\delta_K}{\Delta^2},\delta_K/2}$. Since K' contains the compact set K this concludes the proof for the compact set K. □

Let us now prove the Harnack inequality in Theorem 2.2.15.

Proof of Theorem 2.2.15. Let $K \subset D$ be a compact set. Let $T > 0$ and let u be a non-negative distributional solution of $\partial_t u - \mathscr{L} u = 0$ on $\mathbb{R}_+^* \times D$. The proof is divided into two steps. In the first step, we introduce the necessary background in order to apply the Harnack inequality from [35]. In the second step, we detail the chaining argument, based on Lemma 2.4.2, which allows us to obtain the Harnack inequality of Theorem 2.2.15.

Step 1. Let $M_{K,T} > 0$ and $\delta_K > 0$ be the constants given in Lemma 2.4.2 and let us define the constant $r_{K,T} := \sqrt{\frac{\delta_K}{1+M_{K,T}}} \wedge \frac{1}{2}$. Let $r \in (0, r_{K,T}]$. Let us define

$$D_{K,T,r} = \{(t,q,p) \in \mathbb{R}_+^* \times D : t > r^2, \mathrm{d}_\partial(q) > \delta_K/2, |p| \leq M_{K,T}\}.$$

Notice that $(r^2, \infty) \times K \subset D_{K,T,r}$. Let Q be the following unit box

$$Q := \{(t,q,p) \in \mathbb{R} \times \mathbb{R}^{2d} : t \in (-1,0], |q| < 1, |p| < 1\}.$$

For all $z_0 = (t_0, q_0, p_0) \in D_{K,T,r}$, let us define the following function on Q

$$h_{r,z_0} : (t,q,p) := (r^2 t + t_0, q_0 - r^2 t p_0 + r^3 q, p_0 - rp).$$

Notice that for all $z_0 \in D_{K,T,r}$ and $(t,q,p) \in Q$,

$$|-r^2 t p_0 + r^3 q| \leq M_{K,T} r_{K,T}^2 + r_{K,T}^3 < r_{K,T}^2 (1 + M_{K,T}) \leq \delta_K,$$

since $r_{K,T} \in (0,1)$. As a result, h_{r,z_0} is a function on Q with values in $\mathbb{R}_+^* \times D$.

Since $\partial_t - \mathscr{L}$ is a hypoelliptic operator on $\mathbb{R}_+^* \times D$ it follows that u is in $\mathscr{C}^\infty(\mathbb{R}_+^* \times D)$. Let us now define the following smooth function

$$u_{r,z_0} := u \circ h_{r,z_0}$$

on Q. It satisfies

$$\partial_t u_{r,z_0} = -p \cdot \nabla_q u_{r,z_0} + \gamma(r p_0 - r^2 p) \cdot \nabla_p u_{r,z_0} - rF(q_0 - r^2 t p_0 + r^3 q) \cdot \nabla_p u_{r,z_0} + \frac{\sigma^2}{2} \Delta_p u_{r,z_0}.$$

Besides for $(t,q,p) \in Q$,

$$\left|\gamma(r p_0 - r^2 p) - rF(q_0 - r^2 t p_0 + r^3 q)\right| \leq |\gamma| \left(M_{K,T} + \delta_K\right) + \|F\|_{\mathrm{L}^\infty(\mathscr{O})}$$

which is a constant depending only on the compact K, T and the coefficients of $\mathscr{L}$. As a result, Theorem 4 in [35] ensures the existence of constants $C_{K,T} > 1$ and $R_{K,T}, \Delta_{K,T} \in (0,1)$ (which do not depend on $r \in (0, r_{K,T}]$ or z_0) such that $\Delta_{K,T} + R_{K,T}^2 < 1$ and

$$\sup_{(t,q,p) \in Q_{K,T}^-} u_{r,z_0}(t,q,p) \leq C_{K,T} \inf_{(t,q,p) \in Q_{K,T}^+} u_{r,z_0}(t,q,p) \tag{2.64}$$

where

$$Q_{K,T}^+ := \{(t,q,p) : t \in (-R_{K,T}^2, 0], |q| < R_{K,T}^3, |p| < R_{K,T}\} \subset Q,$$
$$Q_{K,T}^- := \{(t,q,p) : t \in (-R_{K,T}^2 - \Delta_{K,T}, -\Delta_{K,T}], |q| < R_{K,T}^3, |p| < R_{K,T}\} \subset Q.$$

Introducing the notation $Q_{K,T,r}^\pm(z_0) = h_{r,z_0}(Q_{K,T}^\pm)$, (2.64) rewrites, for all $r \in (0, r_{K,T}]$ and $z_0 \in D_{K,T,r}$,

$$\sup_{(t,q,p) \in Q_{K,T,r}^-(z_0)} u(t,q,p) \leq C_{K,T} \inf_{(t,q,p) \in Q_{K,T,r}^+(z_0)} u(t,q,p). \tag{2.65}$$

Step 2. Let $\epsilon > 0$. Let us choose $r_{K,T}^\epsilon$ satisfying

(i) $0 < r^\epsilon_{K,T} \le r_{K,T}$,

(ii) $r^\epsilon_{K,T} < \frac{2R^3_{K,T}}{M_{K,T}\left(\Delta_{K,T}+\frac{R^2_{K,T}}{2}\right)^2} \wedge \frac{R_{K,T}}{M_{K,T}\left(\Delta_{K,T}+\frac{R^2_{K,T}}{2}\right)} \wedge \sqrt{\frac{\epsilon}{1-\Delta_{K,T}-\frac{R^2_{K,T}}{2}}}$,

(iii) the quantity $\alpha^\epsilon_{K,T} := (r^\epsilon_{K,T})^2\left(\Delta_{K,T}+\frac{R^2_{K,T}}{2}\right)$ is such that $n^\epsilon_{K,T} := \frac{T}{\alpha^\epsilon_{K,T}} \in \mathbb{N}$.

Let $t \ge T+\epsilon$. Let (x,y) be two arbitrary points in the compact K. Let $\phi \in \mathscr{H}_{T,x,y,M_{K,T},\delta_K/2}$ (which exists by Lemma 2.4.2) and let

$$\Phi : s \in [0,T] \mapsto \begin{pmatrix} \phi(s) \\ \dot\phi(s) \\ t-s \end{pmatrix} \in \mathbb{R}^{2d+1}.$$

Now let $(s^\epsilon_j)_{0\le j\le n^\epsilon_{K,T}}$ be the sequence defined by $s^\epsilon_j := j\alpha^\epsilon_{K,T}$ for $0 \le j \le n^\epsilon_{K,T}$.

Let us show that $\Phi(s^\epsilon_j) \in D_{K,T,r^\epsilon_{K,T}}$ for all $0 \le j \le n^\epsilon_{K,T}-1$. Indeed, one has

$$t - s_{n^\epsilon_{K,T}-1} = t - (n^\epsilon_{K,T}-1)\alpha^\epsilon_{K,T} = t - T + (r^\epsilon_{K,T})^2\left(\Delta_{K,T}+\frac{R^2_{K,T}}{2}\right) > (r^\epsilon_{K,T})^2,$$

since $(r^\epsilon_{K,T})^2 < \frac{\epsilon}{1-\Delta_{K,T}-\frac{R^2_{K,T}}{2}}$. The rest follows from the definition of $\mathscr{H}_{T,x,y,M_{K,T},\delta_K/2}$. Hence, (2.65) is satisfied for $r = r^\epsilon_{K,T}$ and $z_0 = \Phi(s^\epsilon_j)$ for all $0 \le j \le n^\epsilon_{K,T}-1$, i.e.

$$\sup_{(t,q,p)\in Q^-_{K,T,r^\epsilon_{K,T}}(\Phi(s^\epsilon_j))} u(t,q,p) \le C_{K,T} \inf_{(t,q,p)\in Q^+_{K,T,r^\epsilon_{K,T}}(\Phi(s^\epsilon_j))} u(t,q,p).$$

Let us now prove that for every $0 \le j \le n^\epsilon_{K,T}-1$, $\Phi(s^\epsilon_{j+1}) \in Q^-_{K,T,r^\epsilon_{K,T}}(\Phi(s^\epsilon_j))$. Let

(i) $\widehat{t}_j := -\frac{\alpha^\epsilon_{K,T}}{(r^\epsilon_{K,T})^2} = -\Delta_{K,T} - \frac{R^2_{K,T}}{2}$,

(ii) $\widehat{q}_j := \frac{1}{(r^\epsilon_{K,T})^3}\left(\phi(s^\epsilon_{j+1}) - \phi(s^\epsilon_j) - \alpha^\epsilon_{K,T}\dot\phi(s^\epsilon_j)\right)$,

(iii) $\widehat{p}_j := \frac{1}{r^\epsilon_{K,T}}\left(\dot\phi(s^\epsilon_j) - \dot\phi(s^\epsilon_{j+1})\right)$.

Then it only remains to prove that $(\widehat{t}_j, \widehat{q}_j, \widehat{p}_j) \in Q^-_{K,T}$ for every $0 \le j \le n^\epsilon_{K,T}-1$, i.e. that

$$h_{r^\epsilon_{K,T},\Phi(s^\epsilon_j)}(\widehat{t}_j, \widehat{q}_j, \widehat{p}_j) = \Phi(s^\epsilon_{j+1}).$$

First, concerning $\widehat{t}_j$, it is clear by definition of $\alpha^\epsilon_{K,T}$ that

$$-\Delta_{K,T} - R^2_{K,T} < -\frac{\alpha^\epsilon_{K,T}}{(r^\epsilon_{K,T})^2} \le -\Delta_{K,T}.$$

Second, for $\widehat{q}_j$,

$$\begin{aligned}
\left|\phi(s^\epsilon_{j+1}) - \phi(s^\epsilon_j) - \alpha^\epsilon_{K,T}\dot\phi(s^\epsilon_j)\right| &= \left|\int_{s^\epsilon_j}^{s^\epsilon_{j+1}} \left(\dot\phi(\eta) - \dot\phi(s^\epsilon_j)\right) \mathrm{d}\eta\right| \\
&\le \int_{s^\epsilon_j}^{s^\epsilon_{j+1}} \int_{s^\epsilon_j}^{\eta} \left|\ddot\phi(\mu)\right| \mathrm{d}\mu \mathrm{d}\eta \\
&\le M_{K,T} \int_{s^\epsilon_j}^{s^\epsilon_{j+1}} (\eta - s^\epsilon_j)\, \mathrm{d}\eta \\
&\le M_{K,T}\frac{(\alpha^\epsilon_{K,T})^2}{2}
\end{aligned}$$

and since

$$r^{\epsilon}_{K,T} < \frac{2R^3_{K,T}}{M_{K,T}\left(\Delta_{K,T} + \frac{R^2_{K,T}}{2}\right)^2},$$

we have

$$(r^{\epsilon}_{K,T})^4 \left(\Delta_{K,T} + \frac{R^2_{K,T}}{2}\right)^2 < \frac{2(r^{\epsilon}_{K,T})^3 R^3_{K,T}}{M_{K,T}},$$

and therefore

$$M_{K,T}\frac{(\alpha^{\epsilon}_{K,T})^2}{2} < (r^{\epsilon}_{K,T})^3 R^3_{K,T}.$$

Third, for $\widehat{p}_j$,

$$\left|\dot{\phi}(s^{\epsilon}_{j+1}) - \dot{\phi}(s^{\epsilon}_j)\right| \leq \int_{s^{\epsilon}_j}^{s^{\epsilon}_{j+1}} \left|\ddot{\phi}(\eta)\right| \mathrm{d}\eta \leq M_{K,T}\alpha^{\epsilon}_{K,T}$$

and the assumption that

$$r^{\epsilon}_{K,T} < \frac{R_{K,T}}{M_{K,T}\left(\Delta_{K,T} + \frac{R^2_{K,T}}{2}\right)}$$

ensures that

$$M_{K,T}\alpha^{\epsilon}_{K,T} < r^{\epsilon}_{K,T} R_{K,T}.$$

Hence $\Phi(s^{\epsilon}_{j+1}) \in Q^-_{K,T,r^{\epsilon}_{K,T}}(\Phi(s^{\epsilon}_j))$.

Finally, one gets for $0 \leq j \leq n^{\epsilon}_{K,T} - 1$

$$u(\Phi(s^{\epsilon}_{j+1})) \leq \sup_{Q^-_{K,T,r^{\epsilon}_{K,T}}(\Phi(s^{\epsilon}_j))} u \leq C_{K,T} \inf_{Q^+_{K,T,r^{\epsilon}_{K,T}}(\Phi(s^{\epsilon}_j))} u \leq C_{K,T} u(\Phi(s^{\epsilon}_j))$$

which yields by iterating,

$$u(\Phi(T)) = u(t - T, y) \leq C^{n^{\epsilon}_{K,T}}_{K,T} u(\Phi(0)) = C^{n^{\epsilon}_{K,T}}_{K,T} u(t, x)$$

where $C^{n^{\epsilon}_{K,T}}_{K,T}$ does not depend on (t, x, y) but only on the compact K and T, ϵ. As a result, we have for all $t \geq T + \epsilon$,

$$\sup_{x\in K} u(t - T, x) \leq C^{n^{\epsilon}_{K,T}}_{K,T} \inf_{x\in K} u(t, x)$$

which concludes the proof. □

Remark 2.4.3. *Let $v(t, x)$ be a non-negative distributional solution of $\partial_t v = \mathscr{L}^* v$ on $\mathbb{R}^*_+ \times D$. For $t > 0$, $(q, p) \in D$, let*

$$u(t, (q, p)) = \mathrm{e}^{-d\gamma t} v(t, (q, -p))$$

then u is a non-negative distributional solution of $\partial_t u = \mathscr{L}_{F,-\gamma,\sigma} u$ with the notation of (2.6). As a result, the Harnack inequality is also satisfied for the adjoint generator $\mathscr{L}^*$.

2.4.2 Proof of Theorem 2.2.14

In order to prove the maximum principle stated in Theorem 2.2.14, we need the following lemma.

Lemma 2.4.4 (Irreducibility)**.** *Let Assumptions (F1), (O1) and (O2) hold. Let A be an open subset of D, then*

$$\forall x \in D, \quad \forall t > 0, \quad \forall s \in (0, t), \qquad \mathbb{P}(X^x_s \in A, \tau^x_\partial > t) > 0.$$

Proof. Let $x \in D, t > 0, s \in (0,t)$. Let A be an open subset of D, the Markov property at time s ensures that

$$\mathbb{P}(X_s^x \in A, \tau_\partial^x > t) = \mathbb{E}\left[\mathbb{1}_{X_s^x \in A, \tau_\partial^x > s}\mathbb{P}(\tau_\partial^y > t-s)|_{y=X_s^x}\right].$$

By Theorem 2.2.20, which is proven in Sections 2.5 and 2.6, the kernel $\mathrm{P}_s^D(x,\cdot)$ defined in (2.20) admits a positive density function $\mathrm{p}_t^D(x,\cdot)$. Therefore, $\mathbb{P}(X_s^x \in A, \tau_\partial^x > s) > 0$. Again, by the positivity of $\mathrm{p}_{t-s}^D(\cdot,\cdot)$ in Theorem 2.2.20, on the event $\{X_s^x \in A, \tau_\partial^x > s\}$, one has that $\mathbb{P}(\tau_\partial^y > t-s)|_{y=X_s^x} > 0$ almost surely. This concludes the proof using the Markov property stated above. □

Let us now prove Theorem 2.2.14.

Proof of Theorem 2.2.14. Let $x \in D$. Let $(X_t^x = (q_t^x, p_t^x))_{t\geq 0}$ be the strong solution of (2.10) on $\mathbb{R}^{2d}$. For $k > 0$, let V_k be the following open and bounded subset of D

$$V_k := \left\{(q,p) \in D : |p| < k, \mathrm{d}_\partial(q) > \frac{1}{k}\right\}.$$

Let $\tau_{V_k^c}^x$ be the following stopping time:

$$\tau_{V_k^c}^x = \inf\{t > 0 : X_t^x \notin V_k\}.$$

Let $t > 0$ and $s \in [0,t)$. Since $u \in \mathscr{C}^{1,2}(\mathbb{R}_+^* \times D)$, Itô's formula applied to the process $(u(t-r, X_r^x))_{0\leq r\leq s}$ between 0 and $s \wedge \tau_{V_k^c}^x$ yields: almost surely, for $s \in [0,t)$,

$$\begin{aligned} u(t,x) = \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^x > s} u(t-s, X_s^x)\right] + \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^x \leq s} u(t-\tau_{V_k^c}^x, X_{\tau_{V_k^c}^x}^x)\right] \\ + \mathbb{E}\left[\int_0^{s\wedge\tau_{V_k^c}^x} (\partial_t u(t-r, X_r^x) - \mathscr{L}u(t-r, X_r^x))\,\mathrm{d}r\right]. \end{aligned} \tag{2.66}$$

Step 1. Let us prove Assertion (i) in Theorem 2.2.14 using (2.66). It follows from (2.66) and the inequality $\partial_t u - \mathscr{L}u \leq 0$ on $\mathbb{R}_+^* \times D$, that

$$u(t,x) \leq \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^x > s} u(t-s, X_s^x)\right] + \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^x \leq s} u(t-\tau_{V_k^c}^x, X_{\tau_{V_k^c}^x}^x)\right].$$

By assumption, $u \in \mathscr{C}^b((\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^+ \cup \Gamma^0)))$. Therefore, following the same reasoning as in the proof of Assertion (iv) of Theorem 2.2.10 in Section 2.3.1, one obtains by letting $s \to t$ and $k \to \infty$ that

$$u(t,x) \leq \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t} u(0, X_t^x)\right] + \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x < t} u(t-\tau_\partial^x, X_{\tau_\partial^x}^x)\right].$$

Since $X_{\tau_\partial^x}^x \in \Gamma^+$ almost surely by Proposition 2.2.8, the inequality above immediately yields Assertion (i).

Step 2. We now prove Assertion (ii). Applying the equality (2.66) for $(t,x) = (t_0,x_0)$ and subtracting $u(t_0,x_0)$, we obtain that for all $s \in [0,t_0)$,

$$\begin{aligned} 0 = \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^{x_0} > s}\Big(u(t_0-s, X_s^{x_0}) - u(t_0,x_0)\Big)\right] + \mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^{x_0} \leq s}\Big(u(t_0-\tau_{V_k^c}^{x_0}, X_{\tau_{V_k^c}^{x_0}}^{x_0}) - u(t_0,x_0)\Big)\right] \\ + \mathbb{E}\left[\int_0^{s\wedge\tau_{V_k^c}^{x_0}} \Big(\partial_t u(t_0-r, X_r^{x_0}) - \mathscr{L}u(t_0-r, X_r^{x_0})\Big)\mathrm{d}r\right]. \end{aligned}$$

Using the fact that $u(t_0,x_0) = \|u\|_\infty$ and that $\partial_t u - \mathscr{L}u \leq 0$ on $\mathbb{R}_+^* \times D$, it follows that, necessarily, for all $k > 0$ and $s \in [0,t_0)$, (since $\mathbb{1}_{\tau_{V_k^c}^{x_0} > t_0} \leq \mathbb{1}_{\tau_{V_k^c}^{x_0} > s}$)

$$\mathbb{E}\left[\mathbb{1}_{\tau_{V_k^c}^{x_0} > t_0}\Big(u(t_0-s, X_s^{x_0}) - u(t_0,x_0)\Big)\right] = 0.$$

Taking $k \to \infty$ as in the proof of Assertion (iv) of Theorem 2.2.10, one obtains that for all $s \in [0, t_0)$,

$$\mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x_0} > t_0}\left(u(t_0 - s, X_s^{x_0}) - u(t_0, x_0)\right)\right] = 0. \tag{2.67}$$

Assume now that Assertion (ii) is not satisfied, then there exists $c > 0$, $s_0 \in (0, t_0)$ and an open subset A of D such that for all $y \in A$, $u(t_0 - s_0, y) - u(t_0, x_0) \leq -c$. Therefore,

$$\mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x_0} > t_0, X_{s_0}^{x_0} \in A}\left(u(t_0 - s_0, X_{s_0}^{x_0}) - u(t_0, x_0)\right)\right] \leq -c\mathbb{P}\left(\tau_\partial^{x_0} > t_0, X_{s_0}^{x_0} \in A\right) < 0,$$

by Lemma 2.4.4. Moreover,

$$\mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x_0} > t_0}\left(u(t_0 - s_0, X_{s_0}^{x_0}) - u(t_0, x_0)\right)\right] \leq \mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x_0} > t_0, X_{s_0}^{x_0} \in A}\left(u(t_0 - s_0, X_{s_0}^{x_0}) - u(t_0, x_0)\right)\right] < 0,$$

which is in contradiction with (2.67), hence Assertion (ii). □

2.5 Gaussian upper bound and existence of a smooth transition density for the absorbed Langevin process

The proof of the Gaussian upper bound stated in Theorem 2.2.19 is provided in Section 2.5.1. Section 2.5.2 is devoted to the proof of the existence of a smooth transition density for the absorbed Langevin process from Definition 2.2.5, and the fact that this density satisfies the backward and forward Kolmogorov equations. This yields the first part of Theorem 2.2.20, the boundary continuity will be proved in Section 2.6. Section 2.5.3 is devoted to the study of some preliminary boundary continuity properties of the transition density for the absorbed Langevin process (2.10) which will be useful in Section 2.6.

2.5.1 Gaussian upper bound for the Langevin process in $\mathbb{R}^d$

The purpose of this Section is to provide a Gaussian upper bound satisfied by the transition density $\mathrm{p}_t(x, y)$ of the process $(X_t^x = (q_t^x, p_t^x))_{t\geq 0}$ defined by (2.10) under Assumption (F2). We do not consider absorption in this section.

For $x = (q, p) \in \mathbb{R}^{2d}$, let $(\widehat{X}_t^x = (\widehat{q}_t^x, \widehat{p}_t^x))_{t\geq 0}$ be the strong solution on $\mathbb{R}^{2d}$ of the following SDE

$$\begin{cases} \mathrm{d}\widehat{q}_t^x = \widehat{p}_t^x \mathrm{d}t, \\ \mathrm{d}\widehat{p}_t^x = -\gamma \widehat{p}_t^x \mathrm{d}t + \sigma \mathrm{d}B_t, \\ (\widehat{q}_0^x, \widehat{p}_0^x) = x, \end{cases} \tag{2.68}$$

with infinitesimal generator $\widehat{\mathscr{L}} := \mathscr{L}_{0,\gamma,\sigma}$. Let Φ_1, Φ_2 be the following positive continuous functions on $\mathbb{R}$:

$$\Phi_1 : \rho \in \mathbb{R} \mapsto \begin{cases} \frac{1 - \mathrm{e}^{-\rho}}{\rho} & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0, \end{cases} \tag{2.69}$$

$$\Phi_2 : \rho \in \mathbb{R} \mapsto \begin{cases} \frac{3}{2\rho^3}\left[2\rho - 3 + 4\mathrm{e}^{-\rho} - \mathrm{e}^{-2\rho}\right] & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0. \end{cases} \tag{2.70}$$

The process $(\widehat{q}_t^x, \widehat{p}_t^x)_{t\geq 0}$ is Gaussian and for all $t \geq 0$, the vector $(\widehat{q}_t^x, \widehat{p}_t^x)$ admits the following law

$$\begin{pmatrix} \widehat{q}_t^x \\ \widehat{p}_t^x \end{pmatrix} \sim \mathscr{N}_{2d}\left(\begin{pmatrix} m_q^x(t) \\ m_p^x(t) \end{pmatrix}, C(t)\right), \tag{2.71}$$

where the mean vector is

$$m_q^x(t) := q + tp\Phi_1(\gamma t), \qquad m_p^x(t) := p\mathrm{e}^{-\gamma t},$$

and the covariance matrix is

$$C(t) := \begin{pmatrix} c_{qq}(t)I_d & c_{qp}(t)I_d \\ c_{qp}(t)I_d & c_{pp}(t)I_d \end{pmatrix},$$

where I_d is the identity matrix in $\mathbb{R}^{d\times d}$ and

$$c_{qq}(t) := \frac{\sigma^2 t^3}{3}\Phi_2(\gamma t), \qquad c_{qp}(t) := \frac{\sigma^2 t^2}{2}\Phi_1(\gamma t)^2, \qquad c_{pp}(t) := \sigma^2 t \Phi_1(2\gamma t). \tag{2.72}$$

The determinant of the covariance matrix $C(t)$ is $\det(C(t)) = (\frac{\sigma^4 t^4}{12}\phi(\gamma t))^d$ where ϕ is the positive continuous function defined by

$$\phi : \rho \in \mathbb{R} \mapsto 4\Phi_2(\rho)\Phi_1(2\rho) - 3\Phi_1(\rho)^4 = \begin{cases} \frac{6(1-\mathrm{e}^{-\rho})}{\rho^4}\left[-2+\rho+(2+\rho)\mathrm{e}^{-\rho}\right] & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0. \end{cases} \tag{2.73}$$

As a result, one can easily obtain an explicit expression of the transition density $\widehat{\mathrm{p}}_t((q,p),(q',p'))$ of the process $(\widehat{q}_t^x, \widehat{p}_t^x)_{t\geq 0}$: for $t>0$, $(q,p),(q',p') \in \mathbb{R}^{2d}$,

$$\widehat{\mathrm{p}}_t((q,p),(q',p')) := \frac{1}{\sqrt{(2\pi)^{2d}\left(\frac{\sigma^4 t^4}{12}\phi(\gamma t)\right)^d}}\mathrm{e}^{-\frac{\delta x(t)\cdot C^{-1}(t)\delta x(t)}{2}} \tag{2.74}$$

where

$$\delta x(t) := \begin{pmatrix} \delta q(t) \\ \delta p(t) \end{pmatrix} := \begin{pmatrix} q' - m_q^x(t) \\ p' - m_p^x(t) \end{pmatrix}, \qquad C^{-1}(t) = \frac{1}{\frac{\sigma^4 t^4}{12}\phi(\gamma t)}\begin{pmatrix} c_{pp}(t)I_d & -c_{qp}(t)I_d \\ -c_{qp}(t)I_d & c_{qq}(t)I_d \end{pmatrix}. \tag{2.75}$$

We now give a useful rewriting of $\delta x \cdot C^{-1}(t)\delta x$ as a sum of squares, inspired by [75, Equation 2.5], using an additional function positive continuous function on $\mathbb{R}$:

$$\Phi_3 : \rho \in \mathbb{R} \mapsto \begin{cases} \frac{2(1-\Phi_1(\rho))}{\rho} & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0. \end{cases} \tag{2.76}$$

Lemma 2.5.1 (Covariance decomposition)**.** *For all $t > 0$, $\delta x = \begin{pmatrix} \delta q \\ \delta p \end{pmatrix} \in \mathbb{R}^{2d}$,*

$$\delta x \cdot C^{-1}(t)\delta x = \frac{1}{\sigma^2 t}\left|\Pi_1 \delta x\right|^2 + \frac{12}{\sigma^2 t^3 \phi(\gamma t)}\left|\Pi_2(t)\delta x\right|^2, \tag{2.77}$$

where $\Pi_1 := \begin{pmatrix} \gamma I_d & I_d \end{pmatrix} \in \mathbb{R}^{d\times 2d}$ and $\Pi_2(t) := \begin{pmatrix} \Phi_1(\gamma t)I_d & -\frac{t}{2}\Phi_3(\gamma t)I_d \end{pmatrix} \in \mathbb{R}^{d\times 2d}$.

Proof. On the one hand, from (2.72) and (2.75), easy computations show that

$$\delta x \cdot C^{-1}(t)\delta x = \frac{1}{\frac{\sigma^2 t^3}{12}\phi(\gamma t)}\left[\Phi_1(2\gamma t)|\delta q|^2 - \Phi_1(\gamma t)^2 \delta q \cdot t\delta p + \frac{1}{3}\Phi_2(\gamma t)|t\delta p|^2\right]. \tag{2.78}$$

On the other hand,

$$\begin{aligned} &\frac{1}{\sigma^2 t}\left|\Pi_1 \delta x\right|^2 + \frac{12}{\sigma^2 t^3 \phi(\gamma t)}\left|\Pi_2(t)\delta x\right|^2 \\ &= \frac{1}{\frac{\sigma^2 t^3}{12}\phi(\gamma t)}\left[\left(\frac{(\gamma t)^2}{12}\phi(\gamma t) + \Phi_1(\gamma t)^2\right)|\delta q|^2 + \left(\frac{\gamma t}{6}\phi(\gamma t) - \Phi_1(\gamma t)\Phi_3(\gamma t)\right)\delta q \cdot t\delta p \right. \\ &\qquad \left. + \left(\frac{1}{12}\phi(\gamma t) + \frac{1}{4}\Phi_3(\gamma t)^2\right)|t\delta p|^2\right], \end{aligned}$$

so that the claimed expression follows from the identities

$$\frac{\rho^2}{12}\phi(\rho)+\Phi_1(\rho)^2 = \Phi_1(2\rho), \qquad \frac{\rho}{6}\phi(\rho)-\Phi_1(\rho)\Phi_3(\rho) = -\Phi_1(\rho)^2, \qquad \frac{1}{12}\phi(\rho)+\frac{1}{4}\Phi_3(\rho)^2 = \frac{1}{3}\Phi_2(\rho),$$

for all $\rho \in \mathbb{R}$. □

Now let $\alpha \in (0,1]$. For $x=(q,p), y=(q',p') \in \mathbb{R}^{2d}$ and $t>0$, let $\widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$ be the transition density of the process $(\alpha^{-1/2}\widehat{X}_t^{\sqrt{\alpha}x})_{t\geq 0}$, with infinitesimal generator $\mathscr{L}_{0,\gamma,\sigma/\sqrt{\alpha}}$, i.e.

$$\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')) := \sqrt{\alpha^{2d}}\widehat{\mathrm{p}}_t(\sqrt{\alpha}(q,p),\sqrt{\alpha}(q',p')). \tag{2.79}$$

Let us state the following useful properties.

Lemma 2.5.2 (Transition density properties)**.** *The transition densities* $\widehat{\mathrm{p}}_t$ *and* $\widehat{\mathrm{p}}_t^{(\alpha)}$ *satisfy:*

(i) For all $t>0$, *and* $x=(q,p), y=(q',p') \in \mathbb{R}^{2d}$, *(using the notation (2.75))*

$$\widehat{\mathrm{p}}_t(x,y) = \frac{1}{\sqrt{\alpha^{2d}}}\mathrm{e}^{-\frac{1-\alpha}{2}\delta x(t)\cdot C^{-1}(t)\delta x(t)}\widehat{\mathrm{p}}_t^{(\alpha)}(x,y) \tag{2.80}$$

(ii) Chapman-Kolmogorov relation: For all $t>0$, *for all* $u\in(0,t)$ *and* $x,y\in\mathbb{R}^{2d}$,

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_u^{(\alpha)}(x,z)\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)\mathrm{d}z = \widehat{\mathrm{p}}_t^{(\alpha)}(x,y). \tag{2.81}$$

(iii) For all $t>0$, $\varphi\in\mathscr{C}^b(\mathbb{R}_+\times\mathbb{R}^{2d})$ *and* $y,x_0,y_0\in\mathbb{R}^{2d}$,

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\mathrm{d}x = \mathrm{e}^{d\gamma t} \tag{2.82}$$

and

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\varphi(t,x)\mathrm{d}x \underset{(t,y)\to(0,y_0)}{\longrightarrow} \varphi(0,y_0), \qquad \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\varphi(t,y)\mathrm{d}y \underset{(t,x)\to(0,x_0)}{\longrightarrow} \varphi(0,x_0). \tag{2.83}$$

(iv) For all $\alpha\in(0,1)$, *there exists* $c_\alpha>0$ *depending only on* α *such that for all* $t>0$, $x,y\in\mathbb{R}^{2d}$,

$$|\nabla_p\widehat{\mathrm{p}}_t(x,y)| \leq \frac{c_\alpha(1+\sqrt{\gamma_- t})}{\sqrt{\sigma^2 t}}\widehat{\mathrm{p}}_t^{(\alpha)}(x,y), \tag{2.84}$$

where γ_- *is the negative part of* $\gamma\in\mathbb{R}$.

Proof. The equality (2.80) easily follows from the formulas defining $\widehat{\mathrm{p}}_t$ and $\widehat{\mathrm{p}}_t^{(\alpha)}$. Moreover, since $\widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$ is the transition density of the process $(\alpha^{-1/2}\widehat{X}_t^{\sqrt{\alpha}x})_{t\geq 0}$, the Chapman-Kolmogorov relation (2.81) follows from the Markov property. Let us now prove (2.82). For $\alpha\in(0,1]$,

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\mathrm{d}x = \int_{\mathbb{R}^{2d}} \frac{\sqrt{\alpha^{2d}}}{\sqrt{(2\pi)^{2d}\det(C(t))}}\mathrm{e}^{-\frac{\alpha}{2}\delta x(t)\cdot C^{-1}(t)\delta x(t)}\mathrm{d}x,$$

where $\delta x(t)$ and $C^{-1}(t)$ are defined in (2.75). Let us define the matrix $M(t)$ as follows:

$$M(t) := \begin{pmatrix} I_d & t\Phi_1(\gamma t)I_d \\ 0_d & \mathrm{e}^{-\gamma t}I_d \end{pmatrix}$$

so that for $x=(q,p), y=(q',p')$ one has $M(t)x = \begin{pmatrix} m_q^x(t) \\ m_p^x(t) \end{pmatrix}$. Therefore, $\delta x(t) = y - M(t)x$. As a result, making the following change of variables,

$$x \in \mathbb{R}^{2d} \mapsto z := y - M(t)x$$

one has $\mathrm{d}z = \mathrm{e}^{-d\gamma t}\mathrm{d}x$ and one obtains

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\mathrm{d}x = \mathrm{e}^{d\gamma t} \int_{\mathbb{R}^{2d}} \frac{\sqrt{\alpha^{2d}}}{\sqrt{(2\pi)^{2d}\det(C(t))}} \mathrm{e}^{-\frac{\alpha}{2} z\cdot C^{-1}(t) z}\mathrm{d}z = \mathrm{e}^{d\gamma t}.$$

Let us now prove the first convergence in (2.83). Using the same change of variables as above, one obtains that

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)\varphi(t,x)\mathrm{d}x = \mathrm{e}^{d\gamma t}\mathbb{E}\left[\varphi\left(t, M^{-1}(t)(y - Z(t))\right)\right], \tag{2.85}$$

where $Z(t) \sim \mathscr{N}_{2d}(0, \frac{C(t)}{\alpha}) \xrightarrow[t\to 0]{\mathscr{L}} 0$, since $C(t) \underset{t\to 0}{\longrightarrow} 0_{2d}$. Therefore, since $M(t) \underset{t\to 0}{\longrightarrow} I_{2d}$, one has by Slutsky's theorem that

$$\left(t, M^{-1}(t)(y - Z(t))\right) \xrightarrow[(t,y)\to(0,y_0)]{\mathscr{L}} (0, y_0)$$

which yields the first convergence in (2.83) using (2.85) and the dominated convergence theorem. The second convergence follows easily with a similar change of variables.

Let us finally prove (2.84). By (2.74), (2.75) along with Lemma 2.5.1 we have

$$\frac{\nabla_p \widehat{\mathrm{p}}_t((q,p),(q',p'))}{\widehat{\mathrm{p}}_t((q,p),(q',p'))} = -\frac{1}{2}\left(\frac{2}{\sigma^2 t}\nabla_p\left(\Pi_1\delta x(t)\right)\Pi_1\delta x(t) + \frac{24}{\sigma^2 t^3\phi(\gamma t)}\nabla_p\left(\Pi_2(t)\delta x(t)\right)\Pi_2(t)\delta x(t)\right). \tag{2.86}$$

Since $\nabla_p\Pi_1\delta x(t) = -(\gamma t\Phi_1(\gamma t) + \mathrm{e}^{-\gamma t})I_d = -I_d$, the first term in the right-hand side of the equality (2.86) multiplied by $\widehat{\mathrm{p}}_t$ satisfies (using (2.80), and again Lemma 2.5.1 in the first inequality)

$$\begin{aligned}
&\left|-\frac{1}{2}\frac{2}{\sigma^2 t}\nabla_p\left(\Pi_1\delta x(t)\right)\Pi_1\delta x(t)\right|\widehat{\mathrm{p}}_t((q,p),(q',p')) \\
&= \frac{1}{\sigma^2 t}\left|\Pi_1\delta x(t)\right|\widehat{\mathrm{p}}_t((q,p),(q',p')) \\
&= \frac{1}{\sqrt{\alpha^{2d}}\sigma^2 t}\left|\Pi_1\delta x(t)\right|\mathrm{e}^{-\frac{1-\alpha}{2}\delta x(t)\cdot C^{-1}(t)\delta x(t)}\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')) \\
&\leq \frac{1}{\sqrt{\alpha^{2d}}\sigma^2 t}\left|\Pi_1\delta x(t)\right|\mathrm{e}^{-\frac{1-\alpha}{2\sigma^2 t}|\Pi_1\delta x(t)|^2}\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')) \\
&\leq \frac{\sup_{\theta\geq 0}\theta\mathrm{e}^{-\frac{1-\alpha}{2}\theta^2}}{\sqrt{\alpha^{2d}}\sigma\sqrt{t}}\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')).
\end{aligned} \tag{2.87}$$

Let us now estimate the second term in the right-hand side of the equality (2.86) multiplied by $\widehat{\mathrm{p}}_t$. Since $\nabla_p\Pi_2(t)\delta x(t) = (-t\Phi_1(\gamma t)^2 + \frac{t}{2}\Phi_3(\gamma t)\mathrm{e}^{-\gamma t})I_d$, we have (using the same reasoning as above)

$$\begin{aligned}
&\left|-\frac{1}{2}\frac{24}{\sigma^2 t^3\phi(\gamma t)}\nabla_p\left(\Pi_2(t)\delta x(t)\right)\Pi_2(t)\delta x(t)\right|\widehat{\mathrm{p}}_t((q,p),(q',p')) \\
&= \frac{12t}{\sigma^2 t^3\phi(\gamma t)}\left|-\Phi_1(\gamma t)^2 + \frac{1}{2}\Phi_3(\gamma t)\mathrm{e}^{-\gamma t}\right|\left|\Pi_2(t)\delta x(t)\right|\widehat{\mathrm{p}}_t((q,p),(q',p')) \\
&\leq \frac{\sqrt{12}t}{\sqrt{\alpha^{2d}\sigma^2 t^3\phi(\gamma t)}}\left|-\Phi_1(\gamma t)^2 + \frac{1}{2}\Phi_3(\gamma t)\mathrm{e}^{-\gamma t}\right|\frac{\sqrt{12}\left|\Pi_2(t)\delta x(t)\right|}{\sqrt{\sigma^2 t^3\phi(\gamma t)}}\mathrm{e}^{-\frac{12(1-\alpha)}{2\sigma^2 t^3\phi(\gamma t)}|\Pi_2(t)\delta x(t)|^2}\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')) \\
&\leq \frac{\sqrt{12}}{\sqrt{\alpha^{2d}}\sigma\sqrt{t}}\frac{\left|-\Phi_1(\gamma t)^2 + \frac{1}{2}\Phi_3(\gamma t)\mathrm{e}^{-\gamma t}\right|}{\sqrt{\phi(\gamma t)}}\left(\sup_{\theta\geq 0}\theta\mathrm{e}^{-\frac{1-\alpha}{2}\theta^2}\right)\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')).
\end{aligned} \tag{2.88}$$

Let us now study the behavior of $\frac{|-\Phi_1(\rho)^2+\frac{1}{2}\Phi_3(\rho)e^{-\rho}|}{\sqrt{\phi(\rho)}}$ for $\rho \in \mathbb{R}$. We have that

$$\frac{\left|-\Phi_1(\rho)^2 + \frac{1}{2}\Phi_3(\rho)e^{-\rho}\right|}{\sqrt{\phi(\rho)}} \begin{cases} \underset{\rho\to\infty}{\sim} \dfrac{1}{\sqrt{6}\rho}, \\ \underset{\rho\to 0}{\longrightarrow} \dfrac{1}{2}, \\ \underset{\rho\to-\infty}{\sim} \dfrac{\sqrt{|\rho|}}{\sqrt{6}}. \end{cases}$$

Therefore there exists a universal constant $c > 0$ such that for all $\rho \in \mathbb{R}$

$$\frac{\left|-\Phi_1(\rho)^2 + \frac{1}{2}\Phi_3(\rho)e^{-\rho}\right|}{\sqrt{\phi(\rho)}} \le c(1 + \sqrt{\rho_-}),$$

where ρ_- is the negative part of ρ. As a result, it follows from (2.86), (2.87) and (2.88) that there exists a constant $c_\alpha > 0$ depending only on $\alpha \in (0,1)$ such that for all $t > 0$ and $x, y \in \mathbb{R}^{2d}$,

$$\left|\nabla_p \widehat{\mathrm{p}}_t((q,p),(q',p'))\right| \le \frac{c_\alpha}{\sigma\sqrt{t}}(1 + \sqrt{t\gamma_-})\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p')),$$

which concludes the proof of (2.84). □

We are now in position to prove Theorem 2.2.19.

Proof of Theorem 2.2.19. The idea is to first establish a mild formulation of the difference between the two transition densities $\mathrm{p}_t(x,y)$ and $\widehat{\mathrm{p}}_t(x,y)$, adapting the reasoning from [52]. Secondly, iterating the obtained equality, one obtains, following the steps of [52], an expression of the difference between $\mathrm{p}_t(x,y)$ and $\widehat{\mathrm{p}}_t(x,y)$ in the form of a series, which then yields the Gaussian upper bound stated in Theorem 2.2.19.

Step 1. Let us first obtain the mild formulation linking $\mathrm{p}_t(x,y)$ and $\widehat{\mathrm{p}}_t(x,y)$. Let $T > 0$ and $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Then the function

$$\Phi : (t,(q,p)) \in [0,T) \times \mathbb{R}^{2d} \mapsto \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_{T-t}((q,p),y)\varphi(y)\mathrm{d}y,$$

is in $\mathscr{C}^\infty([0,T) \times \mathbb{R}^{2d})$ by the Lebesgue derivation theorem. Besides, it satisfies $\partial_t\Phi + \widehat{\mathscr{L}}\Phi = 0$ using the backward Kolmogorov equation satisfied by $\widehat{\mathrm{p}}_t(x,y)$ (see Proposition 2.2.17). As a result, the Itô formula ensures that for all $x \in \mathbb{R}^{2d}$, $t \in [0,T)$,

$$\Phi(t, X_t^x) = \underbrace{\Phi(0,x)}_{\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_T(x,y)\varphi(y)\mathrm{d}y} + \int_0^t \underbrace{(\mathscr{L} - \widehat{\mathscr{L}})\Phi(u, X_u^x)}_{F(q_u^x)\cdot\nabla_p\Phi(u,X_u^x)}\mathrm{d}u + \sigma\int_0^t \nabla_p\Phi(u,X_u^x)\cdot \mathrm{d}B_u. \quad (2.89)$$

Besides, one has for $u \in [0,t]$, $(q,p) \in \mathbb{R}^{2d}$,

$$\nabla_p\Phi(u,(q,p)) = \int_{\mathbb{R}^{2d}} \nabla_p\widehat{\mathrm{p}}_{T-u}((q,p),y)\varphi(y)\mathrm{d}y.$$

Let $\alpha \in (0,1)$. It follows from Lemma 2.5.2 that there exist $C_1, C_2 > 0$ depending only on $\alpha, \sigma, \gamma, T$ such that for all $t \in [0,T)$, $u \in [0,t]$, (q,p) and y in $\mathbb{R}^{2d}$,

$$|\nabla_p\widehat{\mathrm{p}}_{T-u}((q,p),y)| \le \frac{C_1}{\sqrt{T-u}}\widehat{\mathrm{p}}_{T-u}^{(\alpha)}((q,p),y) \le \frac{C_2}{(T-t)^{2d+1/2}\phi(\gamma(T-u))^{d/2}}. \quad (2.90)$$

Therefore $\nabla_p\Phi$ is bounded on $[0,t] \times \mathbb{R}^{2d}$ and the integrand of the last term in the right-hand side of the equality (2.89) is bounded, which implies that its expectation vanishes.

Furthermore, using the Fubini-Tonnelli theorem along with (2.90), one gets

$$\mathbb{E}\left(\int_{\mathbb{R}^{2d}} |F(q_u^x)|\,|\nabla_p \widehat{\mathrm{p}}_{T-u}(X_u^x,y)|\,|\varphi(y)|\mathrm{d}y\right) \leq \frac{C_1\|\varphi\|_\infty\|F\|_\infty}{\sqrt{T-u}}\mathbb{E}\Bigg(\underbrace{\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}^{(\alpha)}_{T-u}(X_u^x,y)\mathrm{d}y}_{=1}\Bigg), \tag{2.91}$$

which is integrable on $[0,T)$. Consequently,

$$\mathbb{E}\left(\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_{T-t}(X_t^x,y)\varphi(y)\mathrm{d}y\right) = \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_T(x,y)\varphi(y)\mathrm{d}y + \int_0^t\int_{\mathbb{R}^{2d}} \mathbb{E}\left(F(q_u^x)\cdot\nabla_p\widehat{\mathrm{p}}_{T-u}(X_u^x,y)\right)\varphi(y)\mathrm{d}y\mathrm{d}u. \tag{2.92}$$

It follows from Lemma 2.5.2 that $\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_{T-t}(X_t^x,y)\varphi(y)\mathrm{d}y$ converges almost surely to $\varphi(X_T^x)$ when t converges to T. By considering the limit $t\to T$ (using the dominated convergence theorem in the term in the left-hand side of (2.92)), one obtains from (2.92) and (2.91) that for all $x\in\mathbb{R}^{2d}$,

$$\begin{aligned}\int_{\mathbb{R}^{2d}} \mathrm{p}_T(x,y)\varphi(y)\mathrm{d}y &= \mathbb{E}\left(\varphi(X_T^x)\right)\\ &= \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_T(x,y)\varphi(y)\mathrm{d}y + \int_0^T\int_{\mathbb{R}^{2d}} \mathbb{E}\left(F(q_u^x)\cdot\nabla_p\widehat{\mathrm{p}}_{T-u}(X_u^x,y)\varphi(y)\right)\mathrm{d}y\mathrm{d}u\\ &= \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_T(x,y)\varphi(y)\mathrm{d}y + \int_0^T\int_{\mathbb{R}^{2d}}\int_{\mathbb{R}^{2d}} \mathrm{p}_u(x,(q,p))F(q)\cdot\nabla_p\widehat{\mathrm{p}}_{T-u}((q,p),y)\varphi(y)\mathrm{d}q\mathrm{d}p\mathrm{d}y\mathrm{d}u.\end{aligned}$$

Since this is satisfied for all $T>0$ and $\varphi\in\mathscr{C}_c^\infty(\mathbb{R}^d)$, then by continuity of the transition density, one obtains that for all $t>0$ and $x,y\in\mathbb{R}^{2d}$,

$$\mathrm{p}_t(x,y)-\widehat{\mathrm{p}}_t(x,y) = \int_0^t\int_{\mathbb{R}^{2d}} \mathrm{p}_u(x,(q,p))F(q)\cdot\nabla_p\widehat{\mathrm{p}}_{t-u}((q,p),y)\mathrm{d}q\mathrm{d}p\mathrm{d}u$$

which is a mild formulation of the Fokker-Planck equation associated with (2.10).

In order to rewrite this mild formulation, let us define the following kernel H for $t>0$, (q,p) and y in $\mathbb{R}^{2d}$,

$$\mathrm{H}(t,(q,p),y) := F(q)\cdot\nabla_p\widehat{\mathrm{p}}_t((q,p),y).$$

For $t>0$, x,y in $\mathbb{R}^{2d}$, let us define $\mathrm{p}\otimes\mathrm{H}(t,x,y)$ by

$$(\mathrm{p}\otimes\mathrm{H})(t,x,y) = \int_0^t\int_{\mathbb{R}^{2d}} \mathrm{p}_u(x,z)\mathrm{H}(t-u,z,y)\mathrm{d}z\mathrm{d}u. \tag{2.93}$$

The mild formulation can thus be rewritten: for all $t>0$ and $x,y\in\mathbb{R}^{2d}$,

$$\mathrm{p}_t(x,y)-\widehat{\mathrm{p}}_t(x,y) = \mathrm{p}\otimes\mathrm{H}(t,x,y). \tag{2.94}$$

We notice that $(\mathrm{p}\otimes\mathrm{H})\otimes\mathrm{H} = \mathrm{p}\otimes(\mathrm{H}\otimes\mathrm{H})$, which allows us to define univocally $\mathrm{H}^{(k)} = \underbrace{\mathrm{H}\otimes\cdots\otimes\mathrm{H}}_{k\text{ times}}$. Besides, iterating r times the equality (2.94) we get

$$\mathrm{p}_t(x,y) = \widehat{\mathrm{p}}_t(x,y) + \sum_{j=1}^r \widehat{\mathrm{p}}\otimes\mathrm{H}^{(j)}(t,x,y) + \mathrm{p}\otimes\mathrm{H}^{(r+1)}(t,x,y). \tag{2.95}$$

Step 2. Let us prove that the series $\sum_{j=1}^\infty \widehat{\mathrm{p}}\otimes\mathrm{H}^{(j)}(t,x,y)$ converges by getting upper bounds on $\widehat{\mathrm{p}}\otimes\mathrm{H}^{(j)}$ for $j\geq 1$. Let $\alpha\in(0,1)$. By Lemma 2.5.2, there exists $c_\alpha>0$ such that for all $t>0$,

$x, y \in \mathbb{R}^{2d}$, $|\mathrm{H}(t,x,y)| \leq \|F\|_\infty \frac{c_\alpha(1+\sqrt{\gamma_- t})}{\sqrt{\sigma^2 t}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$. Therefore, for a fixed $T>0$, for all $t \in (0,T]$ and $x, y \in \mathbb{R}^{2d}$,

$$|\mathrm{H}(t,x,y)| \leq \frac{C_3}{\sqrt{t}} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y) \text{ where } C_3 := \|F\|_\infty \frac{c_\alpha(1+\sqrt{\gamma_- T})}{\sigma}. \tag{2.96}$$

Besides, for $u \in (0,t)$ and $t \in (0,T]$, $x,z,y \in \mathbb{R}^{2d}$, one has from (2.96), since $\widehat{\mathrm{p}}_t(x,y) \leq \alpha^{-d}\widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$ (from (2.80)), that

$$|\widehat{\mathrm{p}}_u(x,z)\mathrm{H}(t-u,z,y)| \leq \frac{C_3}{\alpha^d} \widehat{\mathrm{p}}_u^{(\alpha)}(x,z) \frac{\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)}{\sqrt{t-u}}.$$

For $m,n>0$, let $B(m,n) := \int_0^1 u^{m-1}(1-u)^{n-1}\mathrm{d}u = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}$, with Γ the Gamma function. Therefore, for $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$, by the Chapman-Kolmogorov relation (2.81),

$$\begin{aligned}|(\widehat{\mathrm{p}} \otimes \mathrm{H})(t,x,y)| &= \left| \int_0^t \int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}_u(x,z)\mathrm{H}(t-u,z,y)\mathrm{d}z\mathrm{d}u \right| \\ &\leq \frac{C_3}{\alpha^d} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y) t^{\frac{1}{2}} B\left(1, \frac{1}{2}\right).\end{aligned}$$

By induction, for all $j \geq 1$,

$$|\widehat{\mathrm{p}} \otimes \mathrm{H}^{(j)}(t,x,y)| \leq \frac{C_3^j}{\alpha^d} \widehat{\mathrm{p}}_t^{(\alpha)}(x,y) t^{\frac{j}{2}} \prod_{l=1}^j B\left(\frac{l+1}{2}, \frac{1}{2}\right). \tag{2.97}$$

Consequently, since $\prod_{l=1}^j B\left(\frac{l+1}{2}, \frac{1}{2}\right) = \frac{\sqrt{\pi}^j}{\Gamma(\frac{j+2}{2})}$ it is easy to see from the Stirling formula that for all $t>0$, $x, y \in \mathbb{R}^{2d}$, the series $\sum_{j=1}^\infty \widehat{\mathrm{p}} \otimes \mathrm{H}^{(j)}(t,x,y)$ converges absolutely.

Step 3. Let us now prove that $\mathrm{p} \otimes \mathrm{H}^{(r+1)}(t,x,y) \underset{r\to\infty}{\longrightarrow} 0$ for all $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$. By (2.96) and the Chapman-Kolmogorov relation (2.81), we have for all $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$

$$|\mathrm{H} \otimes \mathrm{H}(t,x,y)| \leq C_3^2 B\left(\frac{1}{2}, \frac{1}{2}\right) \widehat{\mathrm{p}}_t^{(\alpha)}(x,y).$$

By induction, for all $j \geq 2$, for all $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$,

$$|\mathrm{H}^{(j)}(t,x,y)| \leq C_3^j \widehat{\mathrm{p}}_t^{(\alpha)}(x,y) t^{\frac{j}{2}-1} \frac{\sqrt{\pi}^{j-1}}{\Gamma(\frac{j+1}{2})}. \tag{2.98}$$

As a consequence,

$$|\mathrm{p} \otimes \mathrm{H}^{(r+1)}(t,x,y)| \leq C_3^{r+1} \frac{\sqrt{\pi}^{r+1}}{\Gamma(\frac{r+3}{2})} \int_0^t \int_{\mathbb{R}^{2d}} \mathrm{p}_u(x,z) \widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)(t-u)^{\frac{r-1}{2}} \mathrm{d}z\mathrm{d}u.$$

From the expression of $\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)$ it follows that there exists $C_4>0$ depending only on α, γ, σ such that

$$\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)(t-u)^{\frac{r-1}{2}} \leq \frac{C_4(t-u)^{\frac{r-1}{2}}}{(t-u)^{2d}\phi(\gamma(t-u))^{d/2}}.$$

Let us choose $r \geq 4d+1$. Since ϕ is positive and continuous then it is bounded from below for $s \in (-|\gamma|T, |\gamma|T)$, therefore there exists $C_5>0$ depending on $\alpha, \gamma, \sigma, d$ and T such that for all $t \in (0,T)$, $r \geq 4d+1$, $u \in (0,t)$ and $z, y \in \mathbb{R}^{2d}$,

$$\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z,y)(t-u)^{\frac{r-1}{2}} \leq C_5.$$

Therefore, for all $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$,

$$|\mathrm{p} \otimes \mathrm{H}^{(r+1)}(t,x,y)| \leq C_3^{r+1} C_5 T B\left(\frac{1}{2},\frac{1}{2}\right) B\left(1,\frac{1}{2}\right) \cdots B\left(\frac{r}{2},\frac{1}{2}\right) \underset{r\longrightarrow\infty}{\longrightarrow} 0.$$

Step 4. As a result, using the results of Step 2 and 3 in the equality (2.95) we get for all $t \in (0,T]$, $x, y \in \mathbb{R}^{2d}$,

$$\mathrm{p}_t(x,y) - \widehat{\mathrm{p}}_t(x,y) = \sum_{j=1}^{\infty} \widehat{\mathrm{p}} \otimes \mathrm{H}^{(j)}(t,x,y).$$

From the formula defining C_3 in (2.96) and (2.97), the inequality (2.19) follows. □

Remark 2.5.3. *In view of the proof of Theorem 2.2.19, it is clear that (2.19) holds for F only bounded (dropping the assumptions that F is $\mathscr{C}^\infty$ and globally Lipschitz continuous in Assumption (F2)), as soon as there exists a weak solution to (2.10). Gaussian upper bounds for the Langevin process thus hold under slightly more general assumptions than those originally stated in [52].*

2.5.2 Existence of a smooth transition density for the absorbed Langevin process

Proposition 2.5.4 (Existence of a measurable transition density)**.** *Under Assumption (F1), there exists a measurable function*

$$(t,x,y) \in \mathbb{R}_+^* \times D \times D \mapsto \mathrm{p}_t^D(x,y)$$

such that for all $t > 0$ and $x \in D$, the kernel $\mathrm{P}_t^D(x,\cdot)$, defined in (2.20), has the density $\mathrm{p}_t^D(x,\cdot)$ with respect to the Lebesgue measure on D.

Proof. For all $t > 0$ and $x \in D$, it follows from (2.21) that the measure $\mathrm{P}_t^D(x,\cdot)$ is absolutely continuous with respect to the measure $\mathrm{P}_t(x,\cdot)$. Since, by Proposition 2.2.17, the latter measure is absolutely continuous with respect to the Lebesgue measure, by the Radon-Nikodym theorem, we deduce that $\mathrm{P}_t^D(x,\cdot)$ possesses a density $\mathrm{q}_t^D(x,\cdot)$ with respect to the Lebesgue measure on D. We now study the joint measurability of the mapping $(t,x,y) \mapsto \mathrm{q}_t^D(x,y)$; more precisely, we construct a measurable function $(t,x,y) \mapsto \mathrm{p}_t^D(x,y)$ such that, for all $t > 0$ and $x \in D$, $\mathrm{p}_t^D(x,y) = \mathrm{q}_t^D(x,y)$, $\mathrm{d}y$-almost everywhere on D.

For all $r > 0$, it follows from Proposition 2.2.17 and Lemmata 2.3.1 and 2.3.2 that the function

$$\varphi_r : (t,x,y) \in \mathbb{R}_+^* \times D \times D \mapsto \frac{\mathrm{P}_t^D(x, \mathrm{B}(y,r) \cap D)}{|\mathrm{B}(y,r)|} = \frac{\mathbb{P}(|X_t^x - y| < r, \tau_\partial^x > t)}{|\mathrm{B}(y,r)|}$$

is continuous. Let $(r_q)_{q\geq 1}$ be a sequence of positive real numbers decreasing towards 0. By definition, for any $t > 0$ and $x \in D$, the density $\mathrm{q}_t^D(x,\cdot)$ is integrable on D. As a result, the Lebesgue differentiation theorem states that almost every $y \in D$ is a Lebesgue point, hence

$$\forall t > 0, \quad \forall x \in D, \qquad \varphi_{r_q}(t,x,y) \underset{q\longrightarrow\infty}{\longrightarrow} \mathrm{q}_t^D(x,y) \quad \mathrm{d}y\text{-almost everywhere on } D.$$

As a consequence, $\mathrm{q}_t^D(x,y)$ coincides, $\mathrm{d}y$-almost everywhere, with the measurable function

$$\mathrm{p}_t^D(x,y) := \limsup_{q\to\infty} \varphi_{r_q}(t,x,y),$$

which completes the proof. □

Let us now prove that this transition density $\mathrm{p}_t^D(x,y)$ is smooth on $\mathbb{R}_+^* \times D \times D$. This will be managed by first showing that it is a distributional solution of the backward and forward Kolmogorov equations. The smoothness of p_t^D will then follow from the hypoellipticity of the differential operators $\partial_t - \mathscr{L}$ and $\partial_t - \mathscr{L}^*$, see Definition 2.2.4. This scheme of proof is inspired from [63, Section 3.5]. Notice that Proposition 2.5.4 only defines the transition density on $\mathbb{R}_+^* \times D \times D$. The extension to a continuous function on $\mathbb{R}_+^* \times \overline{D} \times \overline{D}$ will be done in Section 2.6 (see Theorem 2.6.3).

Proposition 2.5.5 (Kolmogorov equations)**.** *Under Assumption (F1), the transition density* $(t,x,y) \mapsto \mathrm{p}_t^D(x,y)$ *is a* $\mathscr{C}^\infty(\mathbb{R}_+^* \times D \times D)$ *function. Besides it satisfies the backward and forward Kolmogorov equations:*

(i) $(t,x) \mapsto \mathrm{p}_t^D(x,y)$ *is a solution of* $\partial_t \mathrm{p}^D = \mathscr{L}_x \mathrm{p}^D$ *on* $\mathbb{R}_+^* \times D$*,*

(ii) $(t,y) \mapsto \mathrm{p}_t^D(x,y)$ *is a solution of* $\partial_t \mathrm{p}^D = \mathscr{L}_y^* \mathrm{p}^D$ *on* $\mathbb{R}_+^* \times D$*.*

Proof. Let $\Phi \in \mathscr{C}_c^\infty(\mathbb{R}_+^* \times D)$. Notice that Φ can be extended by zero to a $\mathscr{C}^\infty(\mathbb{R}_+ \times \overline{D})$ function. Let $(X_t^x = (q_t^x, p_t^x))_{t\geq 0}$ be the process satisfying (2.10). Using Itô's formula, one gets for all $x \in D$ and $t > 0$,

$$\Phi(t, X_t^x) = \underbrace{\Phi(0,x)}_{=0} + \int_0^t \left[\partial_s \Phi(s, X_s^x) + \mathscr{L}\Phi(s, X_s^x)\right] \mathrm{d}s + \sigma \int_0^t \nabla_p \Phi(s, X_s^x) \cdot \mathrm{d}B_s.$$

Thus,

$$\Phi(\tau_\partial^x \wedge t, X_{\tau_\partial^x \wedge t}^x) = \int_0^t \mathbb{1}_{\tau_\partial^x > s} \left[\partial_s \Phi(s, X_s^x) + \mathscr{L}\Phi(s, X_s^x)\right] \mathrm{d}s + \sigma \int_0^{\tau_\partial^x \wedge t} \underbrace{\nabla_p \Phi(s, X_s^x)}_{\text{bounded}} \cdot \mathrm{d}B_s.$$

As a result, the stochastic integral in the right-hand side is a martingale. Taking the expectation, we get

$$\mathbb{E}\left[\Phi(\tau_\partial^x \wedge t, X_{\tau_\partial^x \wedge t}^x)\right] = \int_0^t \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > s} \left(\partial_s \Phi(s, X_s^x) + \mathscr{L}\Phi(s, X_s^x)\right)\right] \mathrm{d}s.$$

Since $X_{\tau_\partial^x}^x \in \partial D$ and Φ vanishes on $\mathbb{R}_+ \times \partial D$,

$$\mathbb{E}\left[\Phi(\tau_\partial^x \wedge t, X_{\tau_\partial^x \wedge t}^x)\right] = \mathbb{E}[\mathbb{1}_{\tau_\partial^x > t}\Phi(t, X_t^x) + \mathbb{1}_{\tau_\partial^x \leq t} \underbrace{\Phi(\tau_\partial^x, X_{\tau_\partial^x}^x)}_{=0}] = \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t}\Phi(t, X_t^x)\right].$$

Thus

$$\mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t}\Phi(t, X_t^x)\right] = \int_0^t \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > s} \left(\partial_s \Phi(s, X_s^x) + \mathscr{L}\Phi(s, X_s^x)\right)\right] \mathrm{d}s.$$

For t large enough since Φ has a compact support on $\mathbb{R}_+^* \times D$, the left-hand side in the equality above is zero. Therefore,

$$\iint_{\mathbb{R}_+^* \times D} \left(\partial_s \Phi(s,y) + \mathscr{L}\Phi(s,y)\right) \mathrm{p}_s^D(x,y) \mathrm{d}s \mathrm{d}y = 0.$$

As a result for all $x \in D$,

$$(t,y) \in \mathbb{R}_+^* \times D \mapsto \mathrm{p}_t^D(x,y)$$

is a distributional solution of

$$\partial_t \mathrm{p}_t^D = \mathscr{L}_y^* \mathrm{p}_t^D$$

on $\mathbb{R}_+^* \times D$. Since the operator $\partial_t - \mathscr{L}^*$ is hypoelliptic one has that

$$(t,y) \in \mathbb{R}_+^* \times D \mapsto \mathrm{p}_t^D(x,y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D), \tag{2.99}$$

which proves the forward Kolmogorov equation.

We now address the backward Kolmogorov equation. Let $\Phi_1 \in \mathscr{C}_c^\infty(\mathbb{R}_+^* \times D)$, $\Phi_2 \in \mathscr{C}_c^\infty(D)$, and let us define the function Φ as follows: for all $(t,x,y) \in \mathbb{R}_+^* \times D \times D$,

$$\Phi(t,x,y) = \Phi_1(t,x)\Phi_2(y).$$

Let us compute the following integral

$$I = \iiint_{\mathbb{R}_+^* \times D \times D} \mathrm{p}_t^D(x,y) \left(\partial_t \Phi(t,x,y) + \mathscr{L}_x^* \Phi(t,x,y)\right) \mathrm{d}t\mathrm{d}x\mathrm{d}y$$
$$= \iint_{\mathbb{R}_+^* \times D} \left(\partial_t \Phi_1(t,x) + \mathscr{L}_x^* \Phi_1(t,x)\right) \left(\int_D \mathrm{p}_t^D(x,y)\Phi_2(y)\mathrm{d}y\right) \mathrm{d}t\mathrm{d}x.$$

On the one hand, since $(t,x) \mapsto \int_D \mathrm{p}_t^D(x,y)\Phi_2(y)\mathrm{d}y = \mathbb{E}[\mathbb{1}_{\tau_\partial^x > t}\Phi_2(X_t^x)]$ is a solution of $\partial_t u = \mathscr{L}_x u$ by Theorem 2.2.10, then $I = 0$. On the other hand, it follows from Fubini's theorem that

$$\int_D \Phi_2(y) \left(\iint_{\mathbb{R}_+^* \times D} \mathrm{p}_t^D(x,y) \left(\partial_t \Phi_1(t,x) + \mathscr{L}_x^* \Phi_1(t,x)\right) \mathrm{d}t\mathrm{d}x\right) \mathrm{d}y = 0.$$

Since $y \in D \mapsto \iint_{\mathbb{R}_+^* \times D} \mathrm{p}_t^D(x,y) \left(\partial_t \Phi_1(t,x) + \mathscr{L}_x^* \Phi_1(t,x)\right) \mathrm{d}t\mathrm{d}x \in \mathrm{L}_1^{\mathrm{loc}}(D)$ (since $\Phi_1 \in \mathscr{C}_c^\infty(\mathbb{R}_+^* \times D)$), this ensures that for almost every $y \in D$,

$$\iint_{\mathbb{R}_+^* \times D} \mathrm{p}_t^D(x,y) \left(\partial_t \Phi_1(t,x) + \mathscr{L}_x^* \Phi_1(t,x)\right) \mathrm{d}t\mathrm{d}x = 0.$$

Using the continuity of $y \in D \mapsto \mathrm{p}_t^D(x,y)$ from (2.99), the equality above remains true for all $y \in D$. Thus, for all $y \in D$, $(t,x) \mapsto \mathrm{p}_t^D(x,y)$ is a distributional solution of the backward Kolmogorov equation

$$\partial_t \mathrm{p}_t^D = \mathscr{L}_x \mathrm{p}_t^D$$

on $\mathbb{R}_+^* \times D$.

Consequently, the hypoellipticity of $\partial_t - \mathscr{L}$ on the open set $\mathbb{R}_+^* \times D$ ensures that for all $y \in D$

$$(t,x) \in \mathbb{R}_+^* \times D \mapsto \mathrm{p}_t^D(x,y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D).$$

Therefore, using (2.99), it follows that

$$(t,x,y) \in \mathbb{R}_+^* \times D \times D \mapsto \mathrm{p}_t^D(x,y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D \times D),$$

which concludes the proof of Proposition 2.5.5. □

Corollary 2.2.21 shows that the Gaussian upper bound on the transition density p_t immediately transfers to the transition density p_t^D. In fact, in the next lemma, we show that the latter also satisfies a mild formulation of the form

$$\mathrm{p}_t^D - \widehat{\mathrm{p}}_t = \mathrm{p}^D \otimes \mathrm{H}^D, \tag{2.100}$$

for some kernel H^D, and compute estimates on this kernel to obtain an asymptotic expansion of p_t^D in compact sets of D. This lemma will be useful in Section 2.6.

Lemma 2.5.6 (Local asymptotic expansion around $t = 0$)**.** *Under Assumption (F1), the density* p_t^D *is such that for all compact sets* $K \subset D$, $T > 0$ *and* $\alpha \in (0,1)$, *there exists* $C > 0$ *such that for all* $x, y \in K$ *and* $t \in (0,T)$,

$$\left|\mathrm{p}_t^D(x,y) - \widehat{\mathrm{p}}_t(x,y)\right| \leq C\sqrt{t}\,\widehat{\mathrm{p}}_t^{(\alpha)}(x,y). \tag{2.101}$$

Proof. Since the density p_t^D only depends on the values of F in $\mathscr{O}$ (see Remark 2.2.6), we can assume that F satisfies Assumption (F2) for the sake of simplicity. The first step of the proof consists in establishing the mild formulation (2.100). In contrast with the proof of Theorem 2.2.19, where a mild formulation of the forward Kolmogorov equation satisfied by p_t is established, the absorbing boundary condition makes the use of the Itô formula inappropriate. We adopt a different approach, inspired from [52, Proposition 2.2].

Let $T > 0$ and $K \subset D$ be a compact set. Let $x = (q, p)$, $y = (q', p') \in K$ and $t \in (0, T]$. Let us define $\varphi \in \mathscr{C}_c^\infty(D)$ such that

$$0 \leq \varphi(z) \leq 1 \text{ for all } z \in D, \text{ and } \varphi(z) = 1 \text{ for all } z \in K. \tag{2.102}$$

Let us define the function h_t as follows:

$$h_t : u \in (0, t) \mapsto \int_D \mathrm{p}_u^D(x, z)\widehat{\mathrm{p}}_{t-u}(z, y)\varphi(z)\mathrm{d}z.$$

Let us identify the limits of $h_t(u)$ when $u \to 0$ and $u \to t$. First we have that

$$h_t(u) = \mathbb{E}\left[\widehat{\mathrm{p}}_{t-u}(X_u^x, y)\varphi(X_u^x)\mathbb{1}_{\tau_\partial^x > u}\right] \underset{u\to 0}{\longrightarrow} \widehat{\mathrm{p}}_t(x, y)\varphi(x) = \widehat{\mathrm{p}}_t(x, y),$$

by the dominated convergence theorem using Lemma 2.3.2 and the continuity and boundedness of $\widehat{\mathrm{p}}_s(\cdot, y)\varphi(\cdot)$ when s is close to t. Second, it follows from the convergence (2.83) in Lemma 2.5.2 and the boundedness and continuity of the product $\mathrm{p}_u^D(x, \cdot)\varphi(\cdot)$ when u is close to t that (remember that $y \in K$)

$$h_t(u) \underset{u\to t}{\longrightarrow} \mathrm{p}_t^D(x, y)\varphi(y) = \mathrm{p}_t^D(x, y).$$

Therefore, using the fact that $h_t \in \mathscr{C}^1((0, t))$, we have that

$$\begin{aligned}
\mathrm{p}_t^D(x, y) - \widehat{\mathrm{p}}_t(x, y) &= \int_0^t \frac{\mathrm{d}h_t}{\mathrm{d}u}(u)\mathrm{d}u \\
&= \int_0^t \int_D \left(\partial_u[\mathrm{p}_u^D(x, z)]\widehat{\mathrm{p}}_{t-u}(z, y) + \mathrm{p}_u^D(x, z)\partial_u[\widehat{\mathrm{p}}_{t-u}(z, y)]\right)\varphi(z)\mathrm{d}z\mathrm{d}u,
\end{aligned}$$

by the Lebesgue derivation theorem as $\mathrm{p}_t^D(x, y)$, $\widehat{\mathrm{p}}_t(x, y)$ are smooth on $\mathbb{R}_+^* \times D \times D$ and $\varphi \in \mathscr{C}_c^\infty(D)$.

Recall that we denote by $\widehat{\mathscr{L}} = \mathscr{L}_{0,\gamma,\sigma}$ the infinitesimal generator of $(\widehat{X}_t^x)_{t\geq 0}$. Since $\partial_t \mathrm{p}_t^D(x, y) = \mathscr{L}_y^* \mathrm{p}_t^D(x, y)$ (see Theorem 2.2.20) and $\partial_t \widehat{\mathrm{p}}_t(x, y) = \widehat{\mathscr{L}}_x \widehat{\mathrm{p}}_t(x, y)$ (see Proposition 2.2.17), one has (using the notation $\mathrm{d}z = \mathrm{d}q''\mathrm{d}p''$ in $\mathbb{R}^{2d}$),

$$\begin{aligned}
\mathrm{p}_t^D(x, y) - \widehat{\mathrm{p}}_t(x, y) &= \int_0^t \int_D \left(\mathscr{L}_z^* \mathrm{p}_u^D(x, z)\widehat{\mathrm{p}}_{t-u}(z, y) - \mathrm{p}_u^D(x, z)\widehat{\mathscr{L}_z}\widehat{\mathrm{p}}_{t-u}(z, y)\right)\varphi(z)\mathrm{d}z\mathrm{d}u \\
&= \int_0^t \int_D \mathrm{p}_u^D(x, z)\left(\mathscr{L}_z\left(\widehat{\mathrm{p}}_{t-u}(z, y)\varphi(z)\right) - \widehat{\mathscr{L}_z}(\widehat{\mathrm{p}}_{t-u}(z, y))\varphi(z)\right)\mathrm{d}z\mathrm{d}u \\
&= \int_0^t \int_D \mathrm{p}_u^D(x, z)\left[\left(\mathscr{L}_z - \widehat{\mathscr{L}_z}\right)(\widehat{\mathrm{p}}_{t-u}(z, y))\varphi(z) + \sigma^2 \nabla_{p''}\widehat{\mathrm{p}}_{t-u}(z, y) \cdot \nabla_{p''}\varphi(z)\right]\mathrm{d}z\mathrm{d}u \\
&\quad + \int_0^t \int_D \mathrm{p}_u^D(x, z)\widehat{\mathrm{p}}_{t-u}(z, y)\mathscr{L}_z\varphi(z)\mathrm{d}z\mathrm{d}u,
\end{aligned}$$

which is the claimed mild formulation (2.100). For $z = (q'', p'') \in \mathbb{R}^{2d}$, $\mathscr{L}_z - \widehat{\mathscr{L}_z} = F(q'') \cdot \nabla_{p''}$. Furthermore, $\varphi \in \mathscr{C}_c^\infty(D)$, therefore its gradient is bounded on D and $\mathscr{L}\varphi \in \mathscr{C}_c^\infty(D)$. Besides, it follows from (2.84) in Lemma 2.5.2 that for any $\alpha \in (0, 1)$ there exists $C_1 > 0$ such that for all $t \in (0, T]$, $u \in [0, t)$ and $(q'', p''), y \in \mathbb{R}^{2d}$,

$$|\nabla_{p''}\widehat{\mathrm{p}}_{t-u}((q'', p''), y)| \leq \frac{C_1}{\sqrt{t-u}}\widehat{\mathrm{p}}_{t-u}^{(\alpha)}((q'', p''), y).$$

In addition, from (2.80), $\widehat{\mathrm{p}}_t(x, y) \leq \alpha^{-d}\widehat{\mathrm{p}}_t^{(\alpha)}(x, y)$ for all $t > 0$, $x, y \in \mathbb{R}^{2d}$. Consequently, under Assumption (F2), there exists a constant $C_K > 0$ such that

$$\left|\mathrm{p}_t^D(x, y) - \widehat{\mathrm{p}}_t(x, y)\right| \leq C_K \int_0^t \int_D \mathrm{p}_u^D(x, z)\frac{\widehat{\mathrm{p}}_{t-u}^{(\alpha)}(z, y)}{\sqrt{t-u}}\mathrm{d}z\mathrm{d}u.$$

Furthermore, by Corollary 2.2.21 there exists $C_2 > 0$ such that for all $u \in (0,t)$, $t \in (0,T)$, $\mathrm{p}^D_u(x,y) \le \mathrm{p}_u(x,y) \le C_2\widehat{\mathrm{p}}^{(\alpha)}_u(x,y)$. Hence the existence of $C'_K > 0$ such that for all $t \in (0,T)$ and $x, y \in K$,

$$\left|\mathrm{p}^D_t(x,y) - \widehat{\mathrm{p}}_t(x,y)\right| \le C'_K \int_0^t \int_D \widehat{\mathrm{p}}^{(\alpha)}_u(x,z)\frac{\widehat{\mathrm{p}}^{(\alpha)}_{t-u}(z,y)}{\sqrt{t-u}}\mathrm{d}z\mathrm{d}u$$
$$\le C'_K\sqrt{t}\widehat{\mathrm{p}}^{(\alpha)}_t(x,y)\int_0^1 \frac{\mathrm{d}s}{\sqrt{1-s}},$$

since $\widehat{\mathrm{p}}^{(\alpha)}_t$ satisfies the Chapman-Kolmogorov relation (2.81) in Lemma 2.5.2. This concludes the proof of (2.101). □

2.5.3 Boundary behavior of the transition density

The purpose of this subsection is to study the behavior of $\mathrm{p}^D_t(x,y)$ at the boundaries $(t,x) \in \mathbb{R}^*_+ \times (\Gamma^+ \cup \Gamma^0)$ and $(t,y) \in \mathbb{R}^*_+ \times \Gamma^-$ (see Proposition 2.5.7 below). This result will be useful for the proof of Theorem 2.6.2, which will then allow to complete the proof of Theorem 2.2.20.

Proposition 2.5.7 (Boundary limits)**.** *Let Assumptions (O1) and (F1) hold. Let $t_0 > 0$, $x_0 \in \Gamma^+ \cup \Gamma^0$ and $y_0 \in \Gamma^-$. Let $(t_n, x_n, y_n)_{n\ge1}$ be a sequence of points in $\mathbb{R}^*_+ \times D \times D$ converging towards (t_0, x_0, y_0), then one has the following convergences:*

(i) For all $y \in D$, $\mathrm{p}^D_{t_n}(x_n, y) \underset{n\to\infty}{\longrightarrow} 0$.

(ii) For all $x \in D$, $\mathrm{p}^D_{t_n}(x, y_n) \underset{n\to\infty}{\longrightarrow} 0$.

The proof of this proposition relies partly on the following lemma which is shown at the end of this subsection.

Lemma 2.5.8. *Let $y_0 \in \mathbb{R}^{2d}$, $M > 0$ and $\alpha \in (0,1)$. There exist $C_0 > 0$, $\mu > 0$, $\delta_0 > 0$ such that for all $s \in (0,\delta_0]$, $(q',p') \in \mathrm{B}(y_0, M/6)$ and $(q,p) \in \mathbb{R}^{2d}$ satisfying $|p-p'| \ge M/3$,*

$$\widehat{\mathrm{p}}^{(\alpha)}_s((q,p),(q',p')) \le C_0 \exp(-\mu/s). \tag{2.103}$$

Proof of Proposition 2.5.7. Since the density p^D_t only depends on the values of F in $\mathscr{O}$ (see Remark 2.2.6), we can assume that F satisfies Assumption (F2) for the sake of simplicity.

Both proofs of (i) and (ii) rely on the elementary remark that, for any $t > 0$ and $x \in D$, since the function $y \mapsto \mathrm{p}^D_t(x,y)$ is continuous on D, we have for any $y \in D$,

$$\mathrm{p}^D_t(x,y) = \lim_{h\to0} \frac{\mathrm{P}^D_t(x, D\cap \mathrm{B}(y,h))}{|\mathrm{B}(y,h)|}. \tag{2.104}$$

Notice that, here and in the sequel, we take the intersection of $\mathrm{B}(y,h)$ with D because $\mathrm{P}^D_t(x,\cdot)$ is defined as a measure on $\mathscr{B}(D)$.

Proof of (i). Let $t_0 > 0$, $x_0 \in \Gamma^+ \cup \Gamma^0$. Let $(t_n, x_n)_{n\ge1}$ be a sequence of points in $\mathbb{R}^*_+ \times D$ converging towards (t_0, x_0). Let $N \ge 1$ be such that, for any $n \ge N$, $t_0/2 \le t_n \le 3t_0/2$. For any $n \ge N$, $h > 0$ and $y \in D$, the Markov property shows that

$$\mathrm{P}^D_{t_n/2}(x_n, D\cap\mathrm{B}(y,h)) = \mathbb{E}\left[\mathbb{1}_{\tau^{x_n}_\partial > t_n/2}\mathrm{P}^D_{t_n/2}(X^{x_n}_{t_n/2}, D\cap\mathrm{B}(y,h))\right].$$

Besides, by Corollary 2.2.21, there exists a constant $C \ge 0$ which depends on t_0 such that for any $n \ge N$, the transition density $\mathrm{p}^D_{t_n/2}$ is uniformly bounded on $D \times D$ by C, therefore

$$\frac{\mathrm{P}^D_{t_n/2}(x_n, D\cap\mathrm{B}(y,h))}{|\mathrm{B}(y,h)|} \le C\mathbb{P}(\tau^{x_n}_\partial > t_n/2).$$

The right-hand side no longer depends on h and vanishes when $n \to +\infty$ by Lemma 2.3.2 and Proposition 2.2.8, therefore by (2.104) we get Assertion (i).

Remark 2.5.9. *The proof shows that the convergence of Assertion (i) is actually uniform in y, that is to say* $\sup_{y\in D} \mathrm{p}^D_{t_n}(x_n, y) \underset{n\to\infty}{\longrightarrow} 0$.

Proof of (ii). The proof of (ii) needs more work. Let $x \in D$, $t_0 > 0$ and $y_0 = (q_0, p_0) \in \Gamma^-$. Let $(t_n, y_n)_{n\geq 1}$, with $y_n := (q_n, p_n)$, be a sequence of points in $\mathbb{R}^*_+ \times D$ converging towards (t_0, y_0). In order to prove the convergence $\mathrm{p}^D_{t_n}(x, y_n) \underset{n\to\infty}{\longrightarrow} 0$, it is enough by (2.104) to prove the following double limit

$$\lim_{n\to\infty} \lim_{h\to 0} \frac{\mathrm{P}^D_{t_n}(x, D\cap \mathrm{B}(y_n, h))}{|\mathrm{B}(y_n, h)|} = 0. \tag{2.105}$$

Let us define for $0 \leq r \leq t$ the following modulus of continuity

$$Z^x_{r,t} := \sup_{r\leq s\leq t} |p^x_s - p^x_t|.$$

For two constants $\delta \in (0, t_0/2]$ and $M > 0$ to be fixed later on, let us rewrite the numerator in (2.105) as follows: for n sufficiently large so that $t_n \geq t_0/2$ (and thus $t_n - \delta \geq 0$),

$$\begin{aligned}\mathrm{P}^D_{t_n}(x, D\cap \mathrm{B}(y_n, h)) &= \mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), \tau^x_\partial > t_n)\\ &= \mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M, \tau^x_\partial > t_n)\\ &\quad + \mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} > M, \tau^x_\partial > t_n).\end{aligned} \tag{2.106}$$

The idea of the proof of (2.105) relies on the decomposition in (2.106) and is divided into two steps. In **Step 1**, we consider the probability corresponding to the first term in the right-hand side of the equality (2.106). We show that there is a value of M and a $\delta_1 \in (0, t_0/2]$ such that, for all $\delta \in (0, \delta_1]$, there exist $N_1 \geq 1$ and $h_1 > 0$ such that for any $n \geq N_1$ and $h \leq h_1$, the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M, \tau^x_\partial > t_n\}$ has probability 0. Indeed, for n large and h small the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h)\}$ implies that $(q^x_{t_n}, p^x_{t_n})$ is "close" to $y_0 \in \Gamma^-$ which is a boundary point with inward velocity. Therefore, using our control on the modulus of continuity of the velocity, we can prove the existence of a time $s \in (0, t_n)$ such that (q^x_s, p^x_s) is outside of D, which contradicts the fact that $\tau^x_\partial > t_n$.

In **Step 2**, we consider the second term in the right-hand side of the equality (2.106), divided by $|\mathrm{B}(y_n, h)|$. For the value of M determined in **Step 1**, we show the existence of $\delta_2 \in (0, t_0/2]$ and $C, \mu > 0$ such that, for all $\delta \in (0, \delta_2]$, there exist $N_2 \geq 1$ and $h_2 > 0$ such that, for any $n \geq N_2$ and $h \leq h_2$,

$$\frac{\mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} > M)}{|\mathrm{B}(y_n, h)|} \leq C\mathrm{e}^{-\frac{\mu}{\delta}}. \tag{2.107}$$

As a result, the two steps yield the following inequality

$$\limsup_{n\to\infty} \limsup_{h\to 0} \frac{\mathrm{P}^D_{t_n}(x, D\cap \mathrm{B}(y_n, h))}{|\mathrm{B}(y_n, h)|} \leq C\mathrm{e}^{-\frac{\mu}{\delta}}$$

for any $\delta \in (0, \delta_1 \wedge \delta_2]$, then taking $\delta \to 0$ we are able to conclude the proof of (2.105).

Step 1. Let us prove here that one can fix $M > 0$ and choose $\delta > 0$ small enough such that the first term in the right-hand side of the equality (2.106) vanishes for n sufficiently large and h sufficiently small. Let us remind the reader that, since $\mathscr{O}$ is a $\mathscr{C}^2$ bounded set of $\mathbb{R}^d$, it satisfies the exterior sphere condition, see Section 2.3.4.1. Therefore, for $\eta > 0$, there exists $c_0 := c_0(\eta) > 0$ such that if $q \in \mathbb{R}^d$ satisfies $(q - q_0)\cdot n(q_0) \geq \eta|q - q_0|$ and $|q - q_0| \leq c_0$ then $q \notin \mathscr{O}$. Now let $M := -\frac{p_0\cdot n(q_0)}{3}$ which is positive because $y_0 = (q_0, p_0) \in \Gamma^-$. Let $\eta := \frac{M}{2M+|p_0|}$ and $c_0 := c_0(\eta)$ as defined above.

Let $\delta_1 := \frac{t_0}{2} \wedge \frac{c_0}{2M+|p_0|}$. We fix $\delta \in (0, \delta_1]$ and define $h_1 := \frac{\delta M}{2(1+\delta)}$. Remembering that $t_n \underset{n\to\infty}{\longrightarrow} t_0$ and $y_n \underset{n\to\infty}{\longrightarrow} y_0$ we can choose $N_1 \geq 1$ such that for $n \geq N_1$,

$$t_n \in [t_0/2, 3t_0/2] \quad \text{and} \quad y_n = (q_n, p_n) \in \mathrm{B}\left(y_0, \frac{\delta M}{2(1+\delta)}\right).$$

Let $n \geq N_1$ and $h \in (0, h_1]$. Notice that

$$\mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M, \tau^x_\partial > t_n) \leq \mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M, q^x_{t_n-\delta} \in \mathscr{O}).$$

Therefore, the first term in (2.106) vanishes if one can prove that $q^x_{t_n-\delta} \notin \mathscr{O}$ on the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M\}$. By (2.10), one has that

$$q^x_{t_n} = q^x_{t_n-\delta} + \int_{t_n-\delta}^{t_n} p^x_s \mathrm{d}s.$$

Therefore,

$$q^x_{t_n-\delta} = q^x_{t_n} - \delta p^x_{t_n} - \int_{t_n-\delta}^{t_n} (p^x_s - p^x_{t_n}) \mathrm{d}s.$$

Let

$$v^x_{t_n} := q^x_{t_n-\delta} - \left(q_0 - \delta p_0 - \int_{t_n-\delta}^{t_n} (p^x_s - p^x_{t_n})\mathrm{d}s\right) = q^x_{t_n} - q_0 - \delta\left(p^x_{t_n} - p_0\right).$$

As a result, on the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h)\}$, the triangle inequality ensures that

$$\begin{aligned}|v^x_{t_n}| &\leq |q^x_{t_n} - q_n| + |q_n - q_0| + \delta|p^x_{t_n} - p_n| + \delta|p_n - p_0| \\ &\leq |X^x_{t_n} - y_n|(1+\delta) + |y_n - y_0|(1+\delta) \\ &\leq h(1+\delta) + \frac{\delta M}{2(1+\delta)}(1+\delta) \leq \delta M,\end{aligned}$$

by definition of N_1 and h_1. Consequently, we have on the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M\}$,

$$(q^x_{t_n-\delta} - q_0)\cdot n(q_0) = \underbrace{-\delta p_0 \cdot n(q_0)}_{=3\delta M} + \underbrace{\int_{t_n-\delta}^{t_n} (p^x_{t_n} - p^x_s)\cdot n(q_0)\mathrm{d}s}_{|\cdot|\leq \delta M} + \underbrace{v^x_{t_n}\cdot n(q_0)}_{|\cdot|\leq\delta M} \geq \delta M.$$

Furthermore, on the event $\{q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} \leq M\}$,

$$\begin{aligned}\left|q^x_{t_n-\delta} - q_0\right| &= \left|-\delta p_0 - \int_{t_n-\delta}^{t_n}(p^x_s - p^x_{t_n})\mathrm{d}s + v^x_{t_n}\right| \\ &\leq \delta(|p_0| + 2M).\end{aligned}$$

As a result, since $(q^x_{t_n-\delta} - q_0)\cdot n(q_0) \geq \delta M \geq \eta|q^x_{t_n-\delta} - q_0|$ and $|q^x_{t_n-\delta} - q_0| \leq \delta(|p_0| + 2M) \leq c_0$, the exterior sphere condition ensures that $q^x_{t_n-\delta} \notin \mathscr{O}$.

Step 2. Let $M > 0$ be defined as in **Step 1**. We fix a value of $\alpha \in (0,1)$, let $C_0, \mu, \delta_0 > 0$ be given by Lemma 2.5.8 and define $\delta_2 := \delta_0 \wedge (t_0/2)$. We now let $\delta \in (0, \delta_2]$, define $N_2 \geq 1$ be such that for any $n \geq N_2$, $|y_n - y_0| \leq M/12$, and finally set $h_2 := M/12$.

Let $n \geq N_2$, $h \in (0, h_2]$ and define the following stopping time

$$\tau^{(\delta)}_n := \inf\{s \geq t_n - \delta : |p^x_s - p_0| \geq M/2\}.$$

On the event $\{(q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} > M\}$, one has by the triangle inequality

$$\sup_{t_n-\delta\leq s\leq t_n} |p^x_s - p_0| \geq \sup_{t_n-\delta\leq s\leq t_n} |p^x_s - p^x_{t_n}| - |p^x_{t_n} - p_n| - |p_n - p_0| \geq M - h - \frac{M}{12} \geq \frac{5M}{6} > \frac{M}{2},$$

by the definitions of N_2 and h_2. Therefore, $\tau^{(\delta)}_n \leq t_n$ and

$$\mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), Z^x_{t_n-\delta,t_n} > M) \leq \mathbb{P}((q^x_{t_n}, p^x_{t_n}) \in \mathrm{B}(y_n, h), \tau^{(\delta)}_n < t_n),$$

since $\mathbb{P}(\tau_n^{(\delta)} = t_n) \leq \mathbb{P}(|p_{t_n}^x - p_0| = M/2) = 0$ because $p_{t_n}^x$ admits a density on $\mathbb{R}^d$ with respect to the Lebesgue measure by Proposition 2.2.17.

Therefore, applying the strong Markov property at $\tau_n^{(\delta)}$, one has

$$\frac{\mathbb{P}((q_{t_n}^x, p_{t_n}^x) \in \mathrm{B}(y_n, h), Z_{t_n-\delta, t_n}^x > M)}{|\mathrm{B}(y_n, h)|} \leq \mathbb{E}\left[\mathbb{1}_{\tau_n^{(\delta)} < t_n} \frac{\mathbb{P}\left((q_{t_n-r}^z, p_{t_n-r}^z) \in \mathrm{B}(y_n, h)\right)\Big|_{z=\left(q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x\right), r=\tau_n^{(\delta)}}}{|\mathrm{B}(y_n, h)|}\right] \tag{2.108}$$

Let $s_n := t_n - \tau_n^{(\delta)}$. On the event $\{\tau_n^{(\delta)} < t_n\}$, one has $s_n \in (0, \delta]$ and

$$\mathbb{P}\left((q_{t_n-r}^z, p_{t_n-r}^z) \in \mathrm{B}(y_n, h)\right)\Big|_{z=\left(q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x\right), r=\tau_n^{(\delta)}} = \int_{\mathrm{B}(y_n,h)} \mathrm{p}_{s_n}((q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x), y')\mathrm{d}y'. \tag{2.109}$$

Besides, since $s_n \leq \delta$ and $\delta \leq t_0/2$, one has by Theorem 2.2.19 that there exists $C' > 0$ depending only on α and t_0, but not on n, such that for any $y' \in \mathrm{B}(y_n, h)$,

$$\mathrm{p}_{s_n}((q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x), y') \leq C' \widehat{\mathrm{p}}_{s_n}^{(\alpha)}((q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x), y'). \tag{2.110}$$

It now follows from the definition of N_2 and h_2 that $\mathrm{B}(y_n, h) \subset \mathrm{B}(y_0, M/6)$ and, from the continuity of the trajectories of $(p_t^x)_{t\geq 0}$, one has almost surely that $|p_{\tau_n^{(\delta)}}^x - p_0| \geq M/2$ so that for any $y' \in \mathrm{B}(y_n, h)$,

$$\left|p_{\tau_n^{(\delta)}}^x - p'\right| \geq \left|p_{\tau_n^{(\delta)}}^x - p_0\right| - \left|p_0 - p'\right| \geq M/2 - M/6 \geq M/3.$$

These estimates allow to apply Lemma 2.5.8 and deduce that, on the event $\{\tau_n^{(\delta)} < t_n\}$,

$$\widehat{\mathrm{p}}_{s_n}^{(\alpha)}((q_{\tau_n^{(\delta)}}^x, p_{\tau_n^{(\delta)}}^x), y') \leq C_0 \exp(-\mu/s_n) \leq C_0 \exp(-\mu/\delta),$$

which, combined with (2.108–2.110), concludes to (2.107). □

It remains now to prove Lemma 2.5.8.

Proof of Lemma 2.5.8. Let $y_0 = (q_0, p_0) \in \mathbb{R}^{2d}$, $M > 0$ and $\alpha \in (0, 1)$. Let $\delta_0 > 0$ be small enough for the assertion

$$\forall s \in (0, \delta_0], \qquad \left(\frac{M}{6} + |p_0|\right) |\mathrm{e}^{\gamma s} - 1| \leq \frac{M}{12} \tag{2.111}$$

to hold.

Let $(q', p') \in \mathrm{B}(y_0, M/6)$ and $(q, p) \in \mathbb{R}^{2d}$ satisfying $|p - p'| \geq M/3$. For $s \in (0, \delta_0]$, we consider the transition density $\widehat{\mathrm{p}}_s^{(\alpha)}((q, p), (q', p'))$ defined in (2.79).

One has that

$$\begin{aligned} &\widehat{\mathrm{p}}_s^{(\alpha)}((q, p), (q', p')) \\ &= \frac{\sqrt{\alpha^{2d}}}{\sqrt{(2\pi)^{2d}\left(\frac{\sigma^4 s^4}{12}\phi(\gamma s)\right)^d}} \mathrm{e}^{-\frac{\alpha}{2\sigma^2 s}|\gamma\delta q + \delta p|^2 - \frac{6\alpha}{\sigma^2 s^3 \phi(\gamma s)}\left|\Phi_1(\gamma s)\delta q - \frac{s}{2}\Phi_3(\gamma s)\delta p\right|^2}, \end{aligned} \tag{2.112}$$

where

$$\begin{pmatrix} \delta q \\ \delta p \end{pmatrix} = \begin{pmatrix} q' - q - s\Phi_1(\gamma s)p \\ p' - p\mathrm{e}^{-\gamma s} \end{pmatrix}.$$

Let us start by introducing some notations. Let $m := 1 + |\gamma|\delta_0 + \sup_{|\rho|\leq|\gamma|\delta_0} \frac{|\rho|}{2}\Phi_3(\rho)$ and $a := \frac{M\mathrm{e}^{-|\gamma|\delta_0}}{4m}$. Let us prove that necessarily

$$|\gamma\delta q + \delta p| \geq a \quad \text{or} \quad \left|\Phi_1(\gamma s)\delta q - \frac{s}{2}\Phi_3(\gamma s)\delta p\right| \geq as, \tag{2.113}$$

then reinjecting this statement onto the expression (2.112) of $\widehat{\mathrm{p}}_s^{(\alpha)}((q,p),(q',p'))$ we will be able to obtain (2.103).

Assume now that

$$|\gamma\delta q + \delta p| < a \quad \text{and} \quad \left|\Phi_1(\gamma s)\delta q - \frac{s}{2}\Phi_3(\gamma s)\delta p\right| < as,$$

we will prove that $\left|p' - p\right| < M/3$, thus contradicting the initial assumption on (q,p) and (q',p').

Using the triangle inequality, since $\Phi_1(\rho) + \frac{\rho}{2}\Phi_3(\rho) = 1$ for all $\rho \in \mathbb{R}$, one has that

$$\begin{aligned}\left|\delta q\right| &= \left|\delta q\left(\Phi_1(\gamma s) + \frac{\gamma s}{2}\Phi_3(\gamma s)\right)\right| \\ &\leq \left|\delta q\Phi_1(\gamma s) - \frac{s}{2}\Phi_3(\gamma s)\delta p\right| + \frac{s}{2}\Phi_3(\gamma s)\left|\gamma\delta q + \delta p\right| \\ &< a\left(s + \frac{s}{2}\Phi_3(\gamma s)\right).\end{aligned}$$

As a result,

$$\left|\delta p\right| \leq \left|\gamma\delta q + \delta p\right| + |\gamma|\left|\delta q\right| < a\left(1 + |\gamma|s + \frac{|\gamma|s}{2}\Phi_3(\gamma s)\right).$$

Since $s \leq \delta_0$, one obtains that $\left|\delta p\right| < am$. Therefore $\left|\delta p\right| < \frac{M\mathrm{e}^{-|\gamma|\delta_0}}{4}$. Furthermore, by the triangle inequality, for $(q',p') \in \mathrm{B}(y_0, M/6)$,

$$\begin{aligned}\left|p' - p\right| &\leq \mathrm{e}^{\gamma s}\underbrace{\left|p' - p\mathrm{e}^{-\gamma s}\right|}_{=\left|\delta p\right|} + \left|p' - p_0\right|\left|\mathrm{e}^{\gamma s} - 1\right| + \left|p_0\right|\left|\mathrm{e}^{\gamma s} - 1\right| \\ &< \mathrm{e}^{|\gamma|\delta_0}\frac{M\mathrm{e}^{-|\gamma|\delta_0}}{4} + \frac{M}{6}\left|\mathrm{e}^{\gamma s} - 1\right| + \left|p_0\right|\left|\mathrm{e}^{\gamma s} - 1\right| \\ &\leq \frac{M}{4} + \left(\frac{M}{6} + |p_0|\right)|\mathrm{e}^{\gamma s} - 1| \\ &\leq \frac{M}{4} + \frac{M}{12} = \frac{M}{3},\end{aligned}$$

by (2.111) since $s \leq \delta_0$, hence (2.113).

Reinjecting the inequality (2.113) into (2.112), we get

$$\widehat{\mathrm{p}}_s^{(\alpha)}((q,p),(q',p')) \leq \frac{\sqrt{\alpha^{2d}}}{\sqrt{(2\pi)^{2d}(\frac{\sigma^4 s^4}{12}\phi(\gamma s))^d}}\exp\left(-\frac{1}{s}\min\left(\frac{a^2\alpha}{2\sigma^2}, \frac{6a^2\alpha}{\sigma^2\phi(\gamma s)}\right)\right),$$

and using the fact that $\phi(\gamma s)$ is a positive and bounded continuous function for $s \in [-|\gamma|\delta_0, |\gamma|\delta_0]$, it follows that there exist some constants $C_0 \geq 0$ and $\mu > 0$, which only depend on γ, σ, M, α and δ_0, such that for any $s \in (0, \delta_0]$,

$$\widehat{\mathrm{p}}_s^{(\alpha)}((q,p),(q',p')) \leq C_0\mathrm{e}^{-\mu/s},$$

which completes the proof. □

Remark 2.5.10. *A formal conditioning argument shows that, for $x, y \in D$,*

$$\begin{aligned}\mathrm{p}_t^D(x,y) &= \lim_{h\to 0} \frac{\mathbb{P}(X_t^x \in \mathrm{B}(y,h), \tau_\partial^x > t)}{|\mathrm{B}(y,h)|} \\ &= \lim_{h\to 0} \frac{\mathbb{P}(\tau_\partial^x > t | X_t^x \in \mathrm{B}(y,h))\mathbb{P}(X_t^x \in \mathrm{B}(y,h))}{|\mathrm{B}(y,h)|} \\ &= \mathbb{P}(\tau_\partial^x > t | X_t^x = y)\mathrm{p}_t(x,y),\end{aligned}$$

so that Proposition 2.5.7 should amount to studying the limiting behavior, when x or y respectively approach Γ^+ or Γ^-, of the probability that the diffusion bridge associated with (2.10) between x and y remain in D. With this interpretation at hand, both convergence results (i) and (ii) become very intuitive, and they seem to be the time-reversal statement of each other — a point which will be clarified with the introduction of the adjoint process, and the proof of the reversibility relation (2.119), in the next section.

Our proof of Proposition 2.5.7, and in particular of (ii) can be related to the work on diffusion bridges, of Chaumont and Uribe-Bravo in [22] where they obtain a formal characterization of the $h \to 0$ limit of such an expression as $\mathbb{P}(\tau_\partial^x > t | X_t^x \in \mathrm{B}(y,h))$. However, it is unclear to us how to obtain Proposition 2.5.7 using directly their results.

2.6 Reversibility and compactness properties for the absorbed Langevin process

In this section we define the "adjoint" Langevin process, which is later shown to be closely related to the Langevin process, through a reversibility result linking both transition densities of the respective absorbed processes. This result is useful for being able to describe precisely the boundary behavior of p_t^D.

2.6.1 Reversibility

Let $x = (q,p) \in \mathbb{R}^{2d}$. Let us call the "adjoint" Langevin process the diffusion process $(\widetilde{X}_t^x = (\widetilde{q}_t^x, \widetilde{p}_t^x))_{t\geq 0}$ with infinitesimal generator $\widetilde{\mathscr{L}} := \mathscr{L}^* - d\gamma$ (see (2.9) for the definition of $\mathscr{L}^*$), satisfying the following SDE:

$$\begin{cases} \mathrm{d}\widetilde{q}_t^x = -\widetilde{p}_t^x \mathrm{d}t, \\ \mathrm{d}\widetilde{p}_t^x = -F(\widetilde{q}_t^x)\mathrm{d}t + \gamma \widetilde{p}_t^x \mathrm{d}t + \sigma \mathrm{d}B_t, \\ (\widetilde{q}_0^x, \widetilde{p}_0^x) = x. \end{cases} \tag{2.114}$$

Let $\widetilde{\tau}_\partial^x$ be the first exit time from D of $(\widetilde{X}_t^x)_{t\geq 0}$, i.e.

$$\widetilde{\tau}_\partial^x = \inf\{t > 0 : \widetilde{X}_t^x \notin D\}.$$

Let $y := (q,-p)$. Let us now define the process $(\widetilde{X}_t^{\diamond,y} = (\widetilde{q}_t^{\diamond,y}, \widetilde{p}_t^{\diamond,y}))_{t\geq 0} := (\widetilde{q}_t^x, -\widetilde{p}_t^x)_{t\geq 0}$, it is easy to see that it satisfies the following SDE

$$\begin{cases} \mathrm{d}\widetilde{q}_t^{\diamond,y} = \widetilde{p}_t^{\diamond,y} \mathrm{d}t, \\ \mathrm{d}\widetilde{p}_t^{\diamond,y} = F(\widetilde{q}_t^{\diamond,y})\mathrm{d}t + \gamma \widetilde{p}_t^{\diamond,y} \mathrm{d}t + \sigma \mathrm{d}B_t^\diamond, \\ (\widetilde{q}_0^{\diamond,y}, \widetilde{p}_0^{\diamond,y}) = (q,-p) = y, \end{cases} \tag{2.115}$$

where $(B_t^\diamond)_{t\geq 0} = (-B_t)_{t\geq 0}$ is a Brownian motion on $\mathbb{R}^d$. Its infinitesimal generator therefore writes

$$\widetilde{\mathscr{L}}^\diamond := \mathscr{L}_{F,-\gamma,\sigma}$$

with the notation of (2.6). Hence all the results proven in the previous sections apply to $(\widetilde{X}_t^{\diamond,y})_{t\geq 0}$ as well. Furthermore, $\widetilde{X}_t^{\diamond,y}$ and $\widetilde{X}_t^x$ share the same first exit time from D, i.e.

$$\widetilde{\tau}_\partial^{\diamond,y} := \inf\{t > 0 : \widetilde{X}_t^{\diamond,y} \notin D\} = \widetilde{\tau}_\partial^x \quad \text{almost surely.}$$

Let us now write and prove the equivalent of Theorem 2.2.10 for the process $(\widetilde{X}_t^x)_{t\geq 0}$.

By Proposition 2.2.8 applied to $(\widetilde{X}_t^{\diamond,y})_{t\geq 0}$, we have, for all $t \geq 0$, almost surely, if $\widetilde{\tau}_\partial^x > t$ then $\widetilde{X}_t^x \in D \cup \Gamma^+$, and if $\widetilde{\tau}_\partial^x \leq t$ then $\widetilde{X}_{\widetilde{\tau}_\partial^x}^x \in \Gamma^- \cup \Gamma^0$. This ensures that the definition of the function $\widetilde{u}$ in Equation (2.116) below is legitimate.

Proposition 2.6.1 (Classical solution and probabilistic representation for the adjoint kinetic Fokker–Planck equation)**.** *Under Assumptions (O1) and (F1), let $\widetilde{f} \in \mathscr{C}^b(D \cup \Gamma^+)$ and $\widetilde{g} \in \mathscr{C}^b(\Gamma^- \cup \Gamma^0)$, and define the function $\widetilde{u}$ on $\mathbb{R}_+ \times \overline{D}$ by*

$$\widetilde{u} : (t, x) \mapsto \mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}_\partial^x > t}\widetilde{f}(\widetilde{X}_t^x) + \mathbb{1}_{\widetilde{\tau}_\partial^x \leq t}\widetilde{g}(\widetilde{X}_{\widetilde{\tau}_\partial^x}^x)\right]. \tag{2.116}$$

Then we have the following results:

(i) *Initial and boundary values: the function $\widetilde{u}$ satisfies*

$$\widetilde{u}(0, x) = \begin{cases} \widetilde{f}(x) & \text{if } x \in D \cup \Gamma^+, \\ \widetilde{g}(x) & \text{if } x \in \Gamma^- \cup \Gamma^0, \end{cases}$$

and

$$\forall t > 0, \quad \forall x \in \Gamma^- \cup \Gamma^0, \qquad \widetilde{u}(t, x) = \widetilde{g}(x).$$

(ii) *Continuity: $\widetilde{u} \in \mathscr{C}^b((\mathbb{R}_+ \times \overline{D}) \setminus (\{0\} \times (\Gamma^- \cup \Gamma^0)))$, and if $\widetilde{f}$ and $\widetilde{g}$ satisfy the compatibility condition*

$$x \in \overline{D} \mapsto \mathbb{1}_{x \in D \cup \Gamma^+}\widetilde{f}(x) + \mathbb{1}_{x \in \Gamma^- \cup \Gamma^0}\widetilde{g}(x) \in \mathscr{C}^b(\overline{D}), \tag{2.117}$$

then $\widetilde{u} \in \mathscr{C}^b(\mathbb{R}_+ \times \overline{D})$.

(iii) *Interior regularity: $\widetilde{u} \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D)$ and, for all $t > 0$, $x \in D$,*

$$\partial_t \widetilde{u}(t, x) = \widetilde{\mathscr{L}}\widetilde{u}(t, x). \tag{2.118}$$

(iv) *Uniqueness: let $\widetilde{v}$ be a classical solution, in the sense of Definition 2.2.2, to the Initial-Boundary Value Problem*

$$\begin{cases} \partial_t \widetilde{v} = \widetilde{\mathscr{L}}\widetilde{v} & t > 0, \quad x \in D, \\ \widetilde{v}(0, x) = \widetilde{f}(x) & x \in D, \\ \widetilde{v}(t, x) = \widetilde{g}(x) & t > 0, \quad x \in \Gamma^-. \end{cases}$$

If, for all $T > 0$, $\widetilde{v}$ is bounded on the set $[0, T] \times D$, then $\widetilde{v}(t, x) = \widetilde{u}(t, x)$ for all $(t, x) \in (\mathbb{R}_+ \times (D \cup \Gamma^-)) \setminus (\{0\} \times \Gamma^-)$.

Proof. Let $\widetilde{f} \in \mathscr{C}^b(D \cup \Gamma^+)$ and $\widetilde{g} \in \mathscr{C}^b(\Gamma^- \cup \Gamma^0)$. Let $\widetilde{f}^\diamond$, $\widetilde{g}^\diamond$ be defined by

$$\widetilde{f}^\diamond(q, p) = \widetilde{f}(q, -p), \qquad \widetilde{g}^\diamond(q, p) = \widetilde{g}(q, -p).$$

It is easy to see that $\widetilde{f}^\diamond \in \mathscr{C}^b(D \cup \Gamma^-)$ and $\widetilde{g}^\diamond \in \mathscr{C}^b(\Gamma^+ \cup \Gamma^0)$. Using the process $(\widetilde{X}_t^\diamond)_{t\geq 0}$ defined in (2.115), the function $\widetilde{u}$ defined in (2.116) also writes for $(q, p) \in D$ as follows:

$$\widetilde{u}(t, (q, p)) = \mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}_\partial^{\diamond,(q,-p)} > t}\widetilde{f}^\diamond(\widetilde{X}_t^{\diamond,(q,-p)}) + \mathbb{1}_{\widetilde{\tau}_\partial^{\diamond,(q,-p)} \leq t}\widetilde{g}^\diamond\left(\widetilde{X}_{\widetilde{\tau}_\partial^{\diamond,(q,-p)}}^{\diamond,(q,-p)}\right)\right].$$

Let us define $\widetilde{u}^\diamond$ for $t \geq 0$, $(q,p) \in \overline{D}$ by $\widetilde{u}^\diamond(t,(q,p)) := \widetilde{u}(t,(q,-p))$. Then, $\widetilde{u}^\diamond$ satisfies all the assertions of Theorem 2.2.10 for the kinetic Fokker-Planck equation

$$\begin{cases} \partial_t \widetilde{u}^\diamond(t,x) = \widetilde{\mathscr{L}^\diamond} \widetilde{u}^\diamond(t,x) & t > 0, \quad x \in D, \\ \widetilde{u}^\diamond(0,x) = \widetilde{f}^\diamond(x) & x \in D, \\ \widetilde{u}^\diamond(t,x) = \widetilde{g}^\diamond(x) & t > 0, \quad x \in \Gamma^+. \end{cases}$$

Therefore, $\widetilde{u}$ as defined in (2.116) satisfies all the assertions of Proposition 2.6.1. □

Let us define the transition kernel $\widetilde{\mathrm{P}}_t^D$ for the absorbed adjoint process $(\widetilde{X}_t^x)_{0 \leq t \leq \widetilde{\tau}_\partial^x}$:

$$\forall t \geq 0, \quad \forall x \in D, \quad \forall A \in \mathscr{B}(D), \qquad \widetilde{\mathrm{P}}_t^D(x,A) := \mathbb{P}(\widetilde{X}_t^x \in A, \widetilde{\tau}_\partial^x > t).$$

In the next theorem, we show that this kernel admits a transition density $\widetilde{\mathrm{p}}_t^D$ which satisfies a simple reversibility relation with p_t^D.

Theorem 2.6.2 (Reversibility)**.** *Let Assumptions (O1) and (F1) hold. For all $t > 0$, $x, y \in D$, let us define*

$$\widetilde{\mathrm{p}}_t^D(x,y) = \mathrm{e}^{-d\gamma t} \mathrm{p}_t^D(y,x). \tag{2.119}$$

For any $t > 0$, $x \in D$ and $A \in \mathscr{B}(D)$,

$$\widetilde{\mathrm{P}}_t^D(x,A) = \int_A \widetilde{\mathrm{p}}_t^D(x,y)\mathrm{d}y.$$

Proof. Let $\varphi \in \mathscr{C}_c^\infty(D)$. Let $\widetilde{u} : \mathbb{R}_+ \times \overline{D} \to \mathbb{R}$ be defined by

$$\widetilde{u}(t,x) := \mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}_\partial^x > t} \varphi(\widetilde{X}_t^x)\right].$$

By Assertion (ii) in Proposition 2.6.1, this function is continuous on $\mathbb{R}_+ \times \overline{D}$. Let us define the function $\widetilde{v}$ on $\mathbb{R}_+ \times \overline{D}$ by

$$\widetilde{v}(t,x) = \begin{cases} \mathrm{e}^{-d\gamma t} \displaystyle\int_D \mathrm{p}_t^D(y,x)\varphi(y)\mathrm{d}y & \text{if } t > 0 \text{ and } x \in D, \\ \varphi(x) & \text{if } (t,x) \in (\mathbb{R}_+ \times \overline{D}) \setminus (\mathbb{R}_+^* \times D). \end{cases}$$

Let us prove that $\widetilde{v}(t,x) = \widetilde{u}(t,x)$ for $t > 0$ and $x \in D$, which will ensure (2.119). In this purpose, we use the uniqueness result of Assertion (iv) in Proposition 2.6.1. By Definition 2.2.2, we need to check that:

(i) $(t,x) \mapsto \widetilde{v}(t,x) \in \mathscr{C}^{1,2}(\mathbb{R}_+^* \times D)$ and $\widetilde{v}$ satisfies $\partial_t \widetilde{v} = \widetilde{\mathscr{L}} \widetilde{v}$,

(ii) $(t,x) \mapsto \widetilde{v}(t,x) \in \mathscr{C}((\mathbb{R}_+ \times (D \cup \Gamma^-)) \setminus (\{0\} \times \Gamma^-))$, $\widetilde{v}(0,\cdot) = \varphi$ on D and, for $t > 0$, $\widetilde{v}(t,\cdot) = 0$ on Γ^-,

(iii) $\forall T > 0$, $\sup_{t \in [0,T], x \in D} |\widetilde{v}(t,x)| < \infty$.

Since φ has a compact support in D and, by Proposition 2.5.5, p^D is $\mathscr{C}^\infty$ on $\mathbb{R}_+^* \times D \times D$ and satisfies $\partial_t \mathrm{p}^D(x,y) = \mathscr{L}_x \mathrm{p}^D(x,y)$, we deduce that $\widetilde{v}$ is $\mathscr{C}^{1,2}$ on $\mathbb{R}_+^* \times D$ and satisfies $\partial_t \widetilde{v} = (\mathscr{L}^* - d\gamma)\widetilde{v} = \widetilde{\mathscr{L}} \widetilde{v}$.

Let $t > 0$ and $x \in \Gamma^-$. By the definition of $\widetilde{v}$, we have $\widetilde{v}(t,x) = \varphi(x) = 0$ since φ has a compact support in D. On the other hand, if $(t_n, x_n)_{n \geq 1}$ is a sequence of elements of $(\mathbb{R}_+ \times (D \cup \Gamma^-)) \setminus (\{0\} \times \Gamma^-)$ which converge to (t,x), then it follows from Assertion (ii) in Proposition 2.5.7, Remark 2.2.21 and the dominated convergence theorem that $\widetilde{v}(t_n, x_n)$ converges to 0.

Similarly, if $x \in D$ then it follows from the definition of $\widetilde{v}$ that $\widetilde{v}(0,x) = \varphi(x)$. Now let $(t_n, x_n)_{n \geq 1}$ be a sequence of elements of $(\mathbb{R}_+ \times (D \cup \Gamma^-)) \setminus (\{0\} \times \Gamma^-)$ which converge to $(0,x)$, and let us check that $\widetilde{v}(t_n, x_n)$ converges to $\varphi(x)$. We first remark that if $t_n = 0$ then $\widetilde{v}(t_n, x_n) = \varphi(x_n)$, so that along the subsequence $\{n \geq 1 : t_n = 0\}$, the claimed convergence is immediate. Therefore, we may now assume that $t_n > 0$ for any $n \geq 1$. Let $K \subset D$ be a compact set which contains the support of φ and an open ball centered at x. There exists $N_1 \geq 1$ such that for all $n \geq N_1$, $x_n \in K$. Moreover, there exists $N_2 \geq 1$ such that for $n \geq N_2$, $t_n \in (0, 1]$ since $t_n \underset{n\to\infty}{\longrightarrow} 0$. Therefore, by Lemma 2.5.6, there exist a constant $C > 0$ and $\alpha \in (0, 1)$ such that for all $y \in K$ and $n \geq N_1 \vee N_2$,

$$\left|\mathrm{p}^D_{t_n}(y, x_n) - \widehat{\mathrm{p}}_{t_n}(y, x_n)\right| \leq C\sqrt{t_n}\widehat{\mathrm{p}}^{(\alpha)}_{t_n}(y, x_n).$$

Consequently, since $\varphi = 0$ outside K,

$$\begin{aligned}\left|\widetilde{v}(t_n, x_n) - \mathrm{e}^{-d\gamma t_n}\int_D \widehat{\mathrm{p}}_{t_n}(y, x_n)\varphi(y)\mathrm{d}y\right| &\leq C\sqrt{t_n}\mathrm{e}^{-d\gamma t_n}\int_D \widehat{\mathrm{p}}^{(\alpha)}_{t_n}(y, x_n)\varphi(y)\mathrm{d}y\\ &\leq C\|\varphi\|_\infty\sqrt{t_n}\mathrm{e}^{-d\gamma t_n}\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}^{(\alpha)}_{t_n}(y, x_n)\mathrm{d}y.\end{aligned}$$

By Lemma 2.5.2, one has that

$$\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}^{(\alpha)}_{t_n}(y, x_n)\mathrm{d}y = \mathrm{e}^{d\gamma t_n}, \qquad \int_D \widehat{\mathrm{p}}_{t_n}(y, x_n)\varphi(y)\mathrm{d}y \underset{n\to\infty}{\longrightarrow} \varphi(x).$$

Therefore, $\widetilde{v}(t_n, x_n) \underset{n\to\infty}{\longrightarrow} \varphi(x)$.

We finally fix $T > 0$ and show that $\sup_{t\in[0,T],x\in D} |\widetilde{v}(t, x)| < \infty$. Again, Corollary 2.2.21 ensures the existence of $C' > 0$ such that for all $t \in (0, T]$, $x \in D$,

$$\begin{aligned}|\widetilde{v}(t, x)| &= \mathrm{e}^{-d\gamma t}\left|\int_D \mathrm{p}^D_t(y, x)\varphi(y)\mathrm{d}y\right|\\ &\leq C'\|\varphi\|_\infty \mathrm{e}^{-d\gamma t}\int_{\mathbb{R}^{2d}} \widehat{\mathrm{p}}^{(\alpha)}_t(y, x)\mathrm{d}y\\ &\leq C'\|\varphi\|_\infty,\end{aligned}$$

using Lemma 2.5.2, which concludes the proof. □

Let us now conclude this subsection with results on the boundary continuity of the density $\mathrm{p}^D_t(x, y)$ for a fixed $t > 0$. The proof relies on Theorem 2.6.2, and this result will complete the proof of Theorem 2.2.20. It also completes the results of Proposition 2.5.7 since we consider the continuity with respect to the three variables (t, x, y) at the same time and extend the limit with respect to y going to a point in Γ^0.

Theorem 2.6.3 (Boundary continuity)**.** *Under Assumptions (O1) and (F1), the transition density* p^D *can be extended to a function in* $\mathscr{C}(\mathbb{R}^*_+ \times \overline{D} \times \overline{D})$ *which satisfies for all* $t > 0$*:*

(i) $\mathrm{p}^D_t(x, y) = 0$ *if* $x \in \Gamma^+ \cup \Gamma^0$ *or if* $y \in \Gamma^- \cup \Gamma^0$*,*

(ii) if Assumption (O2) holds, $\mathrm{p}^D_t(x, y) > 0$ *for all* $x \notin \Gamma^+ \cup \Gamma^0$ *and* $y \notin \Gamma^- \cup \Gamma^0$*.*

Proof. **Step 1**. We first study the behavior of $\mathrm{p}^D_t(x, y)$ when x and y approach ∂D, and show that the function p^D can be continuously extended on $\mathbb{R}^*_+ \times \overline{D} \times \overline{D}$. Let $t_0 > 0$, $x_0 \in \overline{D}$ and $y_0 \in \overline{D}$. Let $(t_n, x_n, y_n)_{n\geq 1}$ be a sequence of points in $\mathbb{R}^*_+ \times D \times D$ converging towards (t_0, x_0, y_0).

In the next three cases, we show that $\mathrm{p}^D_{t_n}(x_n, y_n)$ has a limit which does not depend on the sequence $(t_n, x_n, y_n)_{n\geq 1}$. If $x_0, y_0 \in D$ then by Proposition 2.5.5, this limit coincides with $\mathrm{p}^D_{t_0}(x_0, y_0)$. Otherwise, we denote this limit by $\mathrm{p}^D_{t_0}(x_0, y_0)$, which thereby defines a continuous function p^D on $\mathbb{R}^*_+ \times \overline{D} \times \overline{D}$.

Case 1: Assume that $x_0 \in \Gamma^+ \cup \Gamma^0$. By Assertion (i) in Proposition 2.5.7 and Remark 2.5.9, we immediately get

$$\mathrm{p}^D_{t_n}(x_n, y_n) \underset{n\to\infty}{\longrightarrow} 0,$$

and therefore set $\mathrm{p}^D_{t_0}(x_0, y_0) = 0$.

Case 2: Assume that $y_0 = (q_0, p_0) \in \Gamma^- \cup \Gamma^0$. For any $(q, p) \in \mathbb{R}^{2d}$, let us define $\diamond(q, p) := (q, -p)$. From the definition of the process $(\widetilde{X}^{\diamond,x}_t)_{t\geq 0} = (\diamond \widetilde{X}^{\diamond x}_t)_{t\geq 0}$, we deduce that the absorbed version of the latter possesses a transition density $\widetilde{\mathrm{p}}^{\diamond,D}_t$ which satisfies

$$\widetilde{\mathrm{p}}^{\diamond,D}_t(x, y) = \widetilde{\mathrm{p}}^D_t(\diamond x, \diamond y).$$

As a consequence, using Theorem 2.6.2 we rewrite

$$\mathrm{p}^D_{t_n}(x_n, y_n) = \mathrm{e}^{d\gamma t_n}\widetilde{\mathrm{p}}^D_{t_n}(y_n, x_n) = \mathrm{e}^{d\gamma t_n}\widetilde{\mathrm{p}}^{\diamond,D}_{t_n}(\diamond y_n, \diamond x_n).$$

On the one hand, $\diamond y_n \to \diamond y_0 \in \Gamma^+ \cup \Gamma^0$. On the other hand, the process $(\widetilde{X}^{\diamond,x}_t)_{t\geq 0}$ has infinitesimal generator $\widetilde{\mathscr{L}^\diamond} = \mathscr{L}_{F,-\gamma,\sigma}$, and therefore Assertion (i) in Proposition 2.5.7 and Remark 2.5.9 apply to show that

$$\sup_{x\in D} \widetilde{\mathrm{p}}^{\diamond,D}_{t_n}(\diamond y_n, x) \underset{n\to\infty}{\longrightarrow} 0,$$

from which we deduce that $\mathrm{p}^D_{t_n}(x_n, y_n) \underset{n\to\infty}{\longrightarrow} 0$ and set $\mathrm{p}^D_{t_0}(x_0, y_0) = 0$.

Case 3: Assume that $x_0 \in D \cup \Gamma^-$ and $y_0 = (q_0, p_0) \in D \cup \Gamma^+$. For $h > 0$, by the Markov property,

$$\forall 0 \leq s < t, \quad \forall x, y \in D, \qquad \frac{\mathrm{P}^D_t(x, D \cap \mathrm{B}(y, h))}{|\mathrm{B}(y, h)|} = \mathbb{E}\left[\mathbb{1}_{\tau^x_\partial > s}\frac{\mathrm{P}^D_{t-s}(X^x_s, D \cap \mathrm{B}(y, h))}{|\mathrm{B}(y, h)|}\right].$$

Using the Gaussian upper-bound from Corollary 2.2.21 and the dominated convergence theorem when $h \to 0$, we obtain from the equality above the following Chapman-Kolmogorov relation:

$$\forall 0 \leq s < t, \quad \forall x, y \in D, \qquad \mathrm{p}^D_t(x, y) = \mathbb{E}\left[\mathbb{1}_{\tau^x_\partial > s}\mathrm{p}^D_{t-s}(X^x_s, y)\right]. \tag{2.120}$$

By (2.120) applied with $s = t_n/3$, one has that

$$\mathrm{p}^D_{t_n}(x_n, y_n) = \int_D \mathrm{p}^D_{t_n/3}(x_n, z)\mathrm{p}^D_{2t_n/3}(z, y_n)\mathrm{d}z. \tag{2.121}$$

Let us prove now the convergence of both integrands in (2.121). Using Theorem 2.6.2 and (2.120) again, one has for all $z \in D$,

$$\begin{aligned}
\mathrm{p}^D_{2t_n/3}(z, y_n) &= \mathrm{e}^{2d\gamma t_n/3}\widetilde{\mathrm{p}}^D_{2t_n/3}(y_n, z)\\
&= \mathrm{e}^{2d\gamma t_n/3}\mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}^{y_n}_\partial > t_n/3}\widetilde{\mathrm{p}}^D_{t_n/3}(\widetilde{X}^{y_n}_{t_n/3}, z)\right]\\
&= \mathrm{e}^{2d\gamma t_n/3}\mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}^{\diamond,\diamond y_n}_\partial > t_n/3}\widetilde{\mathrm{p}}^{\diamond,D}_{t_n/3}(\widetilde{X}^{\diamond,\diamond y_n}_{t_n/3}, \diamond z)\right].
\end{aligned}$$

By construction, $\widetilde{\mathrm{p}}^{\diamond,D}$ is continuous on $\mathbb{R}^*_+ \times D \times D$ and is the transition density of the process $(\widetilde{X}^{\diamond,x}_t)_{t\geq 0}$ with infinitesimal generator $\widetilde{\mathscr{L}^\diamond} = \mathscr{L}_{F,-\gamma,\sigma}$. Therefore, Lemma 2.3.2 and Corollary 2.2.21 apply here and ensure, using the dominated convergence theorem, that for $z \in D$,

$$\mathrm{p}^D_{2t_n/3}(z, y_n) \underset{n\to\infty}{\longrightarrow} h^{(1)}_t(z) := \mathrm{e}^{2d\gamma t_0/3}\mathbb{E}\left[\mathbb{1}_{\widetilde{\tau}^{\diamond,\diamond y_0}_\partial > t_0/3}\widetilde{\mathrm{p}}^{\diamond,D}_{t_0/3}(\widetilde{X}^{\diamond,\diamond y_0}_{t_0/3}, \diamond z)\right]. \tag{2.122}$$

Furthermore, considering now the first integrand in (2.121), for all $z \in D$,

$$\mathrm{p}^D_{t_n/3}(x_n, z) = \mathbb{E}\left[\mathbb{1}_{\tau^{x_n}_\partial > t_n/6}\mathrm{p}^D_{t_n/6}(X^{x_n}_{t_n/6}, z)\right] \underset{n\to\infty}{\longrightarrow} h^{(2)}_t(z) := \mathbb{E}\left[\mathbb{1}_{\tau^{x_0}_\partial > t_0/6}\mathrm{p}^D_{t_0/6}(X^{x_0}_{t_0/6}, z)\right], \tag{2.123}$$

using the continuity of p^D and Lemma 2.3.2. It remains to prove that the integral (2.121) converges to the integral $\int_D h_t^{(1)}(z)h_t^{(2)}(z)\mathrm{d}z$.

Since the term $\mathrm{p}^D_{2t_n/3}(z,y_n)$ is bounded by a constant depending only on t_n by Corollary 2.2.21 and since $t_n \underset{n\to\infty}{\longrightarrow} t_0 > 0$ the associated constant can easily be obtained independent of n. In order to use the dominated convergence theorem to the product of both integrands in (2.121), it remains to obtain a bound on $\mathrm{p}^D_{t_n/3}(x_n,z)$ in $\mathrm{L}^1(D)$ which is independent of n. This follows from Lemma 2.6.4 below since (t_n,x_n) converges to $(t_0,x_0)\in\mathbb{R}_+^*\times\overline{D}$, therefore the sequence $(t_n,x_n)_{n\geq1}$ stays in some compact set K of $\mathbb{R}_+^*\times\overline{D}$. We thus obtain a limit independent on the sequence $(t_n,x_y,y_n)_{n\geq1}$. By Proposition 2.5.5, if $x_0,y_0\in D$, it coincides with $\mathrm{p}^D_{t_0}(x_0,y_0)$, otherwise we denote it by $\mathrm{p}^D_{t_0}(x_0,y_0)$.

Step 2. Let us now work under Assumption (O2) and first prove that for all $t>0$ and $x,y\in D$,

$$\mathrm{p}^D_t(x,y)>0. \tag{2.124}$$

Let us argue by contradiction. Assume there exists $t_0>0$ and $x_0,y_0\in D$ such that $\mathrm{p}^D_{t_0}(x_0,y_0)=0$. Let us introduce

$$\Psi:(t,y)\in\mathbb{R}_+^*\times D\mapsto \mathrm{e}^{-d\gamma t}\mathrm{p}^D_t(x_0,\diamond y).$$

It follows from the forward Kolmogorov equation satisfied by $\mathrm{p}^D_t(x_0,\cdot)$ (see Proposition 2.5.5), that on $\mathbb{R}_+^*\times D$,

$$\partial_t\Psi=\widetilde{\mathscr{L}^\diamond}\Psi.$$

Using the Harnack inequality stated in Theorem 2.2.15, we have that for any $K\subset D$ compact set and $t\in(0,t_0)$ there exists $C>0$ such that

$$\sup_{y\in K}\Psi(t,y)\leq C\inf_{y\in K}\Psi(t_0,y).$$

In particular, it yields that for all $y\in D$, $t\in(0,t_0)$, $\Psi(t,y)=0$. As a result, for all $t\in(0,t_0)$ and $y\in D$, $\mathrm{p}^D_t(x_0,y)=0$. Integrating over $y\in D$, it follows that for all $t\in(0,t_0)$,

$$\mathbb{P}(\tau_\partial^{x_0}>t)=0.$$

Besides, it follows from Lemma 2.3.2 and Proposition 2.2.8 that $\mathbb{P}(\tau_\partial^{x_0}>t)\underset{t\to0}{\longrightarrow}1$. This is contradiction with the equality above, and this thus concludes the proof of (2.124).

Step 3. It remains to extend the result of **Step 2** to show that $\mathrm{p}^D_t(x,y)>0$ for $t>0$, $x\in D\cup\Gamma^-$ and $y\in D\cup\Gamma^+$. In this purpose, we first show that, for any $x_0\in D\cup\Gamma^-$, for all $t>0$,

$$\mathbb{P}(\tau_\partial^{x_0}>t)>0. \tag{2.125}$$

Indeed, using again Lemma 2.3.2 and Proposition 2.2.8, there exists necessarily $s\in(0,t)$ such that $\mathbb{P}(\tau_\partial^{x_0}>s)>0$. As a result, the Markov property at time s ensures that

$$\mathbb{P}(\tau_\partial^{x_0}>t)=\mathbb{E}\left[\mathbb{1}_{\tau_\partial^{x_0}>s}\mathbb{P}(\tau_\partial^{z}>t-s)|_{z=X_s^{x_0}}\right]>0$$

by (2.124), which yields (2.125).

We now recall from **Case 3** in **Step 1** that for $t>0$, $x\in D\cup\Gamma^-$ and $y\in D\cup\Gamma^+$,

$$\mathrm{p}^D_t(x,y)=\int_D h_t^{(1)}(z)h_t^{(2)}(z)\mathrm{d}z,$$

where h_1,h_2 are defined in (2.122) and (2.123). By **Step 2** applied to $\widetilde{\mathrm{p}}^{\diamond,D}_{t/3}$, for all $z\in D$ we have $\widetilde{\mathrm{p}}^{\diamond,D}_{t/3}(\widetilde{X}^{\diamond,\diamond y}_{t/3},\diamond z)>0$ on the event $\{\widetilde{\tau}^{\diamond,\diamond y}_\partial>t/3\}$. And by (2.125) applied to $(\widetilde{X}^{\diamond,\diamond y}_t)_{t\geq0}$, this event has positive probability, so that $h_t^{(1)}(z)>0$. Similarly, one has $h_t^{(2)}(z)>0$. Therefore, we conclude that $\mathrm{p}^D_t(x,y)>0$. □

Let us now state and prove Lemma 2.6.4.

Lemma 2.6.4 (Transition density domination). *Let Assumptions (O1) and (F1) hold. Let U be a compact set of $\mathbb{R}_+^* \times D$. There exist a constant $C > 0$ and a function $h \in \mathrm{L}^1(D)$ such that for all $(t,x) \in U$ and $y \in D$,*

$$\mathrm{p}_t^D(x,y) \leq Ch(y).$$

Proof. Let U be a compact set of $\mathbb{R}_+^* \times D$ and let (t_0, x_0) be a fixed element of U. Let $(t,x) \in U$, by Corollary 2.2.21, for any $\alpha \in (0,1)$, there exists $C_1 > 0$ such that

$$\mathrm{p}_t^D(x,y) \leq C_1 \widehat{\mathrm{p}}_t^{(\alpha)}(x,y).$$

Besides, by Proposition 2.2.17 and the equality (2.79), for all $y \in D$, the function $(t,x) \in \mathbb{R}_+^* \times \mathbb{R}^{2d} \mapsto \widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$ satisfies

$$\partial_t \widehat{\mathrm{p}}^{(\alpha)} = \mathscr{L}_{0,\gamma,\sigma/\sqrt{\alpha}} \widehat{\mathrm{p}}^{(\alpha)}.$$

As a result, the Harnack inequality in Theorem 2.2.15 along with Remark 2.2.16, applied on the compact set U, ensure the existence of $C_2 > 0$ only depending on U such that

$$\widehat{\mathrm{p}}_t^{(\alpha)}(x,y) \leq C_2 \widehat{\mathrm{p}}_{t+1}^{(\alpha)}(x_0,y).$$

Finally, one has

$$\mathrm{p}_t^D(x,y) \leq C_1 C_2 \widehat{\mathrm{p}}_{t+1}^{(\alpha)}(x_0,y), \tag{2.126}$$

where we eliminated the dependence with respect to the variable x. It remains to eliminate the dependence with respect to t on the time variable. Consider now the expression of $\widehat{\mathrm{p}}^{(\alpha)}$ following from (2.79) and (2.74). Using Lemma 2.5.1, especially the first term in the right-hand side of the equality (2.77), one has for $x_0 = (q_0, p_0)$ and $y = (q', p') \in D$,

$$\widehat{\mathrm{p}}_{t+1}^{(\alpha)}((q_0,p_0),(q',p')) \leq \frac{\sqrt{\alpha^{2d}}}{\sqrt{(2\pi)^{2d}\left(\frac{\sigma^4(t+1)^4}{12}\phi(\gamma(t+1))\right)^d}} \mathrm{e}^{-\frac{\alpha}{\sigma^2(t+1)}|\gamma(q'-q_0)+p'-p_0|^2}.$$

Hence, since $(t,x) \in U$, t is bounded from above and below by positive constants. Therefore, reinjecting into (2.126) there exist $C_3 > 0$ and $\beta > 0$, which do not depend on (t,x), such that for any $y = (q', p') \in D$,

$$\mathrm{p}_t^D(x,y) \leq C_3 \mathrm{e}^{-\beta|\gamma(q'-q_0)+p'-p_0|^2},$$

which is an integrable function of y. □

To complete the proof of Theorem 2.2.20, it remains to check that, for any $t > 0$, the extension of p_t^D constructed in Theorem 2.6.3 remains the density of the kernel $\mathrm{P}_t^D(x,\cdot)$. This is already the case for $x \in D$ by Proposition 2.5.4, and we prove this fact for $x \in \partial D$ in the next proposition.

Proposition 2.6.5 (Identification of the transition density on ∂D). *Under Assumptions (O1) and (F1), for all $t > 0$, $x \in \partial D$ and $A \in \mathscr{B}(D)$,*

$$\mathrm{P}_t^D(x,A) = \int_A \mathrm{p}_t^D(x,y)\mathrm{d}y.$$

Proof. Let $t_0 > 0$, $x_0 = (q_0,p_0) \in \partial D$ and $(t_n,x_n)_{n\geq 1}$ be a sequence of points in $\mathbb{R}_+^* \times D$ converging to (t_0,x_0). Let us show that for any open set $A \subset D$, $\mathrm{P}_{t_n}^D(x_n,A)$ admits two limits when $n \to \infty$ which are $\mathrm{P}_{t_0}^D(x_0,A)$ and $\int_A \mathrm{p}_{t_0}^D(x_0,y)\mathrm{d}y$. This yields the desired equality $\mathrm{P}_{t_0}^D(x_0,A) = \int_A \mathrm{p}_{t_0}^D(x_0,y)\mathrm{d}y$.

Let A be an open subset of D. The limit $\mathrm{P}^D_{t_n}(x_n, A) \underset{n\to\infty}{\longrightarrow} \mathrm{P}^D_{t_0}(x_0, A)$ is a straightforward consequence of Lemmata 2.3.1 and 2.3.2, which ensure that

$$\mathbb{P}(X^{x_n}_{t_n} \in A, \tau^{x_n}_\partial > t_n) \underset{n\to\infty}{\longrightarrow} \mathbb{P}(X^{x_0}_{t_0} \in A, \tau^{x_0}_\partial > t_0),$$

using the dominated convergence theorem since $\mathbb{P}(X^{x_0}_{t_0} \in \partial A, \tau^{x_0}_\partial > t_0) = 0$.

Let us now prove that $\mathrm{P}^D_{t_n}(x_n, A) = \int_A \mathrm{p}^D_{t_n}(x_n, y)\mathrm{d}y \underset{n\to\infty}{\longrightarrow} \int_A \mathrm{p}^D_{t_0}(x_0, y)\mathrm{d}y$. In order to do that we apply the dominated convergence theorem on the integrand of $\int_A \mathrm{p}^D_{t_n}(x_n, y)\mathrm{d}y$ which requires an upper bound of $\mathrm{p}^D_{t_n}(x_n, y)$ independent of n for n large enough, and integrable on D. Such an upper bound is provided in Lemma 2.6.4 if for all $n \geq 1$, (t_n, x_n) is in a compact of $\mathbb{R}^*_+ \times \overline{D}$ which is the case since $t_n \underset{n\to\infty}{\longrightarrow} t_0 > 0$ and $x_n \underset{n\to\infty}{\longrightarrow} x_0 \in \overline{D}$. □

Remark 2.6.6. *Let $(t_n, x_n)_{n\geq 1}$ be a sequence in $\mathbb{R}^*_+ \times \overline{D}$ converging to $(t, x) \in \mathbb{R}^*_+ \times \overline{D}$. By the previous construction, it follows that for any $y \in D$, $\mathrm{p}^D_{t_n}(x_n, y) \underset{n\to\infty}{\longrightarrow} \mathrm{p}^D_t(x, y)$. Futhermore, the proof of Proposition 2.6.5 shows that*

$$\int_D \mathrm{p}^D_{t_n}(x_n, y)\mathrm{d}y \underset{n\to\infty}{\longrightarrow} \int_D \mathrm{p}^D_t(x, y)\mathrm{d}y.$$

These two convergences guarantee by Scheffé's lemma that

$$\int_D \left|\mathrm{p}^D_{t_n}(x_n, y) - \mathrm{p}^D_t(x, y)\right| \mathrm{d}y \underset{n\to\infty}{\longrightarrow} 0.$$

2.6.2 Compactness of the semigroup $(P^D_t)_{t\geq 0}$

Let us end this section with some compactness properties satisfied by the semigroup $(P^D_t)_{t\geq 0}$. Let us first prove that $\mathrm{p}^D_t \in \mathrm{L}^1(D \times D) \cap \mathrm{L}^\infty(D \times D)$.

Lemma 2.6.7 ($\mathrm{p}^D_t \in \mathrm{L}^1(D\times D)\cap\mathrm{L}^\infty(D\times D)$)**.** *Let Assumptions (O1) and (F1) hold. For all $t > 0$, p^D_t is bounded on $D \times D$ and*

$$\int_D \int_D \mathrm{p}^D_t(x, y)\mathrm{d}x\mathrm{d}y < \infty. \tag{2.127}$$

Remark 2.6.8. *In particular, this ensures that $\mathrm{p}^D_t \in \mathrm{L}^q(D \times D)$ for all $q \in [1, \infty]$ and $t > 0$.*

Proof. Let $\alpha \in (0, 1)$ and $t > 0$. By Corollary 2.2.21, there exists $C > 0$ such that for all $(q, p), (q', p') \in D$, $\mathrm{p}^D_t((q, p), (q', p')) \leq C\widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))$, where $\widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))$ is defined in (2.79). Therefore, $\mathrm{p}^D_t \in \mathrm{L}^\infty(D \times D)$ and it is left to prove that

$$\int_D \int_D \widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))\mathrm{d}q\mathrm{d}p\mathrm{d}q'\mathrm{d}p' < \infty.$$

Let us first integrate with respect to $p, p' \in \mathbb{R}^d$ using Fubini-Tonelli's theorem. Since $\widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))$ is the transition density of the process $(\alpha^{-1/2}\widehat{X}^{\sqrt{\alpha}x}_t)_{t\geq 0}$, one can obtain an explicit expression of $\int_{\mathbb{R}^d} \widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))\mathrm{d}p'$ which corresponds to the marginal density of $\alpha^{-1/2}\widehat{q}^{\sqrt{\alpha}x}_t$. Following Section 2.5.1, we have

$$\frac{1}{\sqrt{\alpha}}\widehat{q}^{\sqrt{\alpha}x}_t \sim \mathscr{N}_d\left(\frac{m^{\sqrt{\alpha}x}_q(t)}{\sqrt{\alpha}}, \frac{c_{qq}(t)}{\alpha}I_d\right), \qquad \frac{m^{\sqrt{\alpha}x}_q(t)}{\sqrt{\alpha}} = q + tp\Phi_1(\gamma t), \qquad \frac{c_{qq}(t)}{\alpha} = \frac{\sigma^2 t^3}{3\alpha}\Phi_2(\gamma t),$$

so that

$$\int_{\mathbb{R}^d} \widehat{\mathrm{p}}^{(\alpha)}_t((q, p), (q', p'))\mathrm{d}p' = \frac{(3\alpha)^{d/2}}{(2\pi\sigma^2 t^3\Phi_2(\gamma t))^{d/2}}\mathrm{e}^{-\frac{3\alpha}{2\sigma^2 t^3\Phi_2(\gamma t)}|q'-q-tp\Phi_1(\gamma t)|^2}$$

where Φ_1 and Φ_2 are defined in (2.69) and (2.70). Then,

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p'))\mathrm{d}p\mathrm{d}p' = \frac{\alpha^{d/2}(3)^{\frac{d}{2}}}{(2\pi\sigma^2t^3\Phi_2(\gamma t))^{d/2}}\int_{\mathbb{R}^d}\mathrm{e}^{-\frac{3\alpha}{2\sigma^2t^3\Phi_2(\gamma t)}|q'-q-tp\Phi_1(\gamma t)|^2}\mathrm{d}p$$
$$= \frac{1}{t^d\Phi_1(\gamma t)^d}.$$

Consequently,

$$\int_D\int_D\widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p'))\mathrm{d}q\mathrm{d}p\mathrm{d}q'\mathrm{d}p' = \frac{|\mathscr{O}|^2}{t^d\Phi_1(\gamma t)^d},$$

which concludes the proof. □

Let us now prove Theorem 2.2.22.

Proof of Theorem 2.2.22. It follows from Lemma 2.6.7 that for all $t>0$,

$$\iint_{D\times D}\mathrm{p}_t^D(x,y)^2\mathrm{d}x\mathrm{d}y<\infty.$$

Therefore, by Theorems VI.22 and VI.23 in [70], the operator P_t^D is a compact operator from $\mathrm{L}^2(D)$ to $\mathrm{L}^2(D)$.

Let $s>0$. In **Step 1**, we show that P_s^D maps $\mathrm{L}^p(D)$, $p\in[1,+\infty)$, continuously into $\mathrm{L}^\infty(D)$. In **Step 2**, we show that P_s^D maps $\mathrm{L}^\infty(D)$ continuously into $\mathrm{L}^q(D)$, $q\in[1,+\infty)$. In **Step 3**, we show that P_s^D maps $\mathrm{L}^\infty(D)$ continuously into $\mathscr{C}^b(\overline{D})$. We conclude the proof in **Step 4**.

Step 1. Let $s>0$, $p\geq 1$. Let us prove that P_s^D maps $\mathrm{L}^p(D)$ continuously into $\mathrm{L}^\infty(D)$. Recall that by Lemma 2.6.7, $\|\mathrm{p}_s^D\|_{\mathrm{L}^\infty(D\times D)}<+\infty$. Therefore if $p=1$, then for any $\eta\in\mathrm{L}^1(D)$ we have

$$\|P_s^D\eta\|_{\mathrm{L}^\infty(D)}\leq\|\mathrm{p}_s^D\|_{\mathrm{L}^\infty(D\times D)}\|\eta\|_{\mathrm{L}^1(D)},$$

while if $p\in(1,+\infty)$, then for any $\eta\in\mathrm{L}^p(D)$ and $x\in D$, letting $q\in(1,+\infty)$ be such that $1/p+1/q=1$, we get by Hölder's inequality

$$\begin{aligned}\left|P_s^D\eta(x)\right| &\leq \|\mathrm{p}_s^D(x,\cdot)\|_{\mathrm{L}^q(D)}\|\eta\|_{\mathrm{L}^p(D)}\\ &\leq\left(\|\mathrm{p}_s^D\|^{q-1}_{\mathrm{L}^\infty(D\times D)}\mathbb{P}(\tau_\partial^x>s)\right)^{1/q}\|\eta\|_{\mathrm{L}^p(D)}\\ &\leq\|\mathrm{p}_s^D\|^{\frac{q-1}{q}}_{\mathrm{L}^\infty(D\times D)}\|\eta\|_{\mathrm{L}^p(D)},\end{aligned}$$

which yields $\|P_s^D\eta\|_{\mathrm{L}^\infty(D)}\leq\|\mathrm{p}_s^D\|^{\frac{q-1}{q}}_{\mathrm{L}^\infty(D\times D)}\|\eta\|_{\mathrm{L}^p(D)}$.

Step 2. Let $s>0$, $q\geq 1$. Let us prove that P_s^D maps $\mathrm{L}^\infty(D)$ continuously into $\mathrm{L}^q(D)$. Let $\eta\in\mathrm{L}^\infty(D)$. For $x\in D$, one has that

$$\begin{aligned}\left|P_s^D\eta(x)\right|^q &= \left|\int_D\mathrm{p}_s^D(x,y)\eta(y)\mathrm{d}y\right|^q\\ &\leq\mathbb{P}(\tau_\partial^x>s)^q\|\eta\|^q_{\mathrm{L}^\infty(D)}\\ &\leq\mathbb{P}(\tau_\partial^x>s)\|\eta\|^q_{\mathrm{L}^\infty(D)}.\end{aligned}$$

Therefore, using Lemma 2.6.7 we get $\|P_s^D\eta\|_{\mathrm{L}^q(D)}\leq\|\mathrm{p}_s^D\|^{1/q}_{\mathrm{L}^1(D\times D)}\|\eta\|_{\mathrm{L}^\infty(D)}$.

Step 3. Let $s>0$. It is an immediate consequence of Remark 2.6.6 that if $\eta\in\mathrm{L}^\infty(D)$, then $P_s^D\eta\in\mathscr{C}^b(\overline{D})$. In other words, the operator P_s^D has the strong Feller property. Besides, one has obviously

$$\|P_s^D\eta\|_{\mathscr{C}^b(\overline{D})}:=\|P_s^D\eta\|_\infty\leq\|\eta\|_{L^\infty(D)},$$

so that P_s^D maps $\mathrm{L}^\infty(D)$ into $\mathscr{C}^b(\overline{D})$ continuously.

Step 4. We first deduce from the Markov property that

$$P_{t+s}^D \eta(x) = \mathbb{E}\left[\eta(X_{t+s}^x)\mathbb{1}_{\tau_\partial^x > t+s}\right] = \mathbb{E}\left[\mathbb{1}_{\tau_\partial^x > t} P_s^D \eta(X_t^x)\right] = P_t^D P_s^D \eta,$$

which together with the obvious observation that $P_0^D \eta = \eta$, shows that $(P_t^d)_{t\geq 0}$ is a semigroup on $\mathrm{L}^p(D)$ for any $p \in [1, +\infty]$ (by **Steps 1** and **2**) and on $\mathscr{C}^b(\overline{D})$ (by **Step 3**).

In order to study compactness, we shall use repeatedly the fact that the composition of a continuous operator with a compact operator is a compact operator.

Let $p \in [1, +\infty]$ and $t > 0$. Writing $P_t = P_{t/3}P_{t/3}P_{t/3}$, using the continuity of the mappings $P_{t/3} : \mathrm{L}^p(D) \to \mathrm{L}^2(D)$ and $P_{t/3} : \mathrm{L}^2(D) \to \mathrm{L}^p(D)$, and the compactness of $P_{t/3} : \mathrm{L}^2(D) \to \mathrm{L}^2(D)$, we obtain that P_t is a compact operator from $\mathrm{L}^p(D)$ to $\mathrm{L}^p(D)$.

Similarly, writing $P_t = \iota P_{t/2}P_{t/2}$, where ι is the injection from $\mathscr{C}^b(\overline{D})$ to $\mathrm{L}^\infty(D)$, using the continuity of the operators ι and $P_{t/2} : \mathrm{L}^\infty(D) \to \mathscr{C}^b(\overline{D})$, as well as the compactness of the operator $P_{t/2} : \mathrm{L}^\infty(D) \to \mathrm{L}^\infty(D)$ that we have just proved, we conclude that P_t is a compact operator from $\mathscr{C}^b(\overline{D})$ to $\mathscr{C}^b(\overline{D})$. □

Part II

Quasi-stationary distributions

CHAPTER 3

QUASI-STATIONARY DISTRIBUTIONS FOR THE LANGEVIN PROCESS ON CYLINDRICAL DOMAINS

The following chapter focuses on the study of quasi-stationary distributions for the Langevin diffusion process using the tools developed in the previous chapter.

Abstract: Consider the Langevin process, described by a vector (position,momentum) in $\mathbb{R}^d\times\mathbb{R}^d$. Let $\mathscr{O}$ be a $\mathscr{C}^2$ open bounded and connected set of $\mathbb{R}^d$. In this article, we prove the existence of a unique quasi-stationary distribution (QSD) for the Langevin process on the domain $D := \mathscr{O} \times \mathbb{R}^d$. We also provide a spectral interpretation of this QSD and obtain an exponential convergence of the conditional distribution of the Langevin process remaining in D, towards this QSD. Finally, the overdamped limit of the Langevin QSD on D is studied, linking the Langevin QSD to the well-known QSD of the overdamped Langevin process on $\mathscr{O}$.

3.1 Introduction

In statistical physics, the evolution of a molecular system at a given temperature is typically modeled by the Langevin dynamics

$$\begin{cases} \mathrm{d}q_t = M^{-1}p_t\mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma M^{-1}p_t\mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}B_t, \end{cases} \tag{3.1}$$

where $d = 3N$ for a number N of particles, $(q_t, p_t) \in \mathbb{R}^d \times \mathbb{R}^d$ denotes the set of positions and momenta of the particles, $M \in \mathbb{R}^{d\times d}$ is the mass matrix, $F : \mathbb{R}^d \to \mathbb{R}^d$ is the force acting on the particles, $\gamma > 0$ is the friction parameter, and $\beta^{-1} = k_BT$ with k_B the Boltzmann constant and T the temperature of the system. Alternatively, the overdamped Langevin dynamics

$$\mathrm{d}\overline{q}_t = F(\overline{q}_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t, \tag{3.2}$$

which describes the $\gamma \to \infty$ limit of the process $(q_{\gamma t})_{t\geq 0}$ in (3.1), may also be employed. Remarkably, both processes are related by the fact that when the force field F is conservative, that is to say that there exists $V : \mathbb{R}^d \to \mathbb{R}$ such that $F = -\nabla V$, then the stationary distribution of $(\overline{q}_t)_{t\geq 0}$ writes

$$\overline{\nu}(\mathrm{d}q) = \frac{1}{Z}\mathrm{e}^{-\beta V(q)}, \qquad Z = \int_{\mathbb{R}^d} \mathrm{e}^{-\beta V(q)}\mathrm{d}q, \tag{3.3}$$

while the stationary distribution of $(q_t, p_t)_{t\geq 0}$ has the product structure

$$\nu(\mathrm{d}q\mathrm{d}p) = \overline{\nu}(\mathrm{d}q)\frac{\mathrm{e}^{-\frac{\beta|p|^2}{2}}}{(2\pi\beta^{-1})^{\frac{d}{2}}}\mathrm{d}p, \tag{3.4}$$

the marginal in momentum of which is usually called the Maxwell distribution with inverse temperature β.

Such dynamics are used in particular to compute thermodynamic and dynamic quantities, with numerous applications in biology, chemistry and materials science. In many practical situations of interest, the system remains trapped for very long times in subsets of the phase space, called metastable states, see for example [58, Sections 6.3 and 6.4]. This makes the simulation of these systems over the times of interest impossible. Typically, these states are defined in terms of positions only, and are thus open sets $\mathscr{O}$ of $\mathbb{R}^d$ for (3.2) or cylinders of the form $D = \mathscr{O} \times \mathbb{R}^d$ for (3.1). In such a case, it is expected that the process reaches a local equilibrium distribution within the metastable state before leaving it. This distribution is called the quasi-stationary distribution (QSD). Proving the existence of this limiting behavior is in particular important to prove the consistency of accelerated dynamics algorithms, e.g. the parallel replica method, see for example [67]. It is also the building block to justify the use of jump Markov processes among the metastable states (kinetic Monte-Carlo or Markov state Models) to model the evolution over long timescales [78, 73].

While several works have already studied the properties of QSD for the overdamped Langevin dynamics (3.2), using in particular the ellipticity of this process as well as the fact that the domain $\mathscr{O}$ is often assumed to be bounded, to the best of our knowledge there are no available results for the Langevin dynamics (3.1), which is not elliptic but only hypoelliptic, and for which the natural domain $D = \mathscr{O} \times \mathbb{R}^d$ is not bounded, even if $\mathscr{O}$ is bounded. Building on several analytical results for the Langevin process (3.1) obtained in Chapter 2, including a compactness property satisfied by the semigroup of the Langevin process absorbed at the boundary ∂D, we apply the Krein-Rutman theorem to obtain spectral properties on the infinitesimal generator of the Langevin process on D with Dirichlet boundary conditions, and deduce the existence and uniqueness of a QSD $\mu^{(\gamma)}$, as well as the fact that it describes the long time behavior of the process conditioned on non absorption.

Alternatively, a more probabilistic approach, based on general criteria developed by Champagnat and Villemonais [20], is employed to obtain similar results in Chapter 4. As we were finishing this work, we also became aware of the related work [39], using different techniques based on Lyapounov functions.

Last, we study the limit of the QSD $\mu^{(\gamma)}$ on D when the friction parameter γ goes to infinity, and show that it converges to the product measure

$$\mu^{(\infty)}(\mathrm{d}q\mathrm{d}p) = \overline{\mu}(\mathrm{d}q)\frac{\mathrm{e}^{-\frac{\beta|p|^2}{2}}}{(2\pi\beta^{-1})^{\frac{d}{2}}}\mathrm{d}p, \tag{3.5}$$

where $\overline{\mu}$ is the QSD of the overdamped Langevin process $(\overline{q}_t)_{t\geq 0}$ in $\mathscr{O}$. While the similarity of this expression with (3.4) is striking, we shall see that unlike the latter identity, it is not true that for $\gamma < \infty$, $\mu^{(\gamma)}$ displays such a product structure.

Outline of the chapter. In Section 3.2, we give the main results, which are then proven in the subsequent sections. More precisely, Section 3.3 is devoted to the proof of the existence, uniqueness and convergence results obtained for the QSD of the Langevin process on D and Section 3.4 focuses on the weak overdamped limit of this QSD.

Notation. Let us introduce here some notation that will be used in the following. We denote by $x = (q, p)$ generic elements in $\mathbb{R}^{2d}$, and $|\cdot|$ the Euclidean norm both on $\mathbb{R}^d$ and on $\mathbb{R}^{2d}$. For $x \in \mathbb{R}^{2d}$, $\mathrm{B}(x, \rho)$ is the open ball centered in x with radius $\rho > 0$. For a measurable subset A of $\mathbb{R}^{2d}$, $\mathbb{R}_+^* \times \mathbb{R}^{2d}$ or $\mathbb{R}_+^* \times \mathbb{R}^{2d} \times \mathbb{R}^{2d}$,

- $|A|$ is the Lebesgue measure of A,
- for $1 \leq p \leq \infty$, $\mathrm{L}^p(A)$ is the set of L^p scalar-valued functions on A and $\|\cdot\|_{\mathrm{L}^p(A)}$ the associated norm,
- $\mathscr{C}(A)$ (resp. $\mathscr{C}^b(A)$) is the set of scalar-valued continuous (resp. continuous and bounded) functions on A,

- $\mathscr{C}^\infty(A)$ (resp. $\mathscr{C}_c^\infty(A)$) is the set of scalar-valued $\mathscr{C}^\infty$ (resp. $\mathscr{C}^\infty$ with compact support) functions on A.

We denote by $\|\cdot\|_\infty$ the sup norm on the Banach space $\mathscr{C}^b(A)$. For T a linear bounded operator on $\mathscr{C}^b(A)$, we denote its operator norm by:

$$|||T|||_{\mathscr{C}^b(A)} := \sup_{f\in\mathscr{C}^b(A), \|f\|_\infty\leq 1} \|Tf\|_\infty.$$

Quasi-stationary distribution. The notion of quasi-stationary distribution (QSD) is central in this text. We recall here its definition in a general setting, and refer to [23] for a complete introduction.

Let E be a Polish space endowed with its Borel σ-algebra $\mathscr{B}(E)$, and let $(X_t)_{t\geq 0}$ be a time-homogeneous, strong Markov process in E with continuous sample-paths. For any $x \in E$, we denote by $\mathbb{P}_x$ the probability measure under which $X_0 = x$ almost surely, and for any probability measure θ on E, we define

$$\mathbb{P}_\theta(\cdot) := \int_E \mathbb{P}_x(\cdot)\theta(\mathrm{d}x).$$

Let D be an open subset of E and τ_∂ be the stopping time defined by

$$\tau_\partial := \inf\{t > 0 : X_t \notin D\}.$$

Definition 3.1.1 (QSD). *A probability measure μ on D is said to be a QSD on D of the process $(X_t)_{t\geq 0}$, if for all $A \in \mathscr{B}(D) := \{A \cap D, A \in \mathscr{B}(E)\}$, for all $t \geq 0$,*

$$\mathbb{P}_\mu(X_t \in A, \tau_\partial > t) = \mu(A)\mathbb{P}_\mu(\tau_\partial > t). \tag{3.6}$$

When $\mathbb{P}_\mu(\tau_\partial > t) > 0$, the identity (3.6) equivalently writes $\mathbb{P}_\mu(X_t \in A|\tau_\partial > t) = \mu(A)$.

A closely related notion is that of Quasi-Limiting Distribution (QLD), which is a probability measure μ on D such that there exists a probability measure θ on D for which

$$\forall A \in \mathscr{B}(D), \qquad \mu(A) = \lim_{t\to\infty} \mathbb{P}_\theta(X_t \in A|\tau_\partial > t). \tag{3.7}$$

A QLD is necessarily a QSD (and the converse is obvious), and we say that μ "attracts" θ when (3.7) holds. When a QSD attracts all Dirac masses on D, it is called a Yaglom limit.

Last, when X_0 is initially distributed according to a QSD on D, the exit event from D of the process $(X_t)_{t\geq 0}$ satisfies the following properties, see [23, Theorem 2.6].

Proposition 3.1.2 (Exit event). *Let μ be a QSD on D of the process $(X_t)_{t\geq 0}$, then there exists $\lambda_0 \geq 0$ such that*

1. *τ_∂ follows the exponential law of parameter λ_0, that is to say $\mathbb{P}_\mu(\tau_\partial > t) = \mathrm{e}^{-\lambda_0 t}$ for all $t \geq 0$,*
2. *X_{τ_∂} is independent of τ_∂.*

In the previous statement, the case $\lambda_0 = 0$ means that $\tau_\partial = \infty$, $\mathbb{P}_\mu$-almost surely.

3.2 Main results

This section presents the main results we obtained.

As a motivation, we first recall in Section 3.2.1 what is known about the QSD of the overdamped Langevin process.

In order to prepare the exposition of our main results, we state various analytical properties of the Langevin process and the related kinetic Fokker-Planck equation in Section 3.2.2. The proofs of these auxiliary results are detailed in Chapter 2.

Our main results, concerning the degenerate case of the Langevin process, are presented in Section 3.2.3. We state the existence of a unique QSD in a bounded-in-position domain D. Besides, this QSD is the unique solution of an eigenvalue problem related to the kinetic Fokker-Planck operator and it attracts all probability measures on D, at an exponential rate.

Last, we address the overdamped limit $\gamma \to \infty$ of the QSD of the Langevin process in Section 3.2.4.

3.2.1 Elliptic case and the overdamped Langevin process

Quasi-stationary distributions on smooth bounded domains for elliptic diffusion processes, have been widely studied in the literature. We refer for example to [36, 55, 21, 19]. Let us recall here some of their important results.

Let $\beta > 0$ and $F : \mathbb{R}^d \mapsto \mathbb{R}^d$ satisfying the following assumption.

Assumption (F1). $F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$.

Let $(\Omega, \mathscr{F}, (\mathscr{F}_t)_{t\geq 0}, \mathbb{P})$ be a filtered probability space and $(B_t)_{t\geq 0}$ a d-dimensional $(\mathscr{F}_t)_{t\geq 0}$-Brownian motion. Under Assumption (F1), the vector field F is locally Lipschitz continuous and therefore the stochastic differential equation (3.2) possesses a unique strong solution $(\overline{q}_t)_{0\leq t<\overline{\tau}_\infty}$ defined up to some explosion time $\overline{\tau}_\infty \in (0, +\infty]$. The overdamped Langevin process admits the following infinitesimal generator:

$$\overline{\mathscr{L}} = F \cdot \nabla + \beta^{-1}\Delta, \tag{3.8}$$

with formal adjoint $\overline{\mathscr{L}}^*$ in $\mathrm{L}^2(\mathrm{d}x)$ given by:

$$\overline{\mathscr{L}}^* = -\mathrm{div}(F\cdot) + \beta^{-1}\Delta.$$

Let $\mathscr{O}$ be an open set of $\mathbb{R}^d$ satisfying the following assumption.

Assumption (O). *$\mathscr{O}$ is an open $\mathscr{C}^2$ bounded connected set of $\mathbb{R}^d$.*

Let $\overline{\tau}_\partial := \inf\{t > 0 : \overline{q}_t \notin \mathscr{O}\}$ be the first exit time from $\mathscr{O}$ of the process $(\overline{q}_t)_{0\leq t<\overline{\tau}_\infty}$. Under Assumption (O), the vector field F is Lipschitz continuous on $\mathscr{O}$ and therefore $\overline{\tau}_\partial \leq \overline{\tau}_\infty$.

It has been shown in [19, 36, 55, 50] that the overdamped Langevin process admits a unique QSD on $\mathscr{O}$, which moreover satisfies the following properties.

Theorem 3.2.1 (QSD of the overdamped Langevin process)**.** *Under Assumptions (F1) and (O), there exists a unique QSD $\overline{\mu}$ on $\mathscr{O}$ of the process $(\overline{q}_t)_{t\geq 0}$. Furthermore,*

(i) there exists $\overline{\psi} \in \mathscr{C}^2(\mathscr{O}) \cap \mathscr{C}^b(\overline{\mathscr{O}})$ such that $\overline{\mu}(\mathrm{d}q) = \overline{\psi}(q)\mathrm{d}q$, where $\mathrm{d}q$ is the Lebesgue measure on $\mathbb{R}^d$,

(ii) $\mathrm{Span}(\overline{\psi})$ is the eigenspace associated with the smallest eigenvalue $\overline{\lambda}$ of the operator $-\overline{\mathscr{L}}^*$ with homogeneous Dirichlet boundary conditions on $\partial\mathscr{O}$,

(iii) there exist $C > 0$ and $\alpha > 0$ such that for all probability measures θ on $\mathscr{O}$, for all $t \geq 0$,

$$\left\|\mathbb{P}_\theta(\overline{q}_t \in \cdot|\overline{\tau}_\partial > t) - \overline{\mu}(\cdot)\right\|_{TV} \leq C\mathrm{e}^{-\alpha t},$$

where $\|\cdot\|_{TV}$ is the total-variation norm on the space of bounded signed measures on $\mathbb{R}^d$.

Multiple approaches are used in the literature to obtain the properties above. In the conservative case $F = -\nabla V$, under suitable assumptions on V we have $\overline{\tau}_\infty = \infty$ and the process $(\overline{q}_t)_{t\geq 0}$ is reversible with respect to the measure $\overline{\nu}$ introduced in (3.3). As a consequence, $\overline{\mathscr{L}}$ is symmetric with respect to the canonical scalar product on $\mathrm{L}^2(\mathrm{d}\overline{\nu})$ and since the inverse of the operator $\overline{\mathscr{L}}$ with homogeneous Dirichlet boundary condition on $\partial\mathscr{O}$ is compact from $\mathrm{L}^2(\mathrm{d}\overline{\nu})$ to $\mathrm{L}^2(\mathrm{d}\overline{\nu})$, one can obtain a discrete spectral decomposition of $\overline{\mathscr{L}}$ with this boundary condition. This then yields the theorem above, see [55].

In the general case when F is non conservative, the process $(\overline{q}_t)_{t\geq 0}$ is not necessarily reversible but a spectral approach can still be used. In [36] the authors prove the compactness of the semigroup $(\overline{P}_t^{\mathscr{O}})_{t\geq 0}$ defined on the Banach space

$$\{f \in \mathscr{C}^b(\mathscr{O}) : \forall q \in \mathscr{O}, f(q) = \mathrm{d}_\partial(q)g(q) \quad \text{s.t. } g \text{ is uniformly continuous on } \mathscr{O}\},$$

where d_∂ is the Euclidean distance to the boundary $\partial\mathscr{O}$, by

$$\overline{P}_t^{\mathscr{O}} f : x \in D \mapsto \mathbb{E}_q\left[f(\overline{q}_t)\mathbb{1}_{\tau_\partial > t}\right],$$

using sharp estimates of the Green function of $\overline{\mathscr{L}}$ shown in [38]. Then, applying Krein-Rutman theorem to the operator $\overline{P}_t^{\mathscr{O}}$, the authors manage to deduce Theorem 3.2.1.

Last, a more probabilistic approach is developed in [19] where the authors prove that the semigroup $\overline{P}_t^{\mathscr{O}}$ satisfies a gradient estimate, irreducibility conditions and a controlled probability of absorption near the boundary $\partial\mathscr{O}$ which also yields Theorem 3.2.1.

3.2.2 Analytical properties of the Langevin process

In this section we recall some results from Chapter 2 that will be used henceforth. Let $\gamma \in \mathbb{R}$, $\sigma > 0$. Under Assumption (F1), the stochastic differential equation

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sigma \mathrm{d}B_t, \end{cases} \tag{3.9}$$

possesses a unique strong solution $(X_t = (q_t, p_t))_{0\leq t<\tau_\infty}$, defined up to some explosion time $\tau_\infty \in (0, +\infty]$. Notice that, compared to (3.1), we consider here and henceforth the mass to be identity without loss of generality (see the change of variables in [56, Equation (3.117)]), so that momentum is identified with velocity. Besides, we consider the general case $\gamma \in \mathbb{R}$ and $\sigma > 0$ not necessarily related to γ.

The infinitesimal generator of the Langevin process is called the kinetic Fokker-Planck operator $\mathscr{L}$, defined for $(q, p) \in \mathbb{R}^d \times \mathbb{R}^d$ by:

$$\mathscr{L} = p \cdot \nabla_q + F(q) \cdot \nabla_p - \gamma p \cdot \nabla_p + \frac{\sigma^2}{2}\Delta_p, \tag{3.10}$$

with formal adjoint $\mathscr{L}^*$ in $\mathrm{L}^2(\mathrm{d}x)$ given by:

$$\mathscr{L}^* = -p \cdot \nabla_q - F(q) \cdot \nabla_p + \gamma \mathrm{div}_p(p\cdot) + \frac{\sigma^2}{2}\Delta_p. \tag{3.11}$$

Let us strengthen Assumption (F1) on F.

Assumption (F2). *$F \in \mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ and F is bounded and globally Lipschitz continuous on $\mathbb{R}^d$.*

Under Assumption (F2), $\tau_\infty = \infty$ almost surely and the Langevin process (3.9) admits a smooth transition density $\mathrm{p}_t(x, y)$ [71, Corollary 7.2], which is positive [44, Corollary 3.3]. In addition, this density admits an explicit Gaussian upper-bound, see Theorem 2.2.19 that we now recall.

Theorem 3.2.2 (Gaussian upper-bound). *Under Assumption (F2), the transition density $\mathrm{p}_t(x, y)$ under $\mathbb{P}_x$ of the Langevin process $(X_t)_{t\geq 0}$ satisfying (3.9) is such that for all $\alpha \in (0, 1)$, there exists $c_\alpha > 0$, depending only on α, such that for all $T > 0$ and $t \in (0, T]$, for all $x, y \in \mathbb{R}^{2d}$,*

$$\mathrm{p}_t(x, y) \leq \frac{1}{\alpha^d}\sum_{j=0}^{\infty} \frac{\left(\|F\|_\infty c_\alpha (1 + \sqrt{\gamma_- T})\sqrt{\pi t}\right)^j}{\sigma^j \Gamma\left(\frac{j+1}{2}\right)} \widehat{\mathrm{p}}_t^{(\alpha)}(x, y), \tag{3.12}$$

where $\gamma_- = \max(-\gamma, 0)$ *is the negative part of* $\gamma \in \mathbb{R}$, Γ *is the Gamma function and* $\widehat{\mathrm{p}}_t^{(\alpha)}(x, y)$ *is the transition density of the Gaussian process* $(\widehat{q}_t^{(\alpha)}, \widehat{p}_t^{(\alpha)})_{t\geq 0}$ *defined by*

$$\begin{cases} \mathrm{d}\widehat{q}_t^{(\alpha)} = \widehat{p}_t^{(\alpha)}\mathrm{d}t, \\ \mathrm{d}\widehat{p}_t^{(\alpha)} = -\gamma\widehat{p}_t^{(\alpha)}\mathrm{d}t + \frac{\sigma}{\sqrt{\alpha}}\mathrm{d}B_t, \end{cases} \tag{3.13}$$

see equations (2.69)-(2.79) for explicit formulas.

Remark 3.2.3. *In the case* $\gamma > 0$ *and* $\sigma = \sqrt{2\gamma\beta^{-1}}$ *with* $\beta > 0$, *one easily obtains from (3.12) that for all* $T > 0$, $x, y \in \mathbb{R}^{2d}$,

$$\mathrm{p}_{\gamma T}(x, y) \leq \frac{1}{\alpha^d} \sum_{j=0}^{\infty} \frac{\left(\|F\|_\infty c_\alpha \sqrt{\pi T}\right)^j}{(2\beta^{-1})^{j/2}\Gamma\left(\frac{j+1}{2}\right)} \widehat{\mathrm{p}}_{\gamma T}^{(\alpha)}(x, y). \tag{3.14}$$

Notice that the series above is then independent of $\gamma > 0$. *This will play an important role in Section 3.4, when considering the overdamped limit* $\gamma \to \infty$.

We now let $\mathscr{O} \subset \mathbb{R}^d$ satisfy Assumption (O) and consider the following domain of $\mathbb{R}^{2d}$,

$$D := \mathscr{O} \times \mathbb{R}^d,$$

where the first coordinate (position) is constrained to remain on the bounded open set $\mathscr{O}$ and the second one (velocity) remains free. This is the natural phase space domain of the Langevin process absorbed when leaving $\mathscr{O}$.

For $q \in \partial\mathscr{O}$, let $n(q) \in \mathbb{R}^d$ be the unitary outward normal vector to $\mathscr{O}$ at $q \in \partial\mathscr{O}$. We introduce the following partition of ∂D:

$$\Gamma^0 = \{(q, p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) = 0\},$$

$$\Gamma^+ = \{(q, p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) > 0\},$$

$$\Gamma^- = \{(q, p) \in \partial\mathscr{O} \times \mathbb{R}^d : p \cdot n(q) < 0\}.$$

Let τ_∂ be the first exit time from D of the Langevin process $(X_t)_{t\geq 0}$ from (3.9), i.e.

$$\tau_\partial = \inf\{t > 0 : X_t \notin D\}.$$

Under Assumptions (F1) and (O), F is Lipschitz continuous on $\mathscr{O}$ and therefore $\tau_\partial \leq \tau_\infty$. The Langevin process absorbed outside of the domain D has been thoroughly studied in Chapter 2. Some of the results associated to its semigroup are reminded below and can be found in Theorems 2.2.10, 2.2.20, 2.6.2.

Theorem 3.2.4 (Transition density of the absorbed Langevin process)**.** *Under Assumptions (F1) and (O), there exists a function*

$$(t, x, y) \mapsto \mathrm{p}_t^D(x, y) \in \mathscr{C}^\infty(\mathbb{R}_+^* \times D \times D) \cap \mathscr{C}(\mathbb{R}_+^* \times \overline{D} \times \overline{D})$$

which satisfies for all $t > 0$,

- $\mathrm{p}_t^D(x, y) > 0$ *for all* $x \notin \Gamma^+ \cup \Gamma^0$ *and* $y \notin \Gamma^- \cup \Gamma^0$,
- $\mathrm{p}_t^D(x, y) = 0$ *if* $x \in \Gamma^+ \cup \Gamma^0$ *or if* $y \in \Gamma^- \cup \Gamma^0$,

and is such that for all $t > 0$*,* $x \in D$ *and* $A \in \mathscr{B}(D)$*,*

$$\mathbb{P}_x(X_t \in A, \tau_\partial > t) = \int_A \mathrm{p}_t^D(x,y)\mathrm{d}y.$$

Moreover, for $f \in \mathscr{C}^b(\overline{D})$*, the functions* u, v *defined by:*

$$\forall t > 0, \quad \forall x \in D, \qquad u(t,x) := \int_D \mathrm{p}_t^D(x,y)f(y)\mathrm{d}y, \qquad v(t,x) := \int_D \mathrm{p}_t^D(y,x)f(y)\mathrm{d}y,$$

are in $\mathscr{C}^\infty(\mathbb{R}_+^* \times D)$ *and satisfy:*

$$\forall t > 0, \quad \forall x \in D, \qquad \partial_t u(t,x) = \mathscr{L}u(t,x), \qquad \partial_t v(t,x) = \mathscr{L}^* v(t,x).$$

Remark 3.2.5. *For* F *satisfying Assumption (F2), one has that*

$$\forall t > 0, \quad \forall x, y \in \overline{D}, \qquad \mathrm{p}_t^D(x,y) \leq \mathrm{p}_t(x,y). \tag{3.15}$$

Besides, it follows from Remark 2.2.6 that p_t^D *only depends on the values of* F *inside* $\mathscr{O}$*, therefore* F*, satisfying Assumption (F1) can be modified arbitrarily to satisfy Assumption (F2) without modifying* p_t^D*. As a result, for* F *satisfying Assumption (F1),* $\mathrm{p}_t^D(x,y)$ *also satisfies the Gaussian upper-bound of Theorem 3.2.2. In particular, this is used in Lemma 2.6.7 to prove the following double integral estimate of* p_t^D*:*

$$\forall t > 0, \qquad \int_D \int_D \mathrm{p}_t^D(x,y)\mathrm{d}x\mathrm{d}y < \infty, \tag{3.16}$$

which is used in this work.

Theorem 3.2.6 (Semigroup of the absorbed Langevin process)**.** *Let Assumptions (O) and (F1) hold. For any* $t \geq 0$*,* $p \in [1, +\infty]$ *and* $f \in \mathrm{L}^p(D)$*, the quantity*

$$P_t^D f : x \in \overline{D} \mapsto \mathbb{E}_x\left[\mathbb{1}_{\tau_\partial > t} f(X_t)\right] \tag{3.17}$$

is well-defined. Besides, let $p, q \in [1, +\infty]$*.*

(i) *The family of operators* $(P_t^D)_{t\geq 0}$ *is a semigroup on* $\mathrm{L}^p(D)$ *and on* $\mathscr{C}^b(\overline{D})$*.*

(ii) *For any* $t > 0$*, the operator* P_t^D *maps* $L^p(D)$ *into* $L^q(D)$ *continuously.*

(iii) *For any* $t > 0$*, the operator* P_t^D *is compact from* $\mathrm{L}^p(D)$ *to* $\mathrm{L}^p(D)$*, and from* $\mathscr{C}^b(\overline{D})$ *to* $\mathscr{C}^b(\overline{D})$*.*

We conclude this subsection with a time-reversibility result from Chapter 2 linking the transition densities of the Langevin process (3.9) and of a process called here the "adjoint" Langevin process $(\widetilde{X}_t = (\widetilde{q}_t, \widetilde{p}_t))_{t\geq 0}$ with infinitesimal generator $\widetilde{\mathscr{L}} := \mathscr{L}^* - d\gamma$, and satisfying the following SDE:

$$\begin{cases} \mathrm{d}\widetilde{q}_t = -\widetilde{p}_t \mathrm{d}t, \\ \mathrm{d}\widetilde{p}_t = -F(\widetilde{q}_t)\mathrm{d}t + \gamma \widetilde{p}_t \mathrm{d}t + \sigma \mathrm{d}B_t. \end{cases} \tag{3.18}$$

Let $\widetilde{\tau}_\partial$ be the first exit time from D of $\widetilde{X}_t$, i.e. $\widetilde{\tau}_\partial := \inf\{t > 0 : \widetilde{X}_t \notin D\}$. The transition kernel $\mathbb{P}_x(\widetilde{X}_t \in \cdot, \widetilde{\tau}_\partial > t)$ admits a transition density $\widetilde{\mathrm{p}}_t^D(x,y)$ which satisfies the following equality, see Theorem 2.6.2.

Theorem 3.2.7 (Time-reversibility)**.** *Under Assumptions (F1) and (O),*

$$\forall t > 0, \quad \forall x, y \in D, \qquad \mathrm{p}_t^D(x,y) = \mathrm{e}^{d\gamma t}\widetilde{\mathrm{p}}_t^D(y,x). \tag{3.19}$$

Let $(\widetilde{P}_t^D)_{t\geq 0}$ be the semigroup associated to the transition density $\widetilde{\mathrm{p}}_t^D$, defined by

$$\widetilde{P}_t^D f : x \in \overline{D} \mapsto \mathbb{E}_x\left[\mathbb{1}_{\widetilde{\tau}_\partial > t} f(\widetilde{X}_t)\right]. \tag{3.20}$$

Remark 3.2.8. *Following the proof of Theorem 3.2.6 in Chapter 2 and using the equality in Theorem 3.2.7, one easily deduces that the semigroup* $(\widetilde{P}_t^D)_{t\geq 0}$ *also satisfies Theorem 3.2.6.*

3.2.3 QSD of the Langevin process

In this section and in the next one, we state the main results proven in this work. Let us emphasize the fact that the results stated in the present section hold for any $\gamma \in \mathbb{R}$, $\sigma > 0$ and F satisfying Assumption (F1). The first result focuses on the spectral radii of the semigroups $(P_t^D)_{t\geq 0}$ and $(\widetilde{P}_t^D)_{t\geq 0}$. Let us recall here the definition of the spectral radius of a bounded operator T on the Banach space $\mathscr{C}^b(\overline{D})$, which can be found in [70, p. 192].

Definition 3.2.9 (Spectrum and spectral radius)**.** *Let T be a bounded real operator on $\mathscr{C}^b(\overline{D})$ and I the identity operator. Let us call $\sigma(T)$ the spectrum of T which is defined by:*

$$\sigma(T) := \{\lambda \in \mathbb{C} : T - \lambda I \text{ does not have an inverse that is a bounded linear operator}\}.$$

The spectral radius $r(T)$ of T is then defined as:

$$r(T) := \sup_{\lambda \in \sigma(T)} |\lambda|.$$

We obtain the following result on the operators P_t^D and $\widetilde{P}_t^D$ (defined in (3.17) and (3.20)) and their spectral radius.

Theorem 3.2.10 (Spectral properties of P_t^D and $\widetilde{P}_t^D$)**.** *Under Assumptions (F1) and (O), there exists $\lambda_0 > 0$ such that for all $t \geq 0$,*

$$r(P_t^D) = \mathrm{e}^{-\lambda_0 t}, \qquad r(\widetilde{P}_t^D) = \mathrm{e}^{-(\lambda_0 + d\gamma)t}.$$

Besides, there exist unique functions $\phi, \psi \in \mathscr{C}^b(\overline{D})$, up to a multiplicative constant, such that for all $t \geq 0$,

$$P_t^D \phi = \mathrm{e}^{-\lambda_0 t}\phi \quad \text{and} \quad \widetilde{P}_t^D \psi = \mathrm{e}^{-(\lambda_0 + d\gamma)t}\psi.$$

Last, $\phi, \psi \in \mathrm{L}^1(D) \cap \mathscr{C}^\infty(D)$ and

- *$\phi > 0$ on $D \cup \Gamma^-$, $\phi = 0$ on $\Gamma^+ \cup \Gamma^0$ and $\mathscr{L}\phi = -\lambda_0 \phi$ on D,*
- *$\psi > 0$ on $D \cup \Gamma^+$, $\psi = 0$ on $\Gamma^- \cup \Gamma^0$ and $\mathscr{L}^*\psi = -\lambda_0 \psi$ on D.*

In the following, we choose ϕ and ψ such that $\int_D \phi(x)\mathrm{d}x = \int_D \psi(x)\mathrm{d}x = 1$. The proof of this theorem relies on the application of the Krein-Rutman theorem [72, p. 313] to the compact operators P_t^D and $\widetilde{P}_t^D$ on the Banach space $\mathscr{C}^b(\overline{D})$. We are able to deduce from this result the existence of a unique QSD on D for the processes $(X_t)_{t\geq 0}$ and $(\widetilde{X}_t)_{t\geq 0}$.

Theorem 3.2.11 (Existence and uniqueness of a QSD)**.** *Let Assumptions (F1) and (O) hold. Let μ and $\widetilde{\mu}$ be the following probability measures on D:*

$$\forall A \in \mathscr{B}(D), \qquad \mu(A) = \int_A \psi(x)\mathrm{d}x, \quad \widetilde{\mu}(A) = \int_A \phi(x)\mathrm{d}x. \tag{3.21}$$

Then μ (resp. $\widetilde{\mu}$) is the unique QSD on D of $(X_t)_{t\geq 0}$ (resp. $(\widetilde{X}_t)_{t\geq 0}$) and for all $t \geq 0$,

$$\mathbb{P}_\mu(\tau_\partial > t) = \mathrm{e}^{-\lambda_0 t}, \quad \mathbb{P}_{\widetilde{\mu}}(\widetilde{\tau}_\partial > t) = \mathrm{e}^{-(\lambda_0 + d\gamma)t}.$$

Remark 3.2.12. *The density ψ of the QSD μ satisfies $\psi > 0$ on Γ^+ and $\psi = 0$ on $\Gamma^- \cup \Gamma^0$. Therefore, for a fixed $\gamma \in \mathbb{R}$, the QSD μ does not admit a product structure as is displayed in (3.5).*

Furthermore, the densities of the QSD are the unique classical solutions to an eigenvalue problem.

Theorem 3.2.13 (Spectral interpretation of the QSD)**.** *Under Assumptions (F1) and (O), there exists a unique couple (λ, η) (resp. (λ^*, η^*)), up to a multiplicative constant on η (resp. η^*) such that $\eta \in \mathscr{C}^2(D) \cap \mathscr{C}^b(D \cup \Gamma^+)$ (resp. $\eta^* \in \mathscr{C}^2(D) \cap \mathscr{C}^b(D \cup \Gamma^-)$) is a non-zero, non-negative classical solution to the following problem*

$$\begin{cases} \mathscr{L}\eta(x) = -\lambda\eta(x) & x \in D, \\ \eta(x) = 0 & x \in \Gamma^+, \end{cases} \quad \textit{resp.} \quad \begin{cases} \mathscr{L}^*\eta^*(x) = -\lambda^*\eta^*(x) & x \in D, \\ \eta^*(x) = 0 & x \in \Gamma^-. \end{cases} \tag{3.22}$$

Moreover, $\eta \in \mathrm{L}^1(D)$, $\lambda = \lambda_0$ and $\frac{\eta}{\int_D \eta} = \phi$ (resp. $\eta^* \in \mathrm{L}^1(D)$, $\lambda^* = \lambda_0$ and $\frac{\eta^*}{\int_D \eta^*} = \psi$).

Remark 3.2.14. *In particular, it follows from the expression of the spectral radii in Theorem 3.2.10 that λ_0 is the smallest eigenvalue associated with the operators $-\mathscr{L}$ and $-\mathscr{L}^*$.*

Last, we are able to obtain the following long time asymptotics of the operator P_t^D, in the operator norm of the Banach space $\mathscr{C}^b(\overline{D})$.

Theorem 3.2.15 (Long time asymptotics)**.** *Let Assumptions (F1) and (O) hold. Let α^* be defined by*

$$\mathrm{e}^{-(\lambda_0+\alpha^*)} := \sup_{z \in \sigma(P_1^D)\setminus\{\mathrm{e}^{-\lambda_0}\}} |z|. \tag{3.23}$$

Then $\alpha^* \in (0, +\infty]$, and for all $\alpha \in [0, \alpha^*)$, there exists $C_\alpha > 0$ such that for all $t \geq 0$,

$$\left|\left|\left| P_t^D - \mathrm{e}^{-\lambda_0 t} \frac{\phi \otimes \psi}{\int_D \phi\psi} \right|\right|\right|_{\mathscr{C}^b(\overline{D})} \leq C_\alpha \mathrm{e}^{-(\lambda_0+\alpha)t},$$

where the tensor product $\phi \otimes \psi$ is defined by: for any $f \in \mathscr{C}^b(\overline{D})$, $\phi \otimes \psi(f) = (\int_D \psi f)\phi$.

We deduce from the previous results that the QSD μ attracts all probability measures θ on D at an exponential rate.

Theorem 3.2.16 (Convergence to the QSD in total variation)**.** *Under the assumptions of Theorem 3.2.15, for all $\alpha \in [0, \alpha^*)$, there exists $C'_\alpha > 0$ such that, for all $t \geq 0$, for any probability measure θ on D, $\mathbb{P}_\theta(\tau_\partial > t) > 0$, and*

$$\|\mathbb{P}_\theta(X_t \in \cdot | \tau_\partial > t) - \mu\|_{TV} \leq \frac{C'_\alpha}{\int_D \phi \mathrm{d}\theta} \mathrm{e}^{-\alpha t}, \tag{3.24}$$

where $\|\cdot\|_{TV}$ denotes the total-variation norm on the space of bounded signed measures on $\mathbb{R}^{2d}$.

Remark 3.2.17. *The convergence speed and the prefactor are similar to what is obtained in Chapter 4 using the results by Champagnat and Villemonais, see [20]. However the prefactor depends on the initial distribution θ which is not the case for the overdamped Langevin process in Theorem 3.2.1.*

Remark 3.2.18. *Theorems 3.2.15 and 3.2.16 can be also obtained for the adjoint Langevin process $(\widetilde{X}_t)_{t\geq 0}$ (3.18) following the exact same proofs and using the equality in Theorem 3.2.7 satisfied by its transition density $\widetilde{\mathrm{p}}_t^D(x, y)$.*

The proofs of the theorems above are divided as follows. In Section 3.3.1 we prove Theorem 3.2.10 and in Section 3.3.2 we prove Theorems 3.2.11 and 3.2.13. Finally, Section 3.3.3 is devoted to the proofs of Theorems 3.2.15 and 3.2.16.

3.2.4 Overdamped limit of the QSD of the Langevin process

In this section we consider the case $\gamma > 0$ and $\sigma = \sqrt{2\gamma\beta^{-1}}$ with $\beta > 0$ independent of γ, and we study the overdamped limit, i.e. when γ goes to infinity, of the QSD on D of $(X_t)_{t\geq 0}$. Let us thus rewrite, for future reference, the Langevin process with these specific parameters

$$\begin{cases} \mathrm{d}q_t^{(\gamma)} = p_t^{(\gamma)}\mathrm{d}t, \\ \mathrm{d}p_t^{(\gamma)} = F(q_t^{(\gamma)})\mathrm{d}t - \gamma p_t^{(\gamma)}\mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}B_t, \end{cases} \tag{3.25}$$

and denote by $\mu^{(\gamma)}$ the QSD given by Theorem 3.2.11 as well as $\lambda_0^{(\gamma)}$ the associated smallest eigenvalue of $-\mathscr{L}$.

The motivation behind this comes from the well-known fact that, when $\gamma \to \infty$, for all $T > 0$, the process $(q_{\gamma t}^{(\gamma)})_{t\in[0,T]}$ converges in distribution to $(\overline{q}_t)_{t\in[0,T]}$ [56, Proposition 2.15] on the space of continuous functions on $[0,T]$, endowed with the supremum norm on $[0,T]$. Therefore, it may be expected that the marginal law in position of the QSD on D of $(X_t)_{t\geq 0}$ converges weakly to the QSD on $\mathscr{O}$ of the overdamped Langevin process. Here, we actually prove a more general result and consider the weak convergence of the QSD on D, from which we can easily deduce the weak convergence of the marginal distributions. This convergence result relies heavily on the following generalization of the overdamped limit of the Langevin process. In this statement, it is more convenient to keep track of the initial value q (resp. $x = (q,p)$) of the solution to (3.2) (resp. to (3.25)) by denoting the latter by $(\overline{q}_t^q)_{t\geq 0}$ (resp. $(X_t^{(\gamma),x} = (q_t^{(\gamma),x}, p_t^{(\gamma),x}))_{t\geq 0}$).

Theorem 3.2.19 (Generalization of the overdamped limit of the Langevin process)**.** *Let Assumption (F2) hold. Let $T > 0$ and $x = (q,p) \in \mathbb{R}^{2d}$. Let $Z \sim \mathscr{N}_d(0, \beta^{-1}I_d)$ be a Gaussian vector independent of the process $(\overline{q}_t^q)_{t\in[0,T]}$. The law of the couple $((q_{\gamma t}^{(\gamma),x})_{t\in[0,T]}, p_{\gamma T}^{(\gamma),x})$ converges weakly to the law of $((\overline{q}_t^q)_{t\in[0,T]}, Z)$ when $\gamma \to \infty$.*

Using this convergence, we are able to prove the following result.

Theorem 3.2.20 (QSD overdamped limit)**.** *Let Assumptions (F1) and (O) hold. The QSD $\mu^{(\gamma)}$ converges weakly, when $\gamma \to \infty$, to the probability measure $\mu^{(\infty)}$ on D defined by:*

$$\mu^{(\infty)}(\mathrm{d}q\mathrm{d}p) := \overline{\psi}(q)\frac{\mathrm{e}^{-\frac{\beta|p|^2}{2}}}{(2\pi\beta^{-1})^{\frac{d}{2}}}\mathrm{d}q\mathrm{d}p. \tag{3.26}$$

Furthermore, the eigenvalue $\lambda_0^{(\gamma)}$ associated with the QSD satisfies

$$\lambda_0^{(\gamma)} \underset{\gamma\to\infty}{\sim} \frac{\overline{\lambda}}{\gamma},$$

where $\overline{\lambda}$ and $\overline{\psi}$ are defined in Theorem 3.2.1.

Theorem 3.2.19 is proven in Section 3.4.1 and Theorem 3.2.20 is proven in Section 3.4.2.

3.3 Existence, uniqueness and long time convergence for the QSD

Let us start this section with the proof of Theorem 3.2.10.

3.3.1 Proof of Theorem 3.2.10

In this subsection we apply the Krein-Rutman theorem to the operators P_t^D and $\widetilde{P}_t^D$, defined in (3.17) and (3.20). In order to do that we first recall an important property satisfied by the spectral radius of a bounded operator, see [70, p. 192, Theorem VI.6].

Proposition 3.3.1 ([70])**.** *Let T be a bounded real operator on $\mathscr{C}^b(\overline{D})$. One has that*

$$r(T) = \lim_{n\to\infty} |||T^n|||^{1/n}_{\mathscr{C}^b(\overline{D})}.$$

The Krein-Rutman theorem, recalled below, basically states that under some conditions on the bounded operator T, the spectral radius $r(T)$ is also an eigenvalue of the operator T. The following version of the Krein-Rutman theorem can be found in [72, p. 313].

Theorem 3.3.2. *(Krein-Rutman theorem [72]) Let $K \subset \mathscr{C}^b(\overline{D})$ be a convex cone such that the set $\{f - g : f, g \in K\}$ is dense in $\mathscr{C}^b(\overline{D})$. Let $T : \mathscr{C}^b(\overline{D}) \mapsto \mathscr{C}^b(\overline{D})$ be a non-zero compact operator such that $T(K) \subset K$, and assume that its spectral radius $r(T)$ is strictly positive. Then, $r(T)$ is an eigenvalue of T with an eigenvector u in $K \setminus \{0\}$ such that $T(u) = r(T)u$.*

Let K be the following convex cone of $\mathscr{C}^b(\overline{D})$,

$$K := \{f \in \mathscr{C}^b(\overline{D}) : f \geq 0\}. \tag{3.27}$$

The density of $\{f - g : f, g \in K\}$ in $\mathscr{C}^b(\overline{D})$ is immediate. Our goal now is to apply the Krein-Rutman theorem above to the compact operators P_t^D and $\widetilde{P}_t^D$, for $t > 0$, on the cone K. In order to do that we need to prove the positivity of the spectral radii $r(P_t^D)$ and $r(\widetilde{P}_t^D)$ for $t > 0$.

Proposition 3.3.3 (Spectral radius positivity)**.** *Under Assumptions (F1) and (O), for all $t > 0$, $r(P_t^D) > 0$ and $r(\widetilde{P}_t^D) > 0$.*

Proof. Let $t > 0$. We prove here that $r(P_t^D) > 0$ which relies merely on the positivity of its transition density $\mathrm{p}_t^D(\cdot,\cdot)$ on $D \times D$, see Theorem 3.2.4. Besides, the positivity of the transition density $\widetilde{\mathrm{p}}_t^D(\cdot,\cdot)$ easily follows from the equality in Theorem 3.2.7, therefore the exact same proof applies to $\widetilde{P}_t^D$ and ensures that $r(\widetilde{P}_t^D) > 0$. As a result, we omit here the case of $\widetilde{P}_t^D$ to avoid repetition.

Following Proposition 3.3.1, it is sufficient to prove that there exists a constant $\beta > 0$ such that for all $n \geq 1$, $|||(P_t^D)^n|||^{1/n}_{\mathscr{C}^b(\overline{D})} \geq \beta$. Let $C \subset D$ be a compact set with positive Lebesgue measure, i.e. $|C| > 0$. It follows from Theorem 3.2.4 that P_t^D admits a smooth transition density p_t^D, which is positive on $C \times C$. Therefore, there exists $\alpha > 0$ such that for all $x, y \in C$, $\mathrm{p}_t^D(x, y) \geq \alpha$. Besides, for $n \geq 1$,

$$\left|\left|\left|\left(P_t^D\right)^n\right|\right|\right|_{\mathscr{C}^b(\overline{D})} \geq \left\|\left(P_t^D\right)^n \mathbb{1}_D\right\|_\infty.$$

Moreover, for all $x \in C$,

$$\begin{aligned}
\left\|\left(P_t^D\right)^n \mathbb{1}_D\right\|_\infty &\geq \left(P_t^D\right)^n \mathbb{1}_D(x) \\
&= \int_{D^n} \mathrm{p}_t^D(x, y_1)\ldots\mathrm{p}_t^D(y_{n-1}, y_n)\mathrm{d}y_1\ldots\mathrm{d}y_n \\
&\geq \int_{C^n} \mathrm{p}_t^D(x, y_1)\ldots\mathrm{p}_t^D(y_{n-1}, y_n)\mathrm{d}y_1\ldots\mathrm{d}y_n \\
&\geq (\alpha|C|)^n.
\end{aligned}$$

Consequently, for all $n \geq 1$,

$$\left|\left|\left|\left(P_t^D\right)^n\right|\right|\right|^{1/n}_{\mathscr{C}^b(\overline{D})} \geq \alpha|C| > 0,$$

which concludes the proof. □

We now apply Theorem 3.3.2 to the operators P_t^D and $\widetilde{P}_t^D$ on the cone K to obtain that $r(P_t^D)$ and $r(\widetilde{P}_t^D)$ are eigenvalues of their respective operators. In addition, these eigenvalues are shown to be simple. The following proof is inspired from unpublished lecture notes by P. Collet.

Proposition 3.3.4 (Consequence of the Krein-Rutman theorem)**.** *Let Assumptions (F1) and (O) hold. For all $t > 0$, $r(P_t^D)$ (resp. $r(\widetilde{P}_t^D)$) is a simple eigenvalue of the operator P_t^D (resp. $\widetilde{P}_t^D$) with eigenspace generated by an element ϕ_t (resp. ψ_t) of $K \cap \mathrm{L}^1(D)$ such that $\phi_t > 0$ (resp. $\psi_t > 0$) on D. Furthermore, $r(\widetilde{P}_t^D) = r(P_t^D)\mathrm{e}^{-d\gamma t}$.*

Proof. Let $t > 0$. The compactness of P_t^D and $\widetilde{P}_t^D$ on $\mathscr{C}^b(\overline{D})$ follows from Theorem 3.2.6 and Remark 3.2.8. Besides, the cone K defined in (3.27) evidently satisfies the assumptions of Theorem 3.3.2. Therefore, by Theorem 3.3.2 and Proposition 3.3.3 we obtain the existence of $\phi_t, \psi_t \in K \setminus \{0\}$ such that

$$P_t^D\phi_t = r(P_t^D)\phi_t, \qquad \widetilde{P}_t^D\psi_t = r(\widetilde{P}_t^D)\psi_t. \tag{3.28}$$

Step 1: Let us prove that

$$r(\widetilde{P}_t^D) = r(P_t^D)\mathrm{e}^{-d\gamma t} \tag{3.29}$$

by computing the integral $\int_D \psi_t(x)P_t^D\phi_t(x)\mathrm{d}x$ in two different ways. On the one hand, by (3.28),

$$\int_D \psi_t(x)P_t^D\phi_t(x)\mathrm{d}x = r(P_t^D)\int_D \psi_t(x)\phi_t(x)\mathrm{d}x. \tag{3.30}$$

On the other hand, using Fubini-Tonelli's theorem, Theorem 3.2.7 and (3.28) again,

$$\begin{aligned}\int_D \psi_t(x)P_t^D\phi_t(x)\mathrm{d}x &= \mathrm{e}^{d\gamma t}\int_D \phi_t(x)\widetilde{P}_t^D\psi_t(x)\mathrm{d}x \\ &= \mathrm{e}^{d\gamma t}r(\widetilde{P}_t^D)\int_D \phi_t(x)\psi_t(x)\mathrm{d}x.\end{aligned} \tag{3.31}$$

Let us now prove that $\int_D \phi_t(x)\psi_t(x)\mathrm{d}x \in (0,\infty)$. First, for $x \in D$, $r(P_t^D)\phi_t(x) = P_t^D\phi_t(x) = \int_D \mathrm{p}_t^D(x,y)\phi_t(y)\mathrm{d}y > 0$ since $\phi_t \in K \setminus \{0\}$ and $\mathrm{p}_t^D > 0$ on $D \times D$ by Theorem 3.2.4. Therefore, $\phi_t > 0$ on D. Likewise $\psi_t > 0$ on D so that $\int_D \phi_t(x)\psi_t(x)\mathrm{d}x > 0$. Second, using the boundedness of ϕ_t along with the double integral estimate (3.16) from Remark 3.2.5 in the left equality in (3.28), one obtains that $\phi_t \in \mathrm{L}^1(D)$. Using Theorem 3.2.7 one also has that $\psi_t \in \mathrm{L}^1(D)$. In particular, since ϕ_t and ψ_t are in $\mathrm{L}^\infty(D)$, this yields that $\int_D \phi_t(x)\psi_t(x)\mathrm{d}x < \infty$. As a result, the equalities (3.30) and (3.31) yield (3.29).

Step 2: Let us prove that every real-valued eigenvector of P_t^D associated with the eigenvalue $r(P_t^D)$ has a constant sign. Assume that there exists $h_t \in \mathscr{C}^b(\overline{D})$ such that $P_t^D h_t = r(P_t^D)h_t$ and h_t changes sign on D. Then, by the positivity of p_t^D one has for $x \in D$,

$$\begin{aligned}r(P_t^D)|h_t(x)| &= |P_t^D h_t(x)| \\ &= \left|\int_D \mathrm{p}_t^D(x,y)h_t(y)\mathrm{d}y\right| \\ &< \int_D \mathrm{p}_t^D(x,y)|h_t(y)|\mathrm{d}y = P_t^D|h_t|(x).\end{aligned}$$

As a result, since $\psi_t > 0$ on D, by Theorem 3.2.7 one has that

$$\begin{aligned}r(P_t^D)\int_D \psi_t(x)|h_t(x)|\mathrm{d}x &< \int_D \psi_t(x)P_t^D|h_t|(x)\mathrm{d}x \\ &= \mathrm{e}^{d\gamma t}\int_D \widetilde{P}_t^D\psi_t(x)|h_t(x)|\mathrm{d}x \\ &= r(P_t^D)\int_D \psi_t(x)|h_t(x)|\mathrm{d}x,\end{aligned}$$

by (3.29), which leads to a contradiction. Therefore, h_t has a constant sign on D.

Step 3: Let h_t be a real-valued eigenvector of P_t^D associated with the eigenvalue $r(P_t^D)$, let us prove that $h_t \in \mathrm{Span}(\phi_t)$. Up to changing h_t to $-h_t$, we can assume that $h_t \in K$ by Step 2. Let us define for $x \in D$,

$$\widetilde{h}_t(x) := \frac{h_t(x)}{\int_D \psi_t(y) h_t(y) \mathrm{d}y}, \qquad \widetilde{\phi}_t(x) := \frac{\phi_t(x)}{\int_D \psi_t(y)\phi_t(y)\mathrm{d}y},$$

so that

$$\int_D \widetilde{h}_t(x)\psi_t(x)\mathrm{d}x = \int_D \widetilde{\phi}_t(x)\psi_t(x)\mathrm{d}x = 1. \tag{3.32}$$

Notice that, $\widetilde{\phi}_t - \widetilde{h}_t$ is an eigenvector of P_t^D with eigenvalue $r(P_t^D)$, therefore it has a constant sign. By (3.32), one concludes that necessarily $\widetilde{\phi}_t - \widetilde{h}_t = 0$ on D since $\psi_t > 0$ on D. Hence $h_t \in \mathrm{Span}(\phi_t)$ and $r(P_t^D)$ is a simple eigenvalue.

Step 4: Applying this time **Step 2** and **Step 3** to the operator $\widetilde{P}_t^D$, one also obtains that $r(\widetilde{P}_t^D)$ is also a simple eigenvalue. This concludes the proof of Proposition 3.3.4. □

To prove Theorem 3.2.10, we finally need the following technical lemma.

Lemma 3.3.5 (High velocity exit event). *Under Assumptions (F1) and (O),*

$$\forall t > 0, \qquad \sup_{q\in\mathscr{O}} \mathbb{P}_{(q,p)}(\tau_\partial > t) \underset{|p|\to\infty}{\longrightarrow} 0.$$

Proof. Let $t > 0$. For $\alpha \in (0,1)$, by Remark 3.2.5, there exists $C > 0$ only depending on t and α such that for all $x, y \in D$, $\mathrm{p}_t^D(x,y) \leq C\widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$, where $\widehat{\mathrm{p}}_t^{(\alpha)}(x,y)$ is the transition density of the process $(\widehat{q}_t^{(\alpha)}, \widehat{p}_t^{(\alpha)})_{t\geq 0}$ defined in (3.13).

Furthermore, for $x = (q,p) \in D$, the law of $\widehat{q}_t^{(\alpha)}$ is Gaussian with mean $q + tp\Phi_1(\gamma t)$ and covariance matrix $\frac{\sigma^2 t^3}{3\alpha}\Phi_2(\gamma t) I_d$, where Φ_1 are Φ_2 are defined as follows, see equations (2.69) and (2.70),

$$\Phi_1 : \rho \in \mathbb{R} \mapsto \begin{cases} \dfrac{1 - \mathrm{e}^{-\rho}}{\rho} & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0, \end{cases} \tag{3.33}$$

$$\Phi_2 : \rho \in \mathbb{R} \mapsto \begin{cases} \dfrac{3}{2\rho^3}\left[2\rho - 3 + 4\mathrm{e}^{-\rho} - \mathrm{e}^{-2\rho}\right] & \text{if } \rho \neq 0, \\ 1 & \text{if } \rho = 0. \end{cases} \tag{3.34}$$

Therefore,

$$\int_{\mathbb{R}^d} \widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p'))\mathrm{d}p' = \frac{(3\alpha)^{d/2}}{(2\pi\sigma^2 t^3 \Phi_2(\gamma t))^{d/2}} \mathrm{e}^{-\frac{3\alpha t^2 \Phi_1(\gamma t)^2}{2\sigma^2 t^3 \Phi_2(\gamma t)}\left|p - \frac{q'-q}{t\Phi_1(\gamma t)}\right|^2}.$$

Let $\delta := \sup_{q,q'\in\mathscr{O}} |q - q'|$ (which is finite since $\mathscr{O}$ is bounded), then for $t > 0$ and $q, q' \in \mathscr{O}$, if $|p| \geq \frac{2\delta}{t\Phi_1(\gamma t)}$ (Φ_1 is positive),

$$\int_{\mathbb{R}^d} \widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p'))\mathrm{d}p' \leq \frac{(3\alpha)^{d/2}}{(2\pi\sigma^2 t^3 \Phi_2(\gamma t))^{d/2}} \mathrm{e}^{-\frac{3\alpha t^2 \Phi_1(\gamma t)^2}{8\sigma^2 t^3 \Phi_2(\gamma t)}|p|^2}.$$

As a consequence,

$$\begin{aligned}
\sup_{q\in\mathscr{O}} \mathbb{P}_{(q,p)}(\tau_\partial > t) &= \sup_{q\in\mathscr{O}} \int_{\mathscr{O}} \int_{\mathbb{R}^d} \mathrm{p}_t^D((q,p),(q',p'))\mathrm{d}p'\mathrm{d}q' \\
&\leq \sup_{q\in\mathscr{O}} C \int_{\mathscr{O}} \int_{\mathbb{R}^d} \widehat{\mathrm{p}}_t^{(\alpha)}((q,p),(q',p'))\mathrm{d}p'\mathrm{d}q' \\
&\leq C \frac{(3\alpha)^{d/2}|\mathscr{O}|}{(2\pi\sigma^2 t^3\Phi_2(\gamma t))^{d/2}} \mathrm{e}^{-\frac{3\alpha t^2\Phi_1(\gamma t)^2}{8\sigma^2 t^3 \Phi_2(\gamma t)}|p|^2} \underset{|p|\to\infty}{\longrightarrow} 0,
\end{aligned}$$

which concludes the proof. □

We are now in position to prove Theorem 3.2.10.

Proof of Theorem 3.2.10. For $t>0$, let ϕ_t (resp. ψ_t) be an eigenvector of P_t^D (resp. $\widetilde{P}_t^D$) in $K\setminus\{0\}$ associated with the eigenvalue $r(P_t^D)$ (resp. $r(\widetilde{P}_t^D)$) and such that $\phi_t>0$ (resp. $\psi_t>0$) on D, whose existence is ensured by Proposition 3.3.4. We will prove Theorem 3.2.10 for ϕ_t and P_t^D, but the exact same reasoning with the operator $\widetilde{P}_t^D$ instead yields the proof for ψ_t and $\widetilde{P}_t^D$.

Step 1: Let us start by proving that $\mathrm{Span}(\phi_t, t>0)$ is a one-dimensional space generated by a function $\phi\in K$. This is the case if one can prove that for all $s,t>0$, $\phi_s\in\mathrm{Span}(\phi_t)$.

For $s,t>0$, $P_s^D\phi_s=r(P_s^D)\phi_s$. Furthermore, by the semigroup property satisfied by $(P_r^D)_{r\geq 0}$,

$$P_s^DP_t^D\phi_s=P_t^DP_s^D\phi_s=r(P_s^D)P_t^D\phi_s.$$

Since $r(P_s^D)$ is a simple eigenvalue of P_s^D by Proposition 3.3.4 then $P_t^D\phi_s\in\mathrm{Span}(\phi_s)$, i.e. there exists $\alpha_{t,s}>0$ such that $P_t^D\phi_s=\alpha_{t,s}\phi_s$.

Let us prove that $\alpha_{t,s}=r(P_t^D)$. Consider the integral $\int_D P_t^D\phi_s(x)\psi_t(x)\mathrm{d}x$. One has that

$$\int_D P_t^D\phi_s(x)\psi_t(x)\mathrm{d}x=\alpha_{t,s}\int_D\phi_s(x)\psi_t(x)\mathrm{d}x.$$

Furthermore, Theorem 3.2.7 and Proposition 3.3.4 also ensure that

$$\int_D P_t^D\phi_s(x)\psi_t(x)\mathrm{d}x=\mathrm{e}^{d\gamma t}\int_D\phi_s(x)\widetilde{P}_t^D\psi_t(x)\mathrm{d}x=r(P_t^D)\int_D\phi_s(x)\psi_t(x)\mathrm{d}x.$$

Since ϕ_s,ψ_t are positive on D and belong to $\mathscr{C}^b(\overline{D})\cap\mathrm{L}^1(D)$ then $\int_D\phi_s(x)\psi_t(x)\mathrm{d}x\in(0,\infty)$. Therefore, the equalities above ensure that $\alpha_{t,s}=r(P_t^D)$. In particular, this yields that $\phi_s\in\mathrm{Span}(\phi_t)$ since $r(P_t^D)$ is a simple eigenvalue for P_t^D. Let us now denote by $\phi\in K$ a function generating $\mathrm{Span}(\phi_t,t>0)$.

Step 2: Let us now show that there exists $\lambda_0\geq 0$ such that for all $t>0$, $r(P_t^D)=\mathrm{e}^{-\lambda_0 t}$. For $s,t>0$, $P_{t+s}^D\phi=r(P_{t+s}^D)\phi$. Besides,

$$\begin{aligned}P_{t+s}^D\phi&=P_t^DP_s^D\phi\\&=r(P_t^D)r(P_s^D)\phi.\end{aligned}$$

Therefore, $r(P_{t+s}^D)=r(P_t^D)r(P_s^D)$ since $\phi>0$. Since $|||P_s^D|||_{\mathscr{C}^b(\overline{D})}\leq 1$ for all $s>0$, then $r(P_s^D)\leq 1$. As a result, for all $s,t>0$, $r(P_{t+s}^D)\leq r(P_t^D)$. Consequently, the function $v:t>0\mapsto\log(r(P_t^D))$ is a decreasing function which satisfies the Cauchy equation:

$$\forall s,t>0,\qquad v_{t+s}=v_t+v_s.$$

Classical results for Cauchy equations ensure that v_t is linear. This implies that there exists $\lambda_0\geq 0$ such that for all $t>0$, $r(P_t^D)=\mathrm{e}^{-\lambda_0 t}$.

Step 3: Let us prove that $\lambda_0>0$. Assume that $\lambda_0=0$, then for all $(q,p)\in D$, $t>0$,

$$P_t^D\phi(q,p)=\mathbb{E}_{(q,p)}\left[\mathbb{1}_{\tau_\partial>t}\phi(X_t)\right]=\phi(q,p).$$

Hence, $\sup_{q\in\mathscr{O}}\phi(q,p)\leq\|\phi\|_\infty\sup_{q\in\mathscr{O}}\mathbb{P}_{(q,p)}(\tau_\partial>t)\underset{|p|\to\infty}{\longrightarrow}0$ by Lemma 3.3.5. As a consequence, $\phi\in\mathscr{C}^b(\overline{D})$ attains its maximum $\|\phi\|_\infty$ at some $x_0\in\overline{D}$. Then, $\|\phi\|_\infty=\phi(x_0)\leq\|\phi\|_\infty\mathbb{P}_{x_0}(\tau_\partial>t)$. Hence, $\mathbb{P}_{x_0}(\tau_\partial>t)=1$, which leads to a contradiction since $\mathbb{P}_{x_0}(X_t\in\mathbb{R}^{2d}\setminus D)>0$.

Step 4: Let us finally prove the properties on ϕ stated in Theorem 3.2.10. First, $\phi\in\mathscr{C}^b(\overline{D})\cap\mathrm{L}^1(D)$ by Proposition 3.3.4. In addition, $\phi>0$ on $D\cup\Gamma^-$ and $\phi=0$ on $\Gamma^+\cup\Gamma^0$ using Theorem 3.2.4 and the fact that $P_t^D\phi=\mathrm{e}^{-\lambda_0 t}\phi$. Last, letting $u(t,x)=P_t^D\phi(x)$ in Theorem 3.2.4, we get that $u\in\mathscr{C}^\infty(\mathbb{R}_+^*\times D)$ and $\partial_t u=\mathscr{L}u$, but since $u(t,x)$ also writes $\mathrm{e}^{-\lambda_0 t}\phi(x)$, we conclude that $\phi\in\mathscr{C}^\infty(D)$ and $\mathscr{L}\phi=-\lambda_0\phi$ on D. □

3.3.2 Proof of Theorem 3.2.11 and Theorem 3.2.13

Let us now prove the existence of a unique QSD on the domain D for the processes $(X_t)_{t\geq 0}$ in (3.9) and $(\widetilde{X}_t)_{t\geq 0}$ in (3.18).

Proof of Theorem 3.2.11. We prove this theorem for the process $(X_t)_{t\geq 0}$ and notice that the exact same proof with the process $(\widetilde{X}_t)_{t\geq 0}$ instead of $(X_t)_{t\geq 0}$ yields the result for $(\widetilde{X}_t)_{t\geq 0}$ with the function ϕ instead of ψ.

Step 1: Let us prove that the measure μ defined in (3.21) is a QSD on D of the Langevin process $(X_t)_{t\geq 0}$.

Let $t > 0$, $A \in \mathscr{B}(D)$. Integrating the equality $\widetilde{P}_t^D\psi = \mathrm{e}^{-(\lambda_0+d\gamma)t}\psi$ over A, one obtains that

$$\int_A \widetilde{P}_t^D\psi(x)\mathrm{d}x = \mathrm{e}^{-(\lambda_0+d\gamma)t}\int_A \psi(x)\mathrm{d}x. \tag{3.35}$$

Furthermore, using Fubini-Tonelli's theorem along with Theorem 3.2.7, one has that

$$\int_A \widetilde{P}_t^D\psi(x)\mathrm{d}x = \mathrm{e}^{-d\gamma t}\int_D \psi(x)\mathbb{P}_x(X_t \in A, \tau_\partial > t)\mathrm{d}x.$$

Therefore, reinjecting into (3.35) we obtain since $\mu(\mathrm{d}x) = \psi(x)\mathrm{d}x$ that

$$\mathbb{P}_\mu(X_t \in A, \tau_\partial > t) = \mathrm{e}^{-\lambda_0 t}\mu(A),$$

which gives in particular for $A = D$ that $\mathbb{P}_\mu(\tau_\partial > t) = \mathrm{e}^{-\lambda_0 t}$ and thus μ is a QSD on D for the process $(X_t)_{t\geq 0}$ by Definition 3.1.1.

Step 2: Let $\check{\mu}$ be a QSD on D for the process $(X_t)_{t\geq 0}$. Let us prove that $\check{\mu} = \mu$, where μ is defined in (3.21). We start by proving that $\check{\mu}$ admits a density with respect to the Lebesgue measure on D and that its density is an eigenvector of the semigroup $(\widetilde{P}_t^D)_{t>0}$. By Definition 3.1.1, for all $A \in \mathscr{B}(D)$ and $t > 0$,

$$\mathbb{P}_{\check{\mu}}(X_t \in A, \tau_\partial > t) = \mathbb{P}_{\check{\mu}}(\tau_\partial > t)\check{\mu}(A). \tag{3.36}$$

Moreover, by Proposition 3.1.2 and the positivity of the transition density p_t^D on $D \times D$ stated in Theorem 3.2.4, there exists $\check{\lambda}_0 \in [0,\infty)$ such that $\mathbb{P}_{\check{\mu}}(\tau_\partial > t) = \mathrm{e}^{-\check{\lambda}_0 t}$.

Let $A \in \mathscr{B}(D)$ with zero Lebesgue measure, then for all $x \in D$, $\mathbb{P}_x(X_t \in A, \tau_\partial > t) = 0$ by Theorem 3.2.4. As a result, $\mathbb{P}_{\check{\mu}}(X_t \in A, \tau_\partial > t) = 0$ and $\check{\mu}(A) = 0$ by (3.36). Therefore, by Radon-Nikodym's theorem, $\check{\mu}$ admits a measurable non-negative density $\check{\psi}$ with respect to the Lebesgue measure on D. Therefore, by (3.36), for all $t > 0$, $A \in \mathscr{B}(D)$,

$$\int_D \check{\psi}(x)\mathbb{P}_x(X_t \in A, \tau_\partial > t)\mathrm{d}x = \mathrm{e}^{-\check{\lambda}_0 t}\int_A \check{\psi}(y)\mathrm{d}y. \tag{3.37}$$

By Fubini-Tonelli's theorem,

$$\begin{aligned}\int_D \check{\psi}(x)\mathbb{P}_x(X_t \in A, \tau_\partial > t)\mathrm{d}x &= \int_D\int_D \check{\psi}(x)\mathrm{p}_t^D(x,y)\mathbb{1}_A(y)\mathrm{d}y\mathrm{d}x \\ &= \int_D \mathbb{1}_A(y)\left(\int_D \check{\psi}(x)\mathrm{p}_t^D(x,y)\mathrm{d}x\right)\mathrm{d}y.\end{aligned}$$

As a result, it follows from (3.37) that for almost every $y \in D$,

$$\int_D \check{\psi}(x)\mathrm{p}_t^D(x,y)\mathrm{d}x = \check{\psi}(y)\mathrm{e}^{-\check{\lambda}_0 t}.$$

Then, Theorem 3.2.7 ensures that

$$\int_D \check{\psi}(x)\widetilde{\mathrm{p}}_t^D(y,x)\mathrm{d}x = \check{\psi}(y)\mathrm{e}^{-(\check{\lambda}_0+d\gamma)t},$$

which can be rewritten as: for almost every $y \in D$,

$$\widetilde{P}_t^D \check{\psi}(y) = \check{\psi}(y)\mathrm{e}^{-(\check{\lambda}_0+d\gamma)t}. \tag{3.38}$$

Using the Gaussian upper-bound in Theorem 3.2.2, the continuity of p_t^D in $\overline{D} \times \overline{D}$ and the duality in Theorem 3.2.7, one obtains that the transition density $\widetilde{\mathrm{p}}_t^D$ of $\widetilde{P}_t^D$ is continuous and bounded on $\overline{D}\times\overline{D}$. Therefore, the dominated convergence theorem ensures, since $\check{\psi} \in \mathrm{L}^1(D)$, that $\widetilde{P}_t^D\check{\psi} \in \mathscr{C}^b(\overline{D})$. Thus, the density $\check{\psi}$ can be chosen in $\mathscr{C}^b(\overline{D})$ so that the identity above holds for all $y \in \overline{D}$.

Step 3: Let us prove that $\check{\lambda}_0 = \lambda_0$. In order to do that let us compute the integral $\int_D \widetilde{P}_t^D\check{\psi}(x)\phi(x)\mathrm{d}x$ in two different ways. On the one hand, it follows from (3.38) that

$$\int_D \widetilde{P}_t^D\check{\psi}(x)\phi(x)\mathrm{d}x = \mathrm{e}^{-(\check{\lambda}_0+d\gamma)t}\int_D \check{\psi}(x)\phi(x)\mathrm{d}x.$$

On the other hand, using Fubini-Tonelli's theorem, Theorem 3.2.7 and Theorem 3.2.10,

$$\begin{aligned}\int_D \widetilde{P}_t^D\check{\psi}(x)\phi(x)\mathrm{d}x &= \mathrm{e}^{-d\gamma t}\int_D \check{\psi}(x)P_t^D\phi(x)\mathrm{d}x \\ &= \mathrm{e}^{-(\lambda_0+d\gamma)t}\int_D \check{\psi}(x)\phi(x)\mathrm{d}x.\end{aligned}$$

Since $\phi > 0$, $\check{\psi} \geq 0$ on D and $\check{\psi}$ satisfies $\int_D \check{\psi}(x)\mathrm{d}x = 1$, then $\int_D \check{\psi}(x)\phi(x)\mathrm{d}x > 0$ and $\check{\lambda}_0 = \lambda_0$.

Step 4: For $t > 0$, $r(\widetilde{P}_t^D) = \mathrm{e}^{-(\lambda_0+d\gamma)t}$ is a simple eigenvalue of $\widetilde{P}_t^D$ (seen as an operator on $\mathscr{C}^b(\overline{D})$) with eigenvector ψ by Theorem 3.2.10. As a result, since $\int_D \check{\psi}(x)\mathrm{d}x = \int_D \psi(x)\mathrm{d}x = 1$, then $\check{\psi} = \psi$ and thus $\check{\mu} = \mu$. □

Let us conclude this subsection by proving Theorem 3.2.13. This will provide a spectral interpretation of the QSD on D of the Langevin process, similarly to the spectral interpretation obtained in the overdamped Langevin case, cf. Theorem 3.2.1.

Proof of Theorem 3.2.13. The couple (λ_0, ϕ), defined in Theorem 3.2.10, is clearly a solution to the left eigenvalue problem in (3.22). Let us prove that such a couple (λ_0, ϕ) is unique, up to a multiplicative constant for ϕ. Since the reasoning for the right eigenvalue problem with solution (λ_0, ψ) is the same, with the process $(\widetilde{X}_t)_{t\geq 0}$ instead of $(X_t)_{t\geq 0}$, it will not be detailed.

Let $\lambda \in \mathbb{R}$ and $\eta \in \mathscr{C}^2(D) \cap \mathscr{C}^b(D \cup \Gamma^+)$ be a non-zero and non-negative classical solution of the left eigenvalue problem in (3.22). Let

$$\tau_{V_k^c} := \inf\{t > 0 : X_t \notin V_k\},$$

where $V_k := \{(q,p) \in D : |p| < k, \mathrm{d}_\partial(q) > \frac{1}{k}\}$ and we recall that d_∂ refers to the distance to $\partial\mathscr{O}$. Applying Itô's formula to the process $(\mathrm{e}^{\lambda s}\eta(X_s))_{s\geq 0}$ at the stopping time $t \wedge \tau_{V_k^c}$, one gets, for $x \in D$, $\mathbb{P}_x$-almost surely, for all $t \geq 0$,

$$\mathrm{e}^{\lambda(t\wedge\tau_{V_k^c})}\eta\big(X_{t\wedge\tau_{V_k^c}}\big) = \eta(x) + \sigma\int_0^t \mathbb{1}_{s\leq\tau_{V_k^c}}\mathrm{e}^{\lambda s}\nabla_p\eta(X_s)\cdot\mathrm{d}B_s, \tag{3.39}$$

since $\mathscr{L}\eta + \lambda\eta = 0$ on D. Moreover, $\nabla_p\eta$ is bounded on the compact $\overline{V_k}$ since $\eta \in \mathscr{C}^2(D)$. Therefore, the stochastic integral in the right-hand side of the equality (3.39) is a martingale and its expectation vanishes. Hence,

$$\mathbb{E}_x\left[\mathrm{e}^{\lambda(t\wedge\tau_{V_k^c})}\eta\big(X_{t\wedge\tau_{V_k^c}}\big)\right] = \eta(x),$$

which can be rewritten as

$$\eta(x) = \mathrm{e}^{\lambda t}\mathbb{E}_x\left[\eta\big(X_t\big)\mathbb{1}_{\tau_{V_k^c}>t}\right] + \mathbb{E}_x\left[\mathrm{e}^{\lambda\tau_{V_k^c}}\eta\big(X_{\tau_{V_k^c}}\big)\mathbb{1}_{\tau_{V_k^c}\leq t}\right]. \tag{3.40}$$

Now we would like to let $k \to \infty$. Let us prove the following limit, $\mathbb{P}_x$-almost surely,

$$\lim_{k\to\infty} \tau_{V_k^c} = \tau_\partial,$$

using the same reasoning as in the proof of Assertion (iv) in Theorem 2.2.10.

The sequence $(\tau_{V_k^c})_{k\geq 1}$ is an increasing sequence of random variables, therefore it converges almost surely to $\sup_{k\geq 1} \tau_{V_k^c}$. Besides, using the continuity of the trajectories of $(X_t)_{t\geq 0}$, one gets for all $r > 0$,

$$\begin{aligned}\left\{\sup_{k\geq 1} \tau_{V_k^c} > r\right\} &= \left\{\exists k \geq 1 : \tau_{V_k^c} > r\right\} \\ &= \left\{\exists k \geq 1 : \sup_{u\in[0,r]} |p_u| < k, \inf_{u\in[0,r]} \mathrm{d}_\partial(q_u) > \frac{1}{k}\right\} \\ &= \left\{\sup_{u\in[0,r]} |p_u| < \infty, \inf_{u\in[0,r]} \mathrm{d}_\partial(q_u) > 0\right\} \\ &= \left\{\sup_{u\in[0,r]} |p_u| < \infty, \tau_\partial > r\right\}.\end{aligned}$$

For all $r > 0$, we have that $\sup_{u\in[0,r]} |p_u| < \infty$, almost surely. Therefore, $\sup_{k\geq 1} \tau_{V_k^c} > r$ if and only if $\tau_\partial > r$, that is to say $\sup_{k\geq 1} \tau_{V_k^c} = \tau_\partial$ almost surely. As a result, one gets $\lim_{k\to\infty} \tau_{V_k^c} = \tau_\partial$ almost surely. Besides, since $(\tau_{V_k^c})_{k\geq 1}$ is an increasing sequence, then for all $s > 0$, almost surely,

$$\mathbb{1}_{\tau_{V_k^c} > s} \underset{k\to\infty}{\longrightarrow} \mathbb{1}_{\tau_\partial > s}.$$

As a result, by continuity of the trajectories of $(X_t)_{t\geq 0}$, $\mathbb{P}_x$-almost surely,

$$\mathbb{1}_{\tau_{V_k^c} \leq t}\eta(X_{\tau_{V_k^c}}) \underset{k\to\infty}{\longrightarrow} \mathbb{1}_{\tau_\partial \leq t}\eta(X_{\tau_\partial}).$$

Moreover $\eta(X_{\tau_\partial}) = 0$ almost surely on the event $\{\tau_\partial \leq t\}$ since $X_{\tau_\partial} \in \Gamma^+$ $\mathbb{P}_x$-almost surely by Proposition 2.2.8. Therefore, taking the limit $k \to \infty$ in (3.40), one gets by the dominated convergence theorem that

$$\forall t > 0, \quad \forall x \in D, \qquad \mathbb{E}_x\left[\eta(X_t)\mathbb{1}_{\tau_\partial > t}\right] = \mathrm{e}^{-\lambda t}\eta(x), \tag{3.41}$$

which ensures in particular that necessarily $\lambda \geq 0$. This also writes

$$\forall t > 0, \quad \forall x \in D, \qquad \int_D \mathrm{p}_t^D(x,y)\eta(y)\mathrm{d}y = \mathrm{e}^{-\lambda t}\eta(x).$$

Using the boundedness of η along with (ii) in Theorem 3.2.6, we deduce that $\eta \in \mathrm{L}^1(D)$. Now let $\widetilde{\eta} = \eta / \int_D \eta$, then using Theorem 3.2.7 one obtains that

$$\forall t > 0, \quad \forall x \in D, \qquad \int_D \widetilde{\eta}(y)\widetilde{\mathrm{p}}_t^D(y,x)\mathrm{d}y = \mathrm{e}^{-(\lambda + d\gamma)t}\widetilde{\eta}(x).$$

Integrating over D we obtain that $\mathbb{P}_{\widetilde{\nu}}(\tau_\partial > t) = \mathrm{e}^{-(\lambda+d\gamma)t}$ with $\widetilde{\nu}(\mathrm{d}x) = \widetilde{\eta}(x)\mathrm{d}x$. Then, integrating over any $A \in \mathscr{B}(D)$, we obtain that $\widetilde{\nu}$ is a QSD on D of the process $(\widetilde{X}_t)_{t\geq 0}$. Consequently, the uniqueness of such a QSD, by Theorem 3.2.11, ensures that $\widetilde{\nu} = \widetilde{\mu}$ where $\widetilde{\mu}$ is defined in Theorem 3.2.11. In addition, it implies that $\lambda = \lambda_0$, which concludes the proof. □

3.3.3 Long time convergence to the QSD

This section is devoted to the study of the long time convergence of the semigroup $(P_t^D)_{t>0}$. Note that a similar study could be performed for the semigroup $(\widetilde{P}_t^D)_{t>0}$, using the duality between the two semigroups as stated in Theorem 3.2.7.

We start this subsection by ensuring the existence of a spectral gap for the operator P_t^D. In the next statement, we denote by $\mathscr{C}^b(\overline{D}, \mathbb{C})$ the space of complex-valued continuous bounded functions on $\overline{D}$.

Lemma 3.3.6 (Spectral gap)**.** *Under Assumptions (F1) and (O), for all $t > 0$, the operator P_t^D admits a unique complex eigenvalue with modulus equal to $r(P_t^D) = \mathrm{e}^{-\lambda_0 t}$ and eigenvector in $\mathscr{C}^b(\overline{D}, \mathbb{C})$.*

Proof. Assume that there exists an eigenvector $h_t \in \mathscr{C}^b(\overline{D}, \mathbb{C})$ of P_t^D with eigenvalue $z \in \mathbb{C}\backslash\{\mathrm{e}^{-\lambda_0 t}\}$ such that $|z| = \mathrm{e}^{-\lambda_0 t}$. Let $\psi \in \mathscr{C}^b(\overline{D})$ be the eigenvector of $\widetilde{P}_t^D$ from Theorem 3.2.10.

First, let us prove that $\int_D h_t(x)\psi(x)\mathrm{d}x = 0$ by computing the integral $\int_D h_t(x)\widetilde{P}_t^D\psi(x)\mathrm{d}x$ in two different ways. On the one hand, by Theorem 3.2.10,

$$\int_D h_t(x)\widetilde{P}_t^D\psi(x)\mathrm{d}x = \mathrm{e}^{-(\lambda_0+d\gamma)t}\int_D h_t(x)\psi(x)\mathrm{d}x.$$

On the other hand, by Theorem 3.2.7,

$$\begin{aligned}\int_D h_t(x)\widetilde{P}_t^D\psi(x)\mathrm{d}x &= \mathrm{e}^{-d\gamma t}\int_D P_t^D h_t(x)\psi(x)\mathrm{d}x\\ &= z\mathrm{e}^{-d\gamma t}\int_D h_t(x)\psi(x)\mathrm{d}x.\end{aligned}$$

Therefore, since $z \neq \mathrm{e}^{-\lambda_0 t}$, $\int_D h_t(x)\psi(x)\mathrm{d}x = 0$, and in particular

$$\int_D \mathrm{Re}(h_t(x))\psi(x)\mathrm{d}x = \int_D \mathrm{Im}(h_t(x))\psi(x)\mathrm{d}x = 0. \tag{3.42}$$

Besides, one has for $x \in D$,

$$\begin{aligned}r(P_t^D)|h_t(x)| &= |P_t^D h_t(x)|\\ &= \left|\int_D \mathrm{p}_t^D(x,y)h_t(y)\mathrm{d}y\right|\\ &< \int_D \mathrm{p}_t^D(x,y)|h_t(y)|\mathrm{d}y = P_t^D|h_t|(x),\end{aligned}$$

by the triangle inequality since the equality case requires that $\mathrm{Re}(h_t)$ and $\mathrm{Im}(h_t)$ have constant signs on D, which would imply $h_t = 0$ from (3.42) since $\psi > 0$ on D. As a result,

$$\begin{aligned}r(P_t^D)\int_D \psi(x)|h_t(x)|\mathrm{d}x &< \int_D \psi(x)P_t^D|h_t|(x)\mathrm{d}x\\ &= \mathrm{e}^{d\gamma t}\int_D \widetilde{P}_t^D\psi(x)|h_t(x)|\mathrm{d}x\\ &= r(P_t^D)\int_D \psi(x)|h_t(x)|\mathrm{d}x\end{aligned}$$

which leads to a contradiction, therefore such an eigenvalue does not exist. ∎

We are now able to prove Theorem 3.2.15.

Proof of Theorem 3.2.15. Let us define the following vector space of $\mathscr{C}^b(\overline{D})$,

$$\mathrm{Span}(\psi)^\perp := \left\{ f \in \mathscr{C}^b(\overline{D}) : \int_D f(x)\psi(x)\mathrm{d}x = 0 \right\}.$$

On the one hand, it is clear that this is a closed subset of $\mathscr{C}^b(\overline{D})$, and thus a Banach space. On the other hand, it follows from Theorems 3.2.7 and 3.2.10 that $\mathrm{Span}(\psi)^\perp$ is stable by P_1^D. As a consequence, we may consider in the sequel the operator $P_1^D|_{\mathrm{Span}(\psi)^\perp}$.

The compactness of P_1^D ensures the compactness of $P_1^D|_{\mathrm{Span}(\psi)^\perp}$ as well. Therefore, any non-zero element of the spectrum $\sigma(P_1^D|_{\mathrm{Span}(\psi)^\perp})$ is an eigenvalue of $P_1^D|_{\mathrm{Span}(\psi)^\perp}$ and the eigenvalues can only accumulate at 0. Therefore, if the spectral radius $r(P_1^D|_{\mathrm{Span}(\psi)^\perp}) > 0$, then it is an eigenvalue of $P_1^D|_{\mathrm{Span}(\psi)^\perp}$ by Definition 3.2.9. Moreover, Lemma 3.3.6 ensures that $r(P_1^D|_{\mathrm{Span}(\psi)^\perp}) < r(P_1^D)$ since $r(P_1^D)$ is a simple eigenvalue associated to a positive function ϕ which thus does not belong to $\mathrm{Span}(\psi)^\perp$.

In any case, we thus have $r(P_1^D|_{\mathrm{Span}(\psi)^\perp}) < r(P_1^D)$, so that there exists $\alpha^* \in (0, +\infty]$ such that $r(P_1^D|_{\mathrm{Span}(\psi)^\perp}) = \mathrm{e}^{-\lambda_0 - \alpha^*}$. In addition, for $\alpha \in [0, \alpha^*)$, by Proposition 3.3.1 there exists $N_0 \geq 1$ such that for all $N \geq N_0$,

$$\left|\left|\left| P_N^D|_{\mathrm{Span}(\psi)^\perp} \right|\right|\right|_{\mathscr{C}^b(\overline{D})} \leq \mathrm{e}^{-(\lambda_0+\alpha)N},$$

where we have used the semigroup property to write $(P_1^D|_{\mathrm{Span}(\psi)^\perp})^N = P_N^D|_{\mathrm{Span}(\psi)^\perp}$.

Noticing that for all $f \in \mathscr{C}^b(\overline{D})$, $f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \in \mathrm{Span}(\psi)^\perp$ since $\phi \otimes \psi(f) = (\int_D \psi f)\phi$, one gets for $N \geq N_0$ and $f \in \mathscr{C}^b(\overline{D})$,

$$\left\| P_N^D f - \mathrm{e}^{-\lambda_0 N}\frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right\|_\infty = \left\| P_N^D \left(f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right) \right\|_\infty \leq \mathrm{e}^{-(\lambda_0+\alpha)N} \left\| f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right\|_\infty.$$

Let $t \geq N_0$, then $\lfloor t \rfloor \geq N_0$, and we have that

$$\begin{aligned}
\left\| P_t^D f - \mathrm{e}^{-\lambda_0 t}\frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right\|_\infty &= \left\| P_{t-\lfloor t \rfloor}^D P_{\lfloor t \rfloor}^D \left(f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right) \right\|_\infty \\
&\leq \left\| P_{\lfloor t \rfloor}^D \left(f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right) \right\|_\infty \\
&\leq \mathrm{e}^{-(\lambda_0+\alpha)\lfloor t \rfloor} \left\| f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right\|_\infty \\
&\leq \mathrm{e}^{-(\lambda_0+\alpha)t}\mathrm{e}^{\lambda_0+\alpha} \left\| f - \frac{\phi\otimes\psi}{\int_D \phi\psi}(f) \right\|_\infty \\
&\leq \mathrm{e}^{-(\lambda_0+\alpha)t}\mathrm{e}^{\lambda_0+\alpha} \left(1 + \frac{\|\phi\|_\infty}{\int_D \phi\psi} \right) \|f\|_\infty,
\end{aligned}$$

which concludes the proof, since the behavior of the left-hand side for $t \leq N_0$ can easily be bounded appropriately. □

We conclude this section with a proof of the long-time convergence, in total variation, of the distribution of the Langevin process conditioned to remain in D, towards its QSD on D.

Proof of Theorem 3.2.16. We first recall that for any probability measure θ on D and $t \geq 0$,

$$\|\mathbb{P}_\theta(X_t \in \cdot | \tau_\partial > t) - \mu\|_{TV} = \sup_{f \in \mathrm{L}^\infty(D), \|f\|_{\mathrm{L}^\infty(D)} \leq 1} \left| \mathbb{E}_\theta\left[f(X_t) | \tau_\partial > t\right] - \int_D f \mathrm{d}\mu \right|.$$

Let us fix $\alpha \in [0, \alpha^*)$ and show that there exists C'_α such that for any initial distribution θ, $t \geq 0$ and $f \in \mathscr{C}^b(\overline{D})$,

$$\left| \frac{\mathbb{E}_\theta(f(X_t)\mathbb{1}_{\tau_\partial > t})}{\mathbb{P}_\theta(\tau_\partial > t)} - \int_D f\psi \right| \leq \frac{C'_\alpha}{\int_D \phi \mathrm{d}\theta}\mathrm{e}^{-\alpha t}\|f\|_\infty.$$

We shall then conclude using the density of $\mathscr{C}^b(\overline{D})$ in $\mathrm{L}^\infty(D)$.

First, let us prove that

$$\mathbb{P}_\theta(\tau_\partial > t) \geq \frac{\int_D \phi \mathrm{d}\theta}{\|\phi\|_\infty} \mathrm{e}^{-\lambda_0 t}.$$

For $x \in D$, $t > 0$ one has

$$\begin{aligned}
\mathbb{P}_x(\tau_\partial > t) &= \int_D \mathrm{p}_t^D(x, y)\mathrm{d}y \\
&= \int_D \mathrm{p}_t^D(x, y)\frac{\phi(y)}{\phi(y)}\mathrm{d}y \\
&\geq \frac{\int_D \mathrm{p}_t^D(x, y)\phi(y)\mathrm{d}y}{\|\phi\|_\infty} = \frac{\phi(x)\mathrm{e}^{-\lambda_0 t}}{\|\phi\|_\infty},
\end{aligned}$$

by Theorem 3.2.10. Therefore,

$$\mathbb{P}_\theta(\tau_\partial > t) = \int_D \theta(\mathrm{d}x)\mathbb{P}_x(\tau_\partial > t) \geq \frac{\int_D \phi \mathrm{d}\theta}{\|\phi\|_\infty} \mathrm{e}^{-\lambda_0 t}. \tag{3.43}$$

As a result, it follows from Theorem 3.2.15 and the inequality (3.43), the existence of $C_\alpha > 0$ such that for all $t > 0$,

$$\begin{aligned}
\left| \frac{\mathbb{E}_\theta(f(X_t)\mathbb{1}_{\tau_\partial > t})}{\mathbb{P}_\theta(\tau_\partial > t)} - \int_D f\psi \right| &= \left| \frac{\int_D \left(\mathbb{E}_x(f(X_t)\mathbb{1}_{\tau_\partial > t}) - \left(\int_D f\psi\right) \mathbb{P}_\theta(\tau_\partial > t)\right) \theta(\mathrm{d}x)}{\mathbb{P}_\theta(\tau_\partial > t)} \right| \\
&\leq \int_D \frac{\left|\mathbb{E}_x(f(X_t)\mathbb{1}_{\tau_\partial > t}) - \mathrm{e}^{-\lambda_0 t}\frac{\int_D \psi f}{\int_D \phi\psi}\phi(x)\right|}{\mathbb{P}_\theta(\tau_\partial > t)}\theta(\mathrm{d}x) \\
&+ \left|\int_D \psi f\right| \frac{\left|\mathrm{e}^{-\lambda_0 t}\frac{\int_D \phi \mathrm{d}\theta}{\int_D \phi\psi} - \mathbb{P}_\theta(\tau_\partial > t)\right|}{\mathbb{P}_\theta(\tau_\partial > t)} \\
&\leq \frac{C_\alpha}{\mathbb{P}_\theta(\tau_\partial > t)}\mathrm{e}^{-(\lambda_0+\alpha)t}\|f\|_\infty + \|f\|_\infty \frac{C_\alpha \mathrm{e}^{-(\lambda_0+\alpha)t}}{\mathbb{P}_\theta(\tau_\partial > t)} \\
&\leq \frac{2C_\alpha}{\int_D \phi \mathrm{d}\theta}\mathrm{e}^{-\alpha t}\|f\|_\infty\|\phi\|_\infty.
\end{aligned}$$

□

3.4 Overdamped limit of the QSD of the Langevin process

In this final section, we are interested in the behavior of the QSD of the Langevin process defined in (3.25), with $\beta > 0$ independent of γ, when γ goes to infinity. Therefore, we assume in this section that the friction coefficient γ in (3.25) is **positive**. Besides, we shall use the following notation: under Assumption (F2), for any $x = (q, p) \in \mathbb{R}^d$, we denote by $(X_t^{(\gamma),x} = (q_t^{(\gamma),x}, p_t^{(\gamma),x}))_{t\geq 0}$ the solution to (3.25) with initial condition x, and by $(\overline{q}_t^{(\gamma),q})_{t\geq 0}$ the solution to the stochastic differential equation (3.2) with initial condition q and driven by the Brownian motion $(B_t^{(\gamma)})_{t\geq 0} = (\frac{B_{\gamma t}}{\sqrt{\gamma}})_{t\geq 0}$. All these processes are defined on the same probability space $(\Omega, \mathscr{F}, (\mathscr{F}_t)_{t\geq 0}, \mathbb{P})$ and it is more convenient to keep track of the initial condition of each process with the superscript notation rather than in the probability measure. We also emphasize the fact that under Assumption (F2), uniqueness in distribution holds for the stochastic differential equation (3.2) and therefore the law of the process $(\overline{q}_t^{(\gamma),q})_{t\geq 0}$ does not depend on γ.

3.4.1 Proof of Theorem 3.2.19

Let $x = (q, p) \in \mathbb{R}^{2d}$, $T > 0$. We explain here the idea of the proof of Theorem 3.2.19.

Let us start by considering the convergence of the marginal laws of $(q^{(\gamma),x}_{\gamma t})_{t\in[0,T]}$ and $p^{(\gamma),x}_{\gamma T}$. Considering (3.25), we have almost surely, for $t \in [0,T]$,

$$q^{(\gamma),x}_{\gamma t} = q - \frac{p^{(\gamma),x}_{\gamma t} - p}{\gamma} + \int_0^t F(q^{(\gamma),x}_{\gamma s})\mathrm{d}s + \sqrt{2\beta^{-1}}B^{(\gamma)}_t. \tag{3.44}$$

Using Gronwall's lemma, we are able to deduce from this equality the inequalities (i) and (ii) in Lemma 3.4.2, which ensure that the difference $(q^{(\gamma),x}_{\gamma t})_{t\in[0,T]} - (\overline{q}^{(\gamma),q}_t)_{t\in[0,T]}$ converges in probability to 0, in the space of the bounded continuous functions on $[0,T]$. Furthermore, the process $(\overline{q}^{(\gamma),q}_t)_{t\in[0,T]}$ shares the same law as the process $(\overline{q}^{q}_t)_{t\in[0,T]}$, which does not depend on γ. Therefore, the law of the process $(q^{(\gamma),x}_{\gamma t})_{t\in[0,T]}$ converges weakly to the law of $(\overline{q}^{q}_t)_{t\in[0,T]}$ when γ goes to infinity.

Moreover, it follows from (3.25) that for all $t \geq 0$,

$$p^{(\gamma),x}_t = p\mathrm{e}^{-\gamma t} + \mathrm{e}^{-\gamma t}\int_0^t \mathrm{e}^{\gamma s}F(q^{(\gamma),x}_s)\mathrm{d}s + \sqrt{2\gamma\beta^{-1}}\mathrm{e}^{-\gamma t}\int_0^t \mathrm{e}^{\gamma s}\mathrm{d}B_s. \tag{3.45}$$

For $t \geq 0$, let

$$Y^{(\gamma)}_t := \sqrt{2\gamma\beta^{-1}}\mathrm{e}^{-\gamma^2 t}\int_0^{\gamma t} \mathrm{e}^{\gamma s}\mathrm{d}B_s, \tag{3.46}$$

then evaluating (3.45) at $t = \gamma T$ for $T \geq 0$, we get

$$p^{(\gamma),x}_{\gamma T} = p\mathrm{e}^{-\gamma^2 T} + \gamma\mathrm{e}^{-\gamma^2 T}\int_0^T \mathrm{e}^{\gamma^2 s}F(q^{(\gamma),x}_{\gamma s})\mathrm{d}s + Y^{(\gamma)}_T. \tag{3.47}$$

Under Assumption (F2), F is bounded. Besides, $Y^{(\gamma)}_T \sim \mathscr{N}_d(0, \beta^{-1}(1-\mathrm{e}^{-2\gamma^2 T})I_d)$. Therefore, $Y^{(\gamma)}_T \xrightarrow[\gamma\to\infty]{\mathscr{L}} Z$ where $Z \sim \mathscr{N}_d(0,\beta^{-1}I_d)$ and $p^{(\gamma),x}_{\gamma T} \xrightarrow[\gamma\to\infty]{\mathscr{L}} Z$ by Slutsky's theorem.

The arguments above give the limit in law of the marginals of the couple $((q^{(\gamma),x}_{\gamma t})_{t\in[0,T]}, p^{(\gamma),x}_{\gamma T})$. To prove Theorem 3.2.19, it remains to show that, in the limit $\gamma \to \infty$, the two random variables $(q^{(\gamma),x}_{\gamma t})_{t\in[0,T]}$ and $p^{(\gamma),x}_{\gamma T}$ are independent. This is done by introducing a small perturbation. In order to define the perturbed Langevin process mentioned above, we introduce the following objects. Let $h^{(\gamma)}_T : [0,T] \mapsto \mathbb{R}$ and the process $(Z^{(\gamma)}_{t,T})_{t\in[0,T]}$ be defined as follow:

$$\forall t \in [0,T], \qquad h^{(\gamma)}_T(t) := \frac{2}{\gamma}\frac{\mathrm{e}^{-\gamma^2(T-t)} - \mathrm{e}^{-\gamma^2 T}}{1-\mathrm{e}^{-2\gamma^2 T}}, \tag{3.48}$$

$$Z^{(\gamma)}_{t,T} := \sqrt{2\beta^{-1}}B^{(\gamma)}_t - h^{(\gamma)}_T(t)Y^{(\gamma)}_T.$$

Let $(\mathscr{F}^{(\gamma),Z}_t)_{t\in[0,T]}$ be the natural filtration of $(Z^{(\gamma)}_{t,T})_{t\in[0,T]}$. Under Assumption (F2), Itô's fixed point argument [49, Thm 2.9 p. 289] shows that the stochastic differential equation

$$\begin{cases} \mathrm{d}w^{(\gamma),q}_t = F(w^{(\gamma),q}_t)\mathrm{d}t + \mathrm{d}Z^{(\gamma)}_{t,T}, \\ w^{(\gamma),q}_0 = q. \end{cases} \tag{3.49}$$

possesses a unique strong solution $(w^{(\gamma),q}_t)_{t\in[0,T]}$, which is thus adapted to $(\mathscr{F}^{(\gamma),Z}_t)_{t\in[0,T]}$.

The process $((w^{(\gamma),q}_t)_{t\in[0,T]}, Y^{(\gamma)}_T)$ satisfies the following lemmata.

Lemma 3.4.1 (Independence)**.** *Under Assumption (F2), for all $T > 0$, the process $(w^{(\gamma),q}_t)_{t\in[0,T]}$ is independent of the random variable $Y^{(\gamma)}_T$.*

Proof. Let $T > 0$. Since $(w_t^{(\gamma),q})_{t\in[0,T]}$ is $\mathscr{F}_T^{(\gamma),Z}$-measurable, it is sufficient to prove that the process $(Z_{t,T}^{(\gamma)})_{t\in[0,T]}$ is independent of $Y_T^{(\gamma)}$. It is clear that for any $t_1,\dots,t_k \in [0,T]$, the vector $(Z_{t_1,T}^{(\gamma)},\dots,Z_{t_k,T}^{(\gamma)},Y_T^{(\gamma)})$ is Gaussian, therefore the independence is satisfied if and only if for all $t\in[0,T]$, the covariance matrix of $(Z_{t,T}^{(\gamma)},Y_T^{(\gamma)})$ is null, which is indeed the case by an easy computation. □

Lemma 3.4.2 (Perturbed Langevin). *Let Assumption (F2) hold. There exists $C > 0$ such that for all $T > 0$, $x = (q,p) \in \mathbb{R}^{2d}$, $\gamma > 1$,*

(i) $\mathbb{E}\left[\sup_{t\in[0,T]}\left|q_{\gamma t}^{(\gamma),(q,p)} - w_t^{(\gamma),q}\right|\right] \leq \frac{C}{\gamma}\left(1+|p|+\sqrt{\log(1+\gamma^2 T)}\right)\mathrm{e}^{CT}$,

(ii) $\mathbb{E}\left[\sup_{t\in[0,T]}\left|w_t^{(\gamma),q} - \overline{q}_t^{(\gamma),q}\right|\right] \leq \frac{C}{\gamma}\mathrm{e}^{CT}$.

The proof of Lemma 3.4.2 is postponed to Section 3.4.3.

These two lemmata now yield the following proof of Theorem 3.2.19.

Proof of Theorem 3.2.19. Let $T > 0$, $x = (q,p) \in \mathbb{R}^{2d}$. Let Φ_1 be a bounded k_1-Lipschitz continuous function on $\mathscr{C}([0,T],\mathbb{R}^d)$ equipped with the supremum norm on $[0,T]$ and let g be a bounded k_2-Lipschitz continuous function on $\mathbb{R}^d$. Our goal is to prove the following convergence:

$$\mathbb{E}\left[\Phi_1((q_{\gamma t}^{(\gamma),x})_{t\in[0,T]})g(p_{\gamma T}^{(\gamma),x})\right] \underset{\gamma\to\infty}{\longrightarrow} \mathbb{E}\left[\Phi_1((\overline{q}_t^{q})_{t\in[0,T]})\right]\mathbb{E}\left[g(Z)\right], \tag{3.50}$$

where, in the right-hand side, $(\overline{q}_t^q)_{t\in[0,T]}$ refers to the solution of (3.2) (which we recall has the same law as all processes $(\overline{q}_t^{(\gamma),q})_{t\in[0,T]}$ for $\gamma > 0$).

By *(i)* in Lemma 3.4.2 and (3.47), there exists $C' > 0$, depending on T, such that for all $\gamma > 1$,

$$\begin{aligned}&\left|\mathbb{E}\left[\Phi_1((q_{\gamma t}^{(\gamma),x})_{t\in[0,T]})g(p_{\gamma T}^{(\gamma),x})\right] - \mathbb{E}\left[\Phi_1((w_t^{(\gamma),q})_{t\in[0,t]})g(Y_T^{(\gamma)})\right]\right| \\ &\leq k_1\|g\|_\infty\frac{C'}{\gamma}\left(1+|p|+\sqrt{\log(1+\gamma^2T)}\right) + k_2\|\Phi\|_\infty\left(|p|\mathrm{e}^{-\gamma^2 T} + \frac{\|F\|_\infty}{\gamma}\right),\end{aligned}$$

which converges to 0 when $\gamma\to\infty$. Furthermore, by Lemma 3.4.1,

$$\mathbb{E}\left[\Phi_1((w_t^{(\gamma),q})_{t\in[0,T]})g(Y_T^{(\gamma)})\right] = \mathbb{E}\left[\Phi_1((w_t^{(\gamma),q})_{t\in[0,T]})\right]\mathbb{E}\left[g(Y_T^{(\gamma)})\right].$$

Since, $Y_T^{(\gamma)} \sim \mathscr{N}_d(0,\beta^{-1}(1-\mathrm{e}^{-2\gamma^2 T})I_d)$ then $Y_T^{(\gamma)} \underset{\gamma\to\infty}{\overset{\mathscr{L}}{\longrightarrow}} Z$ with $Z\sim\mathscr{N}_d(0,\beta^{-1}I_d)$. As a result, $\mathbb{E}[g(Y_T^{(\gamma)})] \underset{\gamma\to\infty}{\longrightarrow} \mathbb{E}[g(Z)]$. Besides, using *(ii)* in Lemma 3.4.2, one obtains that

$$\mathbb{E}\left[\Phi_1((w_t^{(\gamma),q})_{t\in[0,T]})\right] - \mathbb{E}\left[\Phi_1((\overline{q}_t^{(\gamma),q})_{t\in[0,T]})\right] \underset{\gamma\to\infty}{\longrightarrow} 0,$$

Moreover, $\mathbb{E}[\Phi_1((\overline{q}_t^{(\gamma),q})_{t\in[0,T]})] = \mathbb{E}[\Phi_1((\overline{q}_t^{q})_{t\in[0,T]})]$, since $(\overline{q}_t^{(\gamma),q})_{t\in[0,T]}$ and $(\overline{q}_t^{q})_{t\in[0,T]}$ share the same law, which concludes the proof of (3.50). □

3.4.2 Proof of Theorem 3.2.20

We still assume here that $\sigma = \sqrt{2\gamma\beta^{-1}}$ and we consider the weak limit of the QSD on D of the Langevin process when $\gamma\to\infty$. Considering that γ is no longer a fixed parameter but a quantity going to infinity, we will use the following notation:

- $\mu^{(\gamma)}$ the QSD on D of the Langevin process (3.25),
- $\psi^{(\gamma)}$ the density of $\mu^{(\gamma)}$ with respect to the Lebesgue measure on D,

- $\lambda_0^{(\gamma)}$ the associated smallest eigenvalue of $-\mathscr{L}$ and $-\mathscr{L}^*$.

The notation for the overdamped Langevin process and its QSD remains the same as in Theorem 3.2.1. The idea of the proof of Theorem 3.2.20 is the following. We pick an arbitrary sequence $(\gamma_n)_{n\geq 1}$ of positive numbers going to infinity. Assuming that the sequence of probability measure $(\mu^{(\gamma_n)})_{n\geq 1}$ is tight, then using Prokhorov's theorem we obtain a convergent subsequence $(\mu^{(\gamma'_n)})_{n\geq 1}$ to a probability measure μ' on D. It is then left to prove that such a μ' is uniquely defined by the equality (3.26), whatever the sequence $(\gamma'_n)_{n\geq 1}$. As a result, $\mu^{(\gamma)}$ necessarily converges weakly, when γ goes to infinity, to $\mu^{(\infty)}$ defined by (3.26).

Now, let $(\gamma_n)_{n\geq 1}$ be an arbitrary sequence of positive numbers going to infinity. Let us prove that the sequence $(\mu^{(\gamma_n)})_{n\geq 1}$ is tight. This is the consequence of the following lemma which is proven in Section 3.4.3.

Proposition 3.4.3 (Estimates on $\psi^{(\gamma)}$)**.** *Under Assumptions (F1) and (O), the density $\psi^{(\gamma)}$ of the QSD $\mu^{(\gamma)}$ of (3.25) satisfies the following properties:*

(i) $\limsup_{\gamma\to\infty} \left\|\psi^{(\gamma)}\right\|_\infty < \infty$,

(ii) $\limsup_{\gamma\to\infty} \sup_{q\in\mathscr{O}} \int_{\mathbb{R}^d} \psi^{(\gamma)}(q,p)\mathrm{d}p < \infty$,

(iii) $\limsup_{\gamma\to\infty} \iint_D |p|\psi^{(\gamma)}(q,p)\mathrm{d}p\mathrm{d}q < \infty$.

Corollary 3.4.4 (Tightness)**.** *Under Assumptions (F1) and (O), the sequence of probability measures supported on D, $(\mu^{(\gamma_n)})_{n\geq 1}$, is tight.*

Proof. For $k\geq 1$, let K_k be the compact subset of D defined by

$$K_k := \left\{(q,p)\in D : |p|\leq k, \mathrm{d}_\partial(q)\geq \frac{1}{k}\right\},$$

where d_∂ is the Euclidean distance to the boundary $\partial\mathscr{O}$. Let $K_k^c := D\setminus K_k$. Therefore, $K_k^c = \{(q,p)\in D : |p|>k\}\cup\{(q,p)\in D : \mathrm{d}_\partial(q)<\frac{1}{k}\}$. Let us prove the following limit

$$\lim_{k\to\infty}\limsup_{n\to\infty}\mu^{(\gamma_n)}(K_k^c) = 0, \tag{3.51}$$

which immediately yields the required tightness.

Let $\mathscr{O}_k := \{q\in\mathscr{O} : \mathrm{d}_\partial(q)<\frac{1}{k}\}$. For all $n\geq 1$,

$$\begin{aligned}
\mu^{(\gamma_n)}(K_k^c) &\leq \iint_{D\cap\{|p|>k\}}\psi^{(\gamma_n)}(q,p)\mathrm{d}p\mathrm{d}q + \iint_{D\cap\{\mathrm{d}_\partial(q)<\frac{1}{k}\}}\psi^{(\gamma_n)}(q,p)\mathrm{d}p\mathrm{d}q\\
&\leq \iint_{D\cap\{|p|>k\}}\psi^{(\gamma_n)}(q,p)\frac{|p|}{k}\mathrm{d}p\mathrm{d}q + \int_{\mathrm{d}_\partial(q)<\frac{1}{k}}\left(\int_{\mathbb{R}^d}\psi^{(\gamma_n)}(q,p)\mathrm{d}p\right)\mathrm{d}q\\
&\leq \frac{\iint_D\psi^{(\gamma_n)}(q,p)|p|\mathrm{d}p\mathrm{d}q}{k} + |\mathscr{O}_k|\sup_{q\in\mathscr{O}}\int_{\mathbb{R}^d}\psi^{(\gamma_n)}(q,p)\mathrm{d}p.
\end{aligned}$$

The convergence (3.51) then follows from Proposition 3.4.3, which concludes the proof. $\square$

Last, we state and prove here the following lemma which is used later in the proof of Theorem 3.2.20.

Lemma 3.4.5 (Convergence in distribution)**.** *Let Assumptions (F2) and (O) hold. Let $f\in\mathscr{C}^b(\mathscr{O})$, $g\in\mathscr{C}^b(\mathbb{R}^d)$. For all $(q,p)\in D$ and $t>0$,*

$$\mathbb{E}\left[f(q_{\gamma t}^{(\gamma),(q,p)})g(p_{\gamma t}^{(\gamma),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma),(q,p)}>\gamma t}\right]\underset{\gamma\to\infty}{\longrightarrow}\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]. \tag{3.52}$$

Proof. Let $(q,p)\in D$ and $T>0$. Since $\mathscr{O}$ is an open set, we have for any $\gamma>0$,

$$f(q^{(\gamma),(q,p)}_{\gamma T})g(p^{(\gamma),(q,p)}_{\gamma t})\mathbb{1}_{\tau^{(\gamma),(q,p)}_{\partial}>\gamma T}=\Phi\left((q^{(\gamma),(q,p)}_{\gamma t})_{t\in[0,T]},p^{(\gamma),(q,p)}_{\gamma t}\right),$$

where $\Phi:\mathscr{C}([0,T],\mathbb{R}^d)\times\mathbb{R}^d\to\mathbb{R}$ is defined by

$$\Phi\left((q_t)_{t\in[0,T]},z\right)=f(q_T)g(z)\mathbb{1}_{\inf_{t\in[0,T]}\mathrm{d}_{\partial}(q_t)>0},$$

and we take the convention that $\mathrm{d}_\partial(q')=0$ if $q'\notin\mathscr{O}$. The functional Φ is not continuous on the space $\mathscr{C}([0,T],\mathbb{R}^d)\times\mathbb{R}^d$, which prevents us from applying Theorem 3.2.19 directly. Indeed, take for example a continuous trajectory $(q_t)_{t\in[0,T]}$ on $[0,T]$ which hits the boundary $\partial\mathscr{O}$ and is reflected back into the domain $\mathscr{O}$. One can construct a sequence of functions $((q^{(n)}_t)_{t\in[0,T]})_{n\geq1}$ converging in the supremum norm to $(q_t)_{t\in[0,T]}$ such that for all $n\geq1$, $\inf_{t\in[0,T]}\mathrm{d}_\partial(q^{(n)}_t)>0$. As a result, $(q_t)_{t\in[0,T]}$ is an example of a discontinuity point of the function Φ.

The discontinuity points of Φ are contained in the set of discontinuity points of $\mathbb{1}_{\inf_{t\in[0,T]}\mathrm{d}_{\partial}(q_t)>0}$, which can be characterized as follows. They correspond to the trajectories $(q_t)_{t\in[0,T]}$ which hit the boundary and remain on the boundary $\partial\mathscr{O}$ or come back inside $\mathscr{O}$. In fact if $(q_t)_{t\in[0,T]}$ is such that $\inf_{t\in[0,T]}\mathrm{d}_\partial(q_t)>0$ or $\sup_{t\in[0,T]}\mathrm{dist}(q_t,\mathbb{R}^d\setminus\overline{\mathscr{O}})>0$, then taking a sequence of functions $(q^{(n)}_t)_{t\in[0,T]}$ in $\mathscr{C}([0,T],\mathbb{R}^d)$ such that $\|q^{(n)}-q\|_\infty\leq\frac{\inf_{t\in[0,T]}\mathrm{d}_\partial(q_t)}{2}$ or $\|q^{(n)}-q\|_\infty\leq\frac{\sup_{t\in[0,T]}\mathrm{dist}(q_t,\mathbb{R}^d\setminus\overline{\mathscr{O}})}{2}$ then it follows from the $1-$Lipschitz continuity of the Euclidean distances $\mathrm{d}_\partial(\cdot)$ and $\mathrm{dist}(\cdot,\mathbb{R}^d\setminus\overline{\mathscr{O}})$ that

$$\mathbb{1}_{\inf_{t\in[0,T]}\mathrm{d}_{\partial}(q^{(n)}_t)>0}\underset{n\to\infty}{\longrightarrow}\mathbb{1}_{\inf_{t\in[0,T]}\mathrm{d}_{\partial}(q_t)>0}.$$

As a consequence, the set of discontinuities of Φ is included in the set S of continuous trajectories $(q_t)_{t\in[0,T]}$ such that there exists $t_\partial\in[0,T]$ for which $q_{t_\partial}\in\partial\mathscr{O}$ but for all $t\in[0,T]$, $q_t\in\overline{\mathscr{O}}$. Let us now justify that for all $q\in\mathscr{O}$, $\mathbb{P}_q((\overline{q}_t)_{t\in[0,T]}\in S)=0$. Using the strong Markov property at $\overline{\tau}_\partial$, this is the case if for all $q\in\partial\mathscr{O}$, $\mathbb{P}_q(\overline{\tau}_\partial>0)=0$. This is clearly the case since for all $t>0$, $q\in\partial\mathscr{O}$, $\mathbb{P}_q(\overline{\tau}_\partial\leq t)=1$, see [33, p. 347]. Thus, the continuous mapping theorem ensures that $\Phi((q^{(\gamma),(q,p)}_{\gamma t})_{t\in[0,T]},p^{(\gamma),(q,p)}_{\gamma t})$ converges in distribution to

$$\Phi\left((\overline{q}^q_t)_{t\in[0,T]},Z\right)=\mathbb{E}\left[f(\overline{q}^q_t)\mathbb{1}_{\overline{\tau}^q_\partial>t}\right]\mathbb{E}\left[g(Z)\right],$$

which completes the proof. □

Proof of Theorem 3.2.20. Notice that since the QSD $\mu^{(\gamma)}$ does not depend on the values of F outside of $\mathscr{O}$, we can consider here, up to a modification of F outside of $\mathscr{O}$, that F satisfies Assumption (F2). Therefore, the result of Theorem 3.2.19 still applies in the current setting.

By Corollary 3.4.4, the sequence $(\mu^{(\gamma_n)})_{n\geq1}$ is tight, and therefore it is sequentially compact by Prokhorov's theorem. Let us consider a subsequence $(\gamma'_n)_{n\geq1}$ such that the sequence $(\mu^{(\gamma'_n)})_{n\geq1}$ converges weakly to a probability measure μ' on D when n goes to infinity. Let us now prove that $\mu'=\mu^{(\infty)}$ defined in (3.26) independently of the sequence $(\gamma'_n)_{n\geq1}$, which will conclude the proof.

By Definition 3.1.1 of a QSD, one easily deduce that for all $f\in\mathscr{C}^b(\mathscr{O})$, $g\in\mathscr{C}^b(\mathbb{R}^d)$ and all $t>0$,

$$\begin{aligned}&\iint_D\mu^{(\gamma'_n)}(\mathrm{d}q\mathrm{d}p)\mathbb{E}\left[f(q^{(\gamma'_n),(q,p)}_{\gamma'_n t})g(p^{(\gamma'_n),(q,p)}_{\gamma'_n t})\mathbb{1}_{\tau^{(\gamma'_n),(q,p)}_{\partial}>\gamma'_n t}\right]\\&=\mathrm{e}^{-\lambda^{(\gamma'_n)}_0\gamma'_n t}\underbrace{\iint_D f(q)g(p)\mu^{(\gamma'_n)}(\mathrm{d}q\mathrm{d}p)}_{\underset{n\to\infty}{\longrightarrow}\iint_D f(q)g(p)\mu'(\mathrm{d}q\mathrm{d}p)},\end{aligned}\qquad(3.53)$$

where $\tau_\partial^{(\gamma_n'),(q,p)}$ denotes the exit time from D for the process $(X_t^{(\gamma_n'),(q,p)})_{t\geq 0}$.

Let $Z \sim \mathscr{N}_d(0,\beta^{-1}I_d)$ be a Gaussian vector independent of the process $(\overline{q}_t^q)_{t\in[0,T]}$ defined in (3.2). Let us prove that the term in the left-hand side of the equality (3.53) converges to $\iint_D \mathbb{E}[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}]\mathbb{E}[g(Z)]\mu'(\mathrm{d}q\mathrm{d}p)$. Considering the difference between the term in the left-hand side of the equality (3.53) and $\iint_D \mathbb{E}[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}]\mathbb{E}[g(Z)]\mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)$ and partitioning the set $\{p\in\mathbb{R}^d\}$ into $\{|p|\leq K\}$ and $\{|p|>K\}$ for $K>0$, one obtains

$$\begin{aligned}
&\left|\iint_D \mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)\left(\mathbb{E}\left[f(q_{\gamma_n't}^{(\gamma_n'),(q,p)})g(p_{\gamma_n't}^{(\gamma_n'),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma_n'),(q,p)}>\gamma_n't}\right]-\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]\right)\right|\\
&=\left|\iint_D \psi^{(\gamma_n')}(q,p)\left(\mathbb{E}\left[f(q_{\gamma_n't}^{(\gamma_n'),(q,p)})g(p_{\gamma_n't}^{(\gamma_n'),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma_n'),(q,p)}>\gamma_n't}\right]-\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]\right)\mathrm{d}p\mathrm{d}q\right|\\
&\leq \|\psi^{(\gamma_n')}\|_\infty\iint_{\mathscr{O}\times\{|p|\leq K\}}\left|\underbrace{\mathbb{E}\left[f(q_{\gamma_n't}^{(\gamma_n'),(q,p)})g(p_{\gamma_n't}^{(\gamma_n'),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma_n'),(q,p)}>\gamma_n't}\right]-\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]}_{\underset{n\to\infty}{\longrightarrow}0\text{ by Lemma 3.4.5}}\right|\mathrm{d}p\mathrm{d}q\\
&+2\|f\|_\infty\|g\|_\infty\iint_{\mathscr{O}\times\{|p|>K\}}\psi^{(\gamma_n')}(q,p)\mathrm{d}p\mathrm{d}q.
\end{aligned}$$

Therefore, using Proposition 3.4.3 and the dominated convergence theorem to get that the limsup of the first term in the right-hand side is zero,

$$\begin{aligned}
&\limsup_{n\to\infty}\left|\iint_D \mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)\left(\mathbb{E}\left[f(q_{\gamma_n't}^{(\gamma_n'),(q,p)})g(p_{\gamma_n't}^{(\gamma_n'),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma_n'),(q,p)}>\gamma_n't}\right]-\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]\right)\right|\\
&\leq 2\|f\|_\infty\|g\|_\infty\limsup_{n\to\infty}\iint_{\mathscr{O}\times\{|p|>K\}}\psi^{(\gamma_n')}(q,p)\mathrm{d}p\mathrm{d}q\\
&\leq 2\|f\|_\infty\|g\|_\infty\limsup_{n\to\infty}\iint_{\mathscr{O}\times\{|p|>K\}}\psi^{(\gamma_n')}(q,p)\frac{|p|}{K}\mathrm{d}p\mathrm{d}q\\
&\leq\frac{2\|f\|_\infty\|g\|_\infty}{K}\limsup_{n\to\infty}\iint_D\psi^{(\gamma_n')}(q,p)|p|\mathrm{d}p\mathrm{d}q\underset{K\to\infty}{\longrightarrow}0.
\end{aligned}$$

Consequently,

$$\iint_D \mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)\left(\mathbb{E}\left[f(q_{\gamma_n't}^{(\gamma_n'),(q,p)})g(p_{\gamma_n't}^{(\gamma_n'),(q,p)})\mathbb{1}_{\tau_\partial^{(\gamma_n'),(q,p)}>\gamma_n't}\right]-\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]\right)\underset{n\to\infty}{\longrightarrow}0.$$

In addition,

$$\begin{aligned}
\iint_D \mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\mathbb{E}\left[g(Z)\right]&=\mathbb{E}\left[g(Z)\right]\int_{\mathscr{O}}\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\left(\int_{p\in\mathbb{R}^d}\mu^{(\gamma_n')}(\mathrm{d}q\mathrm{d}p)\right)\\
&\underset{n\to\infty}{\longrightarrow}\mathbb{E}\left[g(Z)\right]\int_{\mathscr{O}}\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\left(\int_{p\in\mathbb{R}^d}\mu'(\mathrm{d}q\mathrm{d}p)\right),
\end{aligned}$$

since $q\in\mathscr{O}\mapsto\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]$ is a bounded and continuous function on $\mathscr{O}$, see [32, Theorem 5.2 Chapter 6]. Consequently, taking $n\to\infty$ in the left-hand side of the equation (3.53) and choosing $t=1$, it follows that $\lambda_0^{(\gamma_n')}\gamma_n'$ converges to a value $\lambda'\in[0,\infty)$. Hence, taking $n\to\infty$ again in Equation (3.53), it follows that for all $t>0$,

$$\mathbb{E}\left[g(Z)\right]\int_{\mathscr{O}}\mathbb{E}\left[f(\overline{q}_t^q)\mathbb{1}_{\overline{\tau}_\partial^q>t}\right]\left(\int_{p\in\mathbb{R}^d}\mu'(\mathrm{d}q\mathrm{d}p)\right)=\mathrm{e}^{-\lambda't}\iint_D f(q)g(p)\mu'(\mathrm{d}q\mathrm{d}p). \tag{3.54}$$

Let $\mu'_{\mathscr{O}}$ be the probability measure on $\mathscr{O}$ defined by:

$$\mu'_{\mathscr{O}}(\mathrm{d}q) = \int_{p\in\mathbb{R}^d} \mu'(\mathrm{d}q\mathrm{d}p).$$

Taking $g = 1$ and $f = 1$ in (3.54), we obtain that $\mathbb{P}_{\mu'_0}(\overline{\tau}_\partial > t) = \exp(-\lambda' t)$. Since the equality can also be extended to all functions $f \in \mathrm{L}^\infty(\mathscr{O})$, using the density of $\mathscr{C}^b(\mathscr{O})$ in $\mathrm{L}^\infty(\mathscr{O})$, one gets for $g = 1$ and $f = \mathbb{1}_A$ in (3.54) with $A \in \mathscr{B}(\mathscr{O})$,

$$\frac{\mathbb{P}_{\mu'_0}(\overline{q}_t \in A, \overline{\tau}_\partial > t)}{\mathbb{P}_{\mu'_0}(\overline{\tau}_\partial > t)} = \mu'_{\mathscr{O}}(A).$$

Therefore, $\mu'_{\mathscr{O}}$ is the unique QSD on $\mathscr{O}$ of $(\overline{q}_t)_{t\geq 0}$ by Theorem 3.2.1, which admits the density $\overline{\psi}$ with respect to the Lebesgue measure on $\mathscr{O}$. In particular, one has that $\lambda' = \overline{\lambda}$. Finally, reinjecting this equality into (3.54), we obtain that μ' satisfies the equality (3.26) since $Z \sim \mathscr{N}_d(0, \beta^{-1} I_d)$, which concludes the proof. □

3.4.3 Proofs of technical results

This section gathers the proofs of the results stated previously: Lemma 3.4.2 and Proposition 3.4.3.

3.4.3.1 Proof of Lemma 3.4.2

Proof of Lemma 3.4.2. Let $T > 0$, $x = (q, p) \in \mathbb{R}^{2d}$. Let us prove *(i)*. We recall from (3.44) that almost surely, for all $t \in [0, T]$, for all $\gamma > 1$,

$$q^{(\gamma),x}_{\gamma t} = q - \frac{p^{(\gamma),x}_{\gamma t} - p}{\gamma} + \int_0^t F(q^{(\gamma),x}_{\gamma s})\mathrm{d}s + \sqrt{2\beta^{-1}} B^{(\gamma)}_t.$$

Furthermore, by (3.49), almost surely, for all $t \in [0, T]$,

$$w^{(\gamma),q}_t = q + \int_0^t F(w^{(\gamma),q}_s)\mathrm{d}s + Z^{(\gamma)}_{t,T},$$

where we recall $Z^{(\gamma)}_{t,T} = \sqrt{2\beta^{-1}} B^{(\gamma)}_t - h^{(\gamma)}_T(t) Y^{(\gamma)}_T$, with $Y^{(\gamma)}_T$ defined by (3.46). It follows from (3.48) that for all $T > 0$, $\gamma > 0$ and $t \in [0, T]$,

$$\begin{aligned} h^{(\gamma)}_T(t) &\leq \frac{2}{\gamma}\frac{1 - \mathrm{e}^{-\gamma^2 T}}{1 - \mathrm{e}^{-2\gamma^2 T}} \\ &= \frac{2}{\gamma}\frac{1}{1 + \mathrm{e}^{-\gamma^2 T}} \leq \frac{2}{\gamma}. \end{aligned}$$

Therefore, by Grönwall's Lemma, since F is globally Lipschitz continuous with a Lipschitz coefficient $C_1 > 0$,

$$\sup_{t\in[0,T]} \left| q^{(\gamma),x}_{\gamma t} - w^{(\gamma),q}_t \right| \leq \left(\frac{\sup_{t\in[0,T]} \left| p^{(\gamma),x}_{\gamma t} - p \right|}{\gamma} + \frac{2}{\gamma} \left| Y^{(\gamma)}_T \right| \right) \mathrm{e}^{C_1 T}.$$

Moreover, by (3.45) and (3.46), almost surely, for $t \in [0, T]$,

$$\frac{p^{(\gamma),x}_{\gamma t} - p}{\gamma} = -\frac{1 - \mathrm{e}^{-\gamma^2 t}}{\gamma} p + \mathrm{e}^{-\gamma^2 t} \int_0^t \mathrm{e}^{\gamma^2 s} F(q^{(\gamma),x}_{\gamma s})\mathrm{d}s + \frac{Y^{(\gamma)}_t}{\gamma}.$$

Therefore, since $\gamma > 1$,

$$\mathbb{E}\left[\sup_{t\in[0,T]} \frac{\left|p^{(\gamma),x}_{\gamma t} - p\right|}{\gamma}\right] \leq \frac{|p| + \|F\|_\infty + \mathbb{E}\left[\sup_{t\in[0,T]} |Y^{(\gamma)}_t|\right]}{\gamma}. \tag{3.55}$$

Let $(H^{(\gamma)}_t = ((H^{(\gamma)}_t)_1, \dots, (H^{(\gamma)}_t)_d))_{t\in[0,T]}$ be the strong solution on $\mathbb{R}^d$ of the following Ornstein-Uhlenbeck SDE:

$$\mathrm{d}H^{(\gamma)}_t = -\gamma H^{(\gamma)}_t \mathrm{d}t + \mathrm{d}B_t, \qquad H^{(\gamma)}_0 = 0,$$

then it is easy to see that, almost surely, for $t \in [0,T]$, $Y^{(\gamma)}_t = \sqrt{2\gamma\beta^{-1}} H^{(\gamma)}_{\gamma t}$. Therefore, the Minkowski inequality applied to the Euclidean norm on $\mathbb{R}^d$ of $|Y^{(\gamma)}_t|$ ensures that

$$\sup_{t\in[0,T]} |Y^{(\gamma)}_t| \leq \sqrt{2\gamma\beta^{-1}} \sum_{i=1}^{d} \sup_{t\in[0,\gamma T]} |(H^{(\gamma)}_t)_i|. \tag{3.56}$$

A sharp inequality on the expectation in the summand above is provided in [37] and ensures the existence of a universal constant $C_2 > 0$ such that for all $t \in [0,T]$, $\gamma > 0$ and $i \in \llbracket 1, d \rrbracket$,

$$\mathbb{E}\left[\sup_{t\in[0,\gamma T]} |(H^{(\gamma)}_t)_i|\right] \leq \frac{C_2}{\sqrt{\gamma}} \sqrt{\log(1+\gamma^2 T)}.$$

Reinjecting into (3.56), one gets $\mathbb{E}[\sup_{t\in[0,T]} |Y^{(\gamma)}_t|] \leq dC_2\sqrt{2\beta^{-1}}\sqrt{\log(1+\gamma^2 T)}$. Therefore, the inequality (3.55) ensures the existence of a constant $C_3 > 0$ such that for all $\gamma > 1$,

$$\mathbb{E}\left[\sup_{t\in[0,T]} \frac{\left|p^{(\gamma),x}_{\gamma t} - p\right|}{\gamma}\right] \leq \frac{C_3}{\gamma}\left(1 + |p| + \sqrt{\log(1+\gamma^2 T)}\right).$$

Using the Cauchy-Schwarz inequality and the Itô isometry, one easily gets that $\mathbb{E}[\left|Y^{(\gamma)}_T\right|] \leq \sqrt{d\beta^{-1}}$. Therefore, for all $\gamma > 1$, $T > 0$, $t \in [0,T]$ and $x = (q,p) \in \mathbb{R}^{2d}$,

$$\mathbb{E}\left[\sup_{t\in[0,T]} \left|q^{(\gamma),x}_{\gamma t} - w^{(\gamma),q}_t\right|\right] \leq \frac{C_4}{\gamma}\left(1 + |p| + \sqrt{\log(1+\gamma^2 T)}\right) \mathrm{e}^{C_1 T}.$$

This concludes the proof of *(i)* and the proof of *(ii)* also follows from the use of Gronwall's Lemma along with the previous estimates. □

3.4.3.2 Proof of Proposition 3.4.3

Let us now prove Proposition 3.4.3. In order to do so, we resort to the two following results.

Proposition 3.4.6 (Principal eigenvalue)**.** *Under Assumptions (F1) and (O),*

$$\limsup_{\gamma\to\infty} \lambda^{(\gamma)}_0 \gamma < \infty. \tag{3.57}$$

The proof of Proposition 3.4.6 is postponed to the next section. The next lemma gives useful properties of the transition densities p_t and $\widehat{\mathrm{p}}^{(\alpha)}_t$, introduced in Theorem 3.2.2.

Lemma 3.4.7 (Properties of the transition densities)**.** *Let Assumption (F2) hold. For any $t > 0$, $\alpha \in (0,1)$, there exist $C_t > 0$ and $\gamma_t > 1$ such that for all $\gamma \geq \gamma_t$ and $(q,p), (q',p') \in \mathbb{R}^{2d}$,*

$$\widehat{\mathrm{p}}^{(\alpha)}_{\gamma t}((q,p),(q',p')) \leq C_t, \tag{3.58}$$

and

$$\sup_{q'\in\mathscr{O}} \int_{\mathbb{R}^d} \widehat{\mathrm{p}}^{(\alpha)}_{\gamma t}((q,p),(q',p'))\mathrm{d}p' \leq C_t. \tag{3.59}$$

Proof of Lemma 3.4.7. The explicit expression of $\widehat{\mathrm{p}}^{(\alpha)}$ is detailed in (2.79), from which we deduce the following upper-bound: for $t>0$, $\alpha\in(0,1)$ and $(q,p),(q',p')\in\mathbb{R}^{2d}$,

$$\widehat{\mathrm{p}}^{(\alpha)}_{\gamma t}((q,p),(q',p'))\leq \frac{1}{\sqrt{(2\pi)^{2d}\left(\frac{4\beta^{-2}\gamma^6t^4}{12}\phi(\gamma^2 t)\right)^d}},$$

where ϕ is given by (2.73),

$$\phi:\rho\in\mathbb{R}\mapsto 4\Phi_2(\rho)\Phi_1(2\rho)-3\Phi_1(\rho)^4=\begin{cases}\frac{6(1-\mathrm{e}^{-\rho})}{\rho^4}\left[-2+\rho+(2+\rho)\mathrm{e}^{-\rho}\right] & \text{if } \rho\neq 0,\\ 1 & \text{if } \rho=0.\end{cases}$$

Besides, since $\gamma^6t^4\phi(\gamma^2t)\underset{\gamma\to\infty}{\longrightarrow}6t$, the estimate (3.58) easily follows. We now prove (3.59). For $x=(q,p)\in\mathbb{R}^{2d}$, the marginal distribution in q' of $\widehat{\mathrm{p}}^{(\alpha)}_{\gamma t}((q,p),(q',p'))$ is the Gaussian measure on $\mathbb{R}^d$ with mean $q+\gamma tp\Phi_1(\gamma^2t)$ and covariance matrix $\frac{2\beta^{-1}\gamma^4t^3}{3\alpha}\Phi_2(\gamma^2t)I_d$ so that

$$\begin{aligned}\int_{\mathbb{R}^d}\widehat{\mathrm{p}}^{(\alpha)}_{\gamma t}((q,p),(q',p'))\mathrm{d}p' &= \frac{(3\alpha)^{d/2}}{\left(4\pi\beta^{-1}\gamma^4t^3\Phi_2(\gamma^2t)\right)^{d/2}}\mathrm{e}^{-\frac{3\alpha}{4\beta^{-1}\gamma^4t^3\Phi_2(\gamma^2t)}\left|q'-q-\gamma tp\Phi_1(\gamma^2t)\right|^2} \\ &\leq \frac{(3\alpha)^{d/2}}{\left(4\pi\beta^{-1}\gamma^4t^3\Phi_2(\gamma^2t)\right)^{d/2}}.\end{aligned}\tag{3.60}$$

Since $\gamma^4t^3\Phi_2(\gamma^2t)\underset{\gamma\to\infty}{\longrightarrow}3t$, the upper bound (3.59) immediately follows. □

Proof of Proposition 3.4.3. Let $\gamma>0$. By Definition 3.1.1 of a QSD, $\mu^{(\gamma)}$ is such that for all $A\in\mathscr{B}(D)$,

$$\mathbb{P}_{\mu^{(\gamma)}}(X_\gamma\in A,\tau_\partial>\gamma)=\mu^{(\gamma)}(A)\mathrm{e}^{-\lambda_0^{(\gamma)}\gamma},$$

since $\mathbb{P}_{\mu^{(\gamma)}}(\tau_\partial>\gamma)=\mathrm{e}^{-\lambda_0^{(\gamma)}\gamma}$ by Theorem 3.2.11.

The equality above being satisfied for any $A\in\mathscr{B}(D)$, and since $\mu^{(\gamma)}$ has the continuous density $\psi^{(\gamma)}$ with respect to the Lebesgue measure on D, one deduces that for all $(q',p')\in D$,

$$\psi^{(\gamma)}(q',p')=\mathrm{e}^{\lambda_0^{(\gamma)}\gamma}\iint_D\psi^{(\gamma)}(q,p)\mathrm{p}^D_\gamma((q,p),(q',p'))\mathrm{d}p\mathrm{d}q.$$

Let $\alpha\in(0,1)$. Using Remark 3.2.3 and (3.15) in Remark 3.2.5, there exists $C>0$ such that for all $\gamma>0$ and $(q',p')\in D$,

$$\psi^{(\gamma)}(q',p')\leq C\mathrm{e}^{\lambda_0^{(\gamma)}\gamma}\iint_D\psi^{(\gamma)}(q,p)\widehat{\mathrm{p}}^{(\alpha)}_\gamma((q,p),(q',p'))\mathrm{d}p\mathrm{d}q,\tag{3.61}$$

where $\widehat{\mathrm{p}}^{(\alpha)}$ is the transition density of the process $(\widehat{q}^{(\alpha)}_t,\widehat{p}^{(\alpha)}_t)_{t\geq 0}$ defined in (3.13). By Proposition 3.4.6 and the upper-bounds (3.58) and (3.59) in Lemma 3.4.7, the first two estimates in Proposition 3.4.3 follow from (3.61) and the fact that $\psi^{(\gamma)}$ is the density of a probability measure on D. It remains now to prove the last estimate in Proposition 3.4.3.

It follows from Fubini-Tonelli's theorem and the inequality (3.61) that

$$\iint_D\psi^{(\gamma)}(q',p')|p'|\mathrm{d}p'\mathrm{d}q'\leq C\mathrm{e}^{\lambda_0^{(\gamma)}\gamma}\iint_D\psi^{(\gamma)}(q,p)\left(\iint_D\widehat{\mathrm{p}}^{(\alpha)}_\gamma((q,p),(q',p'))|p'|\mathrm{d}p'\mathrm{d}q'\right)\mathrm{d}p\mathrm{d}q.\tag{3.62}$$

Let us now prove that

$$\limsup_{\gamma\to\infty}\sup_{(q,p)\in D}\iint_D\widehat{\mathrm{p}}^{(\alpha)}_\gamma((q,p),(q',p'))|p'|\mathrm{d}p'\mathrm{d}q'<\infty,$$

this will conclude the proof using (3.57) and (3.62).

Let us start by rewriting, for any $(q,p) \in D$ and $\gamma > 0$,

$$\iint_D \widehat{\mathrm{p}}_\gamma^{(\alpha)}((q,p),(q',p'))|p'|\mathrm{d}p'\mathrm{d}q' = \mathbb{E}_{(q,p)}\left[\mathbb{1}_{\widehat{q}_\gamma^{(\alpha)} \in \mathscr{O}} |\widehat{p}_\gamma^{(\alpha)}|\right]$$
$$\leq \mathbb{E}_{(q,p)}\left[|\widehat{p}_\gamma^{(\alpha)} - p\mathrm{e}^{-\gamma^2}|\right] + |p|\mathrm{e}^{-\gamma^2}\mathbb{P}_{(q,p)}\left(\widehat{q}_\gamma^{(\alpha)} \in \mathscr{O}\right),$$

and recall that under $\mathbb{P}_{(q,p)}$, $\widehat{q}_\gamma^{(\alpha)}$ and $\widehat{p}_\gamma^{(\alpha)}$ have marginal distributions

$$\widehat{q}_\gamma^{(\alpha)} \sim \mathscr{N}_d\left(q + \gamma p \Phi_1(\gamma^2), \frac{2\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2) I_d\right), \qquad \widehat{p}_\gamma^{(\alpha)} \sim \mathscr{N}_d\left(p\mathrm{e}^{-\gamma^2}, \frac{2\beta^{-1}\gamma^2\Phi_1(2\gamma^2)}{\alpha} I_d\right).$$

As a consequence, we deduce from the Cauchy-Schwarz inequality that

$$\mathbb{E}_{(q,p)}\left[|\widehat{p}_\gamma^{(\alpha)} - p\mathrm{e}^{-\gamma^2}|\right] \leq \sqrt{\frac{2d\beta^{-1}\gamma^2\Phi_1(2\gamma^2)}{\alpha}},$$

the right-hand side of which is uniform in (q,p) and is bounded when $\gamma \to \infty$. On the other hand, let us define $\delta := \sup_{q,q' \in \mathscr{O}} |q - q'|$ (which is finite since $\mathscr{O}$ is bounded) and note that

$$\mathbb{P}_{(q,p)}\left(\widehat{q}_\gamma^{(\alpha)} \in \mathscr{O}\right) \leq \mathbb{P}_{(q,p)}\left(|\widehat{q}_\gamma^{(\alpha)} - q| \leq \delta\right)$$
$$= \mathbb{P}\left(\left|\gamma p \Phi_1(\gamma^2) + \sqrt{\frac{2\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2)} Z\right| \leq \delta\right),$$

where $Z \sim \mathscr{N}_d(0, I_d)$. By the triangle, Markov and Cauchy-Schwarz inequalities, if $|p| \neq 0$ then

$$\mathbb{P}\left(\left|\gamma p \Phi_1(\gamma^2) + \sqrt{\frac{2\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2)} Z\right| \leq \delta\right) \leq \mathbb{P}\left(\sqrt{\frac{2\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2)}|Z| + \delta \geq \gamma|p|\Phi_1(\gamma^2)\right)$$
$$\leq \frac{\sqrt{\frac{2d\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2)} + \delta}{\gamma|p|\Phi_1(\gamma^2)},$$

so that

$$|p|\mathrm{e}^{-\gamma^2}\mathbb{P}_{(q,p)}\left(\widehat{q}_\gamma^{(\alpha)} \in \mathscr{O}\right) \leq \mathrm{e}^{-\gamma^2}\frac{\sqrt{\frac{2d\beta^{-1}\gamma^4}{3\alpha}\Phi_2(\gamma^2)} + \delta}{\gamma\Phi_1(\gamma^2)},$$

the right-hand side of which is uniform in (q,p) and vanishes when $\gamma \to \infty$. □

3.4.3.3 Proof of Proposition 3.4.6

Let us now prove Proposition 3.4.6. We will need the following intermediate lemma.

Lemma 3.4.8 (Uniform velocity tightness)**.** *Let Assumption (F2) hold. For every $\epsilon > 0$, there exists $M > 0$ such that for all $\gamma \geq 4$,*

$$\sup_{(q,p) \in \mathscr{O} \times \mathrm{B}(0,M)} \mathbb{P}\left(p_\gamma^{(\gamma),(q,p)} \notin \mathrm{B}(0,M)\right) \leq \epsilon, \tag{3.63}$$

where $\mathrm{B}(0,M) := \{p \in \mathbb{R}^d : |p| < M\}$.

Proof. Let $\epsilon > 0$. Let us take $M \geq \frac{2\sqrt{d\beta^{-1}}}{\epsilon} + \|F\|_\infty$. By (3.25), for all $x = (q,p) \in \mathscr{O} \times \mathrm{B}(0,M)$ and $\gamma \geq 4$ (so that $\frac{M}{\gamma^2} + \frac{M}{\gamma} \leq \frac{M}{2}$),

$$\begin{aligned}\left|p_\gamma^{(\gamma),x}\right| &= \left|p\mathrm{e}^{-\gamma^2} + \gamma\mathrm{e}^{-\gamma^2}\int_0^1 \mathrm{e}^{\gamma^2 s}F(q_{\gamma s}^{(\gamma),x})\mathrm{d}s + Y_1^{(\gamma)}\right| \\ &\leq \frac{M}{\gamma^2}\underbrace{\gamma^2\mathrm{e}^{-\gamma^2}}_{<1} + \frac{\|F\|_\infty}{\gamma} + \left|Y_1^{(\gamma)}\right| \\ &< \frac{M}{2} + \left|Y_1^{(\gamma)}\right|\end{aligned}$$

since $M \geq \|F\|_\infty$ and $\gamma \geq 4$. Besides,

$$\mathbb{P}\left(\left|Y_1^{(\gamma)}\right| > M/2\right) \leq \frac{\mathbb{E}\left[\left|Y_1^{(\gamma)}\right|\right]}{M/2} \leq \frac{2\sqrt{d\beta^{-1}}}{M} \leq \epsilon$$

by definition of M. Therefore, for all $(q,p) \in \mathscr{O} \times \mathrm{B}(0,M)$,

$$\mathbb{P}\left(p_\gamma^{(\gamma),(q,p)} \notin \mathrm{B}(0,M)\right) \leq \epsilon.$$

□

Let us now prove Proposition 3.4.6.

Proof of Proposition 3.4.6. Let $q_0 \in \mathscr{O}$. Let $r \in (0,1)$ such that $\mathrm{B}(q_0,2r) \subset \mathscr{O}$. For $q \in \mathbb{R}^d$, we define the following stopping time:

$$\overline{\tau}_0^{(\gamma),q} = \inf\{t > 0 : \overline{q}_t^{(\gamma),q} \notin \mathrm{B}(q_0, 3r/2)\}.$$

Let also $a := \inf_{q\in\mathrm{B}(q_0,r)} \mathbb{P}(\overline{q}_1^{(\gamma),q} \in \mathrm{B}(q_0,r/2), \overline{\tau}_0^{(\gamma),q} > 1)$. Notice that $a > 0$ since the function $q \in \overline{\mathrm{B}(q_0,r)} \mapsto \mathbb{P}(\overline{q}_1^{(\gamma),q} \in \mathrm{B}(q_0,r/2), \overline{\tau}_0^{(\gamma),q} > 1)$ is continuous and positive on the compact set $\overline{\mathrm{B}(q_0,r)}$ by the continuity and positivity of its transition density see [33]. Besides, a does not depend on γ since the law of the process $(\overline{q}_t^{(\gamma),q})_{t\geq 0}$ does not depend on γ. Let us take $\epsilon \in (0, \frac{a}{4})$ and $M > 0$ such that (3.63) in Lemma 3.4.8 is satisfied.

Step 1: Let us prove that there exists $\gamma_1 > 1$ such that

$$c := \inf_{\gamma\geq\gamma_1}\inf_{(q,p)\in\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0,r)\times\mathrm{B}(0,M), \tau_\partial^{(\gamma),(q,p)} > \gamma\right) > 0. \tag{3.64}$$

For $(q,p) \in \mathrm{B}(q_0,r) \times \mathrm{B}(0,M)$,

$$\begin{aligned}&\mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0,r)\times\mathrm{B}(0,M), \tau_\partial^{(\gamma),(q,p)} > \gamma\right) \\ &\geq \mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0,r)\times\mathrm{B}(0,M), \tau_\partial^{(\gamma),(q,p)} > \gamma, \sup_{t\in[0,1]}\left|q_{\gamma t}^{(\gamma),(q,p)} - \overline{q}_t^{(\gamma),q}\right| \leq r/2\right).\end{aligned} \tag{3.65}$$

By *(i)* and *(ii)* in Lemma 3.4.2, there exists $C_1 > 0$, depending on M, such that for all $\gamma > 4$,

$$\sup_{(q,p)\in\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \mathbb{E}\left[\sup_{t\in[0,1]}\left|q_{\gamma t}^{(\gamma),(q,p)} - \overline{q}_t^{(\gamma),q}\right|\right] \leq C_1\frac{1+\sqrt{\log(1+\gamma^2)}}{\gamma}. \tag{3.66}$$

Moreover, by (3.63) in Lemma 3.4.8,

$$\begin{aligned}&\mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0,r)\times\mathrm{B}(0,M), \tau_\partial^{(\gamma),(q,p)} > \gamma, \sup_{t\in[0,1]}\left|q_{\gamma t}^{(\gamma),(q,p)} - \overline{q}_t^{(\gamma),q}\right| \leq r/2\right) \\ &\geq \mathbb{P}\left(\overline{q}_1^{(\gamma),q} \in \mathrm{B}(q_0,r/2), \overline{\tau}_0^{(\gamma),q} > 1, \sup_{t\in[0,1]}\left|q_{\gamma t}^{(\gamma),(q,p)} - \overline{q}_t^{(\gamma),q}\right| \leq r/2\right) - \epsilon,\end{aligned}$$

by definition of $\overline{\tau}_0^{(\gamma),q}$ and since $\mathrm{B}(q_0, 2r) \subset \mathscr{O}$. Using (3.66) and the Markov inequality, it follows that for all $(q, p) \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M)$,

$$\begin{aligned}
&\mathbb{P}\left(\overline{q}_1^{(\gamma),q} \in \mathrm{B}(q_0, r/2), \overline{\tau}_0^{(\gamma),q} > 1, \sup_{t\in[0,1]} \left|q_{\gamma t}^{(\gamma),(q,p)} - \overline{q}_t^{(\gamma),q}\right| \leq r/2\right) \\
&\geq \mathbb{P}\left(\overline{q}_1^{(\gamma),q} \in \mathrm{B}(q_0, r/2), \overline{\tau}_0^{(\gamma),q} > 1\right) - \frac{2C_1}{\gamma r}(1 + \sqrt{\log(1+\gamma^2)}) \\
&\geq a - \frac{2C_1}{\gamma r}(1 + \sqrt{\log(1+\gamma^2)}).
\end{aligned}$$

As a result, by (3.65) and by definition of a and ϵ, for all $\gamma > 4$,

$$\begin{aligned}
&\inf_{(q,p)\in\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M), \tau_\partial^{(\gamma),(q,p)} > \gamma\right) \\
&\geq a - \frac{2C_1}{\gamma r}(1 + \sqrt{\log(1+\gamma^2)}) - \frac{a}{4}.
\end{aligned}$$

Hence, there exists $\gamma_1 > 4$ such that for all $\gamma \geq \gamma_1$,

$$\inf_{(q,p)\in\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \mathbb{P}\left(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M), \tau_\partial^{(\gamma),(q,p)} > \gamma\right) \geq \frac{a}{2}.$$

Step 2: Now let us prove (3.57). By (3.64), for all $\gamma \geq \gamma_1$,

$$\begin{aligned}
&\mathrm{e}^{\lambda_0^{(\gamma)}\gamma} \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathbb{P}(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M), \tau_\partial^{(\gamma),(q,p)} > \gamma)\mathrm{d}q\mathrm{d}p \\
&\geq c\mathrm{e}^{\lambda_0^{(\gamma)}\gamma} \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathrm{d}q\mathrm{d}p.
\end{aligned}$$

Since $\psi^{(\gamma)}$ is the density of the QSD of the Langevin process $(X_t^{(\gamma)})_{t\geq 0}$ then

$$\begin{aligned}
&\mathrm{e}^{\lambda_0^{(\gamma)}\gamma} \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathbb{P}(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M), \tau_\partial^{(\gamma),(q,p)} > \gamma)\mathrm{d}q\mathrm{d}p \\
&\leq \mathrm{e}^{\lambda_0^{(\gamma)}\gamma} \iint_D \psi^{(\gamma)}(q, p)\mathbb{P}(X_\gamma^{(\gamma),(q,p)} \in \mathrm{B}(q_0, r) \times \mathrm{B}(0, M), \tau_\partial^{(\gamma),(q,p)} > \gamma)\mathrm{d}q\mathrm{d}p \\
&= \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathrm{d}q\mathrm{d}p.
\end{aligned}$$

Consequently, for $\gamma \geq \gamma_1$,

$$c\mathrm{e}^{\lambda_0^{(\gamma)}\gamma} \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathrm{d}q\mathrm{d}p \leq \iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathrm{d}q\mathrm{d}p$$

which concludes the proof since $\iint_{\mathrm{B}(q_0,r)\times\mathrm{B}(0,M)} \psi^{(\gamma)}(q, p)\mathrm{d}q\mathrm{d}p > 0$. □

CHAPTER 4

ANOTHER APPROACH FOR THE STUDY OF THE QSD OF THE LANGEVIN PROCESS

In this chapter we prove the existence of a unique quasi-stationary distribution for the Langevin diffusion process using previous results by N. Champagnat and D. Villemonais in [20], along with some tools, like the Harnack inequality, developed in Chapter 2.

Abstract: Consider the Langevin process, described by a vector (position,velocity), in $\mathbb{R}^d \times \mathbb{R}^d$. Let $\mathscr{O}$ be a $\mathscr{C}^2$ open bounded and connected set of $\mathbb{R}^d$. General criteria for the existence and uniqueness of quasi-stationary distributions (QSD) for Markov processes were provided in a recent work by Champagnat and Villemonais. Besides, a Harnack inequality satisfied by weak solutions to the kinetic Fokker-Planck equation associated with the Langevin process, was obtained in Theorem 2.2.15. Applying this Harnack inequality to these criteria we are able to prove the existence of a unique QSD for the Langevin process on the domain $D := \mathscr{O} \times \mathbb{R}^d$ as well as a convergence result of the Langevin process conditioned to remain in D towards its QSD.

4.1 Introduction

Let $d \geq 1$. Let $(\Omega, \mathscr{F}, (\mathscr{F}_t)_{t\geq 0}, \mathbb{P})$ be a filtered probability space and $(B_t)_{t\geq 0}$ a d-dimensional $(\mathscr{F}_t)_{t\geq 0}$-Brownian motion. We start by introducing some notations used throughout this work.

Let $F : \mathbb{R}^d \mapsto \mathbb{R}^d$ and $\mathscr{O}$ be an open set of $\mathbb{R}^d$ satisfying the following assumptions.

Assumption (A1). $F \in \mathscr{C}^\infty(\overline{\mathscr{O}}, \mathbb{R}^d)$.

Assumption (A2). *$\mathscr{O}$ is a non-empty open $\mathscr{C}^2$ bounded connected set of $\mathbb{R}^d$.*

Let $\sigma > 0$, $\gamma \in \mathbb{R}$. The Langevin diffusion process $(X_t)_{t\geq 0} = (q_t, p_t)_{t\geq 0}$ on $\mathbb{R}^{2d}$, described by its position q_t and velocity p_t at time t, is defined by the following stochastic differential equation:

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sigma \mathrm{d}B_t. \end{cases} \tag{4.1}$$

The infinitesimal generator $\mathscr{L}$ of this process is the following kinetic Fokker-Planck operator $\mathscr{L}$, defined for $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$ by

$$\mathscr{L} = p \cdot \nabla_q + F(q) \cdot \nabla_p - \gamma p \cdot \nabla_p + \frac{\sigma^2}{2}\Delta_p. \tag{4.2}$$

Let us consider the domain $D = \mathscr{O} \times \mathbb{R}^d$ of $\mathbb{R}^{2d}$. Let τ_∂ be the first exit time from D of the process $(X_t)_{t\geq 0}$:

$$\tau_\partial := \inf\{t > 0 : X_t \notin D\}.$$

Remark 4.1.1. *Assume that $X_0 \in D$, Remark 2.2.6 ensures the existence of a unique strong solution $(X_t)_{0\le t\le \tau_\partial}$ defined until the exit time τ_∂.*

For $A \in \mathscr{F}$ we denote by $\mathbb{P}_x(A)$ the probability of A under the event $X_0 = x$ and $\mathbb{P}_\mu(A) = \int_D \mathbb{P}_x(A)\mu(\mathrm{d}x)$ if μ is a probability measure on D. Let us now give the definition of a QSD.

Definition 4.1.2 (Quasi-stationary distribution)**.** *A probability measure μ on D is said to be a quasi-stationary distribution (QSD) on D for the process $(X_t)_{t\ge 0}$, if for all $A \in \mathscr{B}(D)$,*

$$\mathbb{P}_\mu(X_t \in A, \tau_\partial > t) = \mu(A)\mathbb{P}_\mu(\tau_\partial > t).$$

If the existence and uniqueness of a QSD for elliptic diffusion processes with smooth coefficients on smooth bounded domains is well-known in the literature (cf. for example [36, 55, 21, 50]), it is most definitely not once we look at degenerate process such as the Langevin process (4.1). Furthermore we consider here a QSD on an unbounded domain D which is not the usual case of study. Fortunately, recent works by Champagnat, Villemonais [20, Theorem 3.5] established general criteria for the existence of a unique QSD for general Markov processes on domains. These criteria are recalled below for a general diffusion process $(X_t)_{t\ge 0}$.

Theorem 4.1.3 ([20])**.** *Let $n \ge 1$. Let $(X_t)_{t\ge 0}$ be a Markov process in $\mathbb{R}^n$ generated by an operator of the form $\mathscr{L} = \frac{1}{2}a :: \nabla^2 + b\cdot\nabla$ for some continuous functions $a : \mathbb{R}^n \mapsto \mathbb{R}^{n\times n}$ and $b : \mathbb{R}^n \mapsto \mathbb{R}^n$. Assume that there exists a compact subset K of a measurable set $D \subset \mathbb{R}^n$ such that the following hypotheses (F_1), (F_2) and (F_3) are satisfied:*
*(F_1) : (**Local Dobrushin condition**) there exist $c_1, t_1 > 0$ and $\widetilde{\nu}$ a probability measure on K such that*

$$\forall x \in K, \qquad \forall A \in \mathscr{B}(D), \qquad \mathbb{P}_x(X_{t_1} \in A, \tau_\partial > t_1) \ge c_1\widetilde{\nu}(A\cap K).$$

*(F_2) : (**Global Lyapunov criterion**) there exist $c_2, t_2 > 0$, $\psi_1 : D \mapsto [1,\infty)$ a measurable function on D and $\alpha_1 > \alpha_2 > 0$ such that*

(i) $\forall x \in D, \qquad \mathbb{E}_x[\psi_1(X_{t_2})\mathbb{1}_{t_2<\tau_K\wedge\tau_\partial}] \le \mathrm{e}^{-\alpha_1 t_2}\psi_1(x),$

(ii) $\forall x \in K, \quad \forall t \in [0,t_2], \qquad \mathbb{E}_x[\psi_1(X_t)\mathbb{1}_{\tau_\partial>t}] \le c_2,$

(iii) $\forall x \in K, \qquad \mathrm{e}^{\alpha_2 t}\mathbb{P}_x(X_t \in K, \tau_\partial > t) \underset{t\to\infty}{\longrightarrow} \infty,$

where $\tau_K := \inf\{t > 0 : X_t \in K\}$.
*(F_3) : (**Local Harnack inequality**) there exists $c_3 > 0$ such that for all $t \ge 0$,*

$$\sup_{x\in K}\mathbb{P}_x(\tau_\partial > t) \le c_3 \inf_{x\in K}\mathbb{P}_x(\tau_\partial > t).$$

Then $(X_t)_{t\ge 0}$ admits a unique QSD μ on D satisfying $\mu(\psi_1) < \infty$ and such that there exists $t_3 > 0$ satisfying $\mathbb{P}_\mu(X_{t_3} \in K) > 0$. Moreover, there exist $C, \beta > 0$ such that for all probability measure ν on D verifying $\nu(\psi_1) < \infty$ and $\nu(\psi_2) > 0$,

$$\forall t \ge 0, \qquad \|\mathbb{P}_\nu(X_t \in \cdot|\tau_\partial > t) - \mu(\cdot)\|_{TV} \le C\mathrm{e}^{-\beta t}\frac{\nu(\psi_1)}{\nu(\psi_2)}, \tag{4.3}$$

where $\|\cdot\|_{TV}$ is the total-variation norm and ψ_2 is defined for some $n_0 \ge 1$ by:

$$\psi_2(x) = \sum_{k=0}^{n_0}\mathrm{e}^{\alpha_2 k t_2}\mathbb{P}_x(X_{kt_2} \in K, \tau_\partial > kt_2). \tag{4.4}$$

Besides, there exists $\lambda_0 \ge 0$ and a measurable function $\phi : D \mapsto \mathbb{R}_+$ such that

(i) $\forall t \ge 0, \qquad \mathbb{P}_\mu(\tau_\partial > t) = \mathrm{e}^{-\lambda_0 t},$

(ii) $e^{\lambda_0 t}\mathbb{P}_x(\tau_\partial > t) \underset{t\to\infty}{\longrightarrow} \phi(x)$, *where the convergence is uniform in* $L^\infty(\psi^{1/p})$ *for some* $p > 0$,

(iii) $\forall t \geq 0, \quad \forall x \in D, \qquad \mathbb{E}_x[\phi(X_t)\mathbb{1}_{\tau_\partial > t}] = e^{-\lambda_0 t}\phi(x)$.

Remark 4.1.4. *The theorem above is stated in [20] with an additional strong Markov property* (F_0) *which we omit here as we consider diffusion processes which always satisfy the strong Markov property, see [49, Theorem 4.20 p.322].*

We denote by (F) the set of all the three hypotheses (F_1), (F_2) and (F_3). The Harnack inequality from Theorem 2.2.15 obtained in Chapter 2 for distributional solutions of the kinetic Fokker-Planck equation is recalled below.

Theorem 4.1.5 (Theorems 2.2.15, 2.2.20)**.** *Let Assumptions (A1) and (A2) hold. For* $A \in \mathscr{B}(D)$*, the function*

$$u_A : (t,x) \in \mathbb{R}_+^* \times D \mapsto \mathbb{P}_x(X_t \in A, \tau_\partial > t) \tag{4.5}$$

is continuous on $\mathbb{R}_+^* \times D$*. It is positive if* $\mathring{A} \neq \emptyset$*. Furthermore, for all compact set* $K \subset D$*,* $\epsilon > 0$ *and* $T > 0$ *there exists a constant* $C_{K,\epsilon,T} > 0$ *such that for all* $A \in \mathscr{B}(D)$ *and for all* $t \geq \epsilon$*,*

$$\sup_{x\in K} u_A(t,x) \leq C_{K,\epsilon,T} \inf_{x\in K} u_A(t+T,x). \tag{4.6}$$

Proof. The continuity and positivity of u_A follows from Thereom 2.2.20 and the Harnack inequality follows from the application of Remark 2.2.11 along with Theorem 2.2.15 to u_A. □

Applying this Harnack inequality to the Langevin process $(X_t)_{t\geq 0}$, we shall prove that $(X_t)_{t\geq 0}$ satisfies the hypotheses of Theorem 4.1.3. Hence, we obtain the main result of this chapter.

Theorem 4.1.6 (QSD for the Langevin process)**.** *Let Assumptions (A1) and (A2) hold. Let* $(X_t)_{t\geq 0}$ *be the Langevin process satisfying (4.1). The process* $(X_t)_{t\geq 0}$ *admits a unique QSD* μ *on* D*. Besides, there exist* $C, \beta > 0$ *such that for all probability measure* ν *on* D*,*

$$\forall t \geq 0, \qquad \|\mathbb{P}_\nu(X_t \in \cdot | \tau_\partial > t) - \mu(\cdot)\|_{TV} \leq \frac{Ce^{-\beta t}}{\nu(\psi_2)}, \tag{4.7}$$

where ψ_2 *is defined as in (4.4). Moreover, there exists* $\lambda_0 \geq 0$ *and a measurable function* $\phi : D \mapsto \mathbb{R}_+$ *such that*

(i) $\forall t \geq 0, \qquad \mathbb{P}_\mu(\tau_\partial > t) = e^{-\lambda_0 t}$,

(ii) $e^{\lambda_0 t}\mathbb{P}_x(\tau_\partial > t) \underset{t\to\infty}{\longrightarrow} \phi(x)$, *where the convergence is uniform on* D,

(iii) $\forall t \geq 0, \quad \forall x \in D, \qquad \mathbb{E}_x[\phi(X_t)\mathbb{1}_{\tau_\partial > t}] = e^{-\lambda_0 t}\phi(x)$.

4.2 Highlights of the proof of 4.1.3

The idea behind the proof of 4.1.3 is briefly explained in this section. The proof is done for a discrete-time Markov chain $(Y_n)_{n\geq 0}$ which is extracted from the process $(X_t)_{t\geq 0}$ satisfying (F) and writes for all $n \geq 0$, $Y_n := X_{nt_0}$ for some $t_0 > 0$. Besides, the Markov chain $(Y_n)_{n\geq 0}$ satisfies Hypotheses [20, Assumption (E) p.8] which are the analogous of the hypotheses (F) in the discrete-time setting. The goal is to prove [20, Theorem 2.1] for the Markov chain $(Y_n)_{n\geq 1}$. Then, in Section 11.5.2 of [20], Champagnat and Villemonais show how to deduce from the result [20, Theorem 2.1] satisfied by $(Y_n)_{n\geq 1}$ the result obtained in 4.1.3 for the process $(X_t)_{t\geq 0}$.

The theorem relies, in particular, on previous work from Hairer and Mattingly [40] where the authors managed to prove, under a geometric drift condition and a minorization condition recalled below, an exponentially fast convergence of the law of a Markov chain towards its stationary distribution in the total-variation norm.

For $x \in \mathbb{R}^n$, let $P(x, \cdot)$ be the transition kernel of a Markov chain on $\mathbb{R}^{2d}$. Let us state the following conditions, see Assumptions 3.1 and 3.4 in [40].

(i) (**Drift condition**) There exists a function $V : \mathbb{R}^{2d} \mapsto \mathbb{R}_+$, $K \geq 0$ and $\alpha \in (0,1)$ such that

$$\forall x \in \mathbb{R}^{2d}, \qquad \int_{\mathbb{R}^{2d}} \mathrm{P}(x, \mathrm{d}y)V(y) \leq \alpha V(x) + K,$$

(ii) (**Minorization condition**) for every $R > 0$, there exists $\beta > 0$ so that

$$\|\mathrm{P}(x,\cdot) - \mathrm{P}(y,\cdot)\|_{TV} \leq 2(1-\beta),$$

for all $x, y \in \mathbb{R}^{2d}$ such that $V(x) + V(y) \geq R$.

Under such conditions one has the following convergence, see [40, Theorem 3.9].

Theorem 4.2.1 ([40]). *Assuming the two conditions above hold then* P *admits a unique invariant measure* μ_∞. *Furthermore, there exist constants* $\theta > 0$ *and* $\rho \in (0,1)$ *such that for all* $n \geq 1$,

$$\left|\!\left|\!\left| \int_{\mathbb{R}^{2d}} \mathrm{P}^n(x, \mathrm{d}y) f(y) - \int_{\mathbb{R}^{2d}} \mu_\infty(\mathrm{d}y) f(y) \right|\!\right|\!\right|_\theta \leq \rho^n,$$

where $|||g|||_\theta := \sup_{x \in \mathbb{R}^{2d}} \frac{|g(x)|}{2 + \theta V(x) + \theta V(y)}$.

Let us come back now to the study of the Markov chain $(Y_n)_{n\geq 0}$. The purpose of 4.1.3 is to transpose and adapt the proof of Theorem 4.2.1 to the following time-inhomogeneous kernel

$$\forall 0 \leq l < k \leq n, \quad \forall x \in D, \qquad S^n_{l,k}(x,\cdot) = \mathbb{P}(Y_k \in \cdot | Y_l = x, \tau_\partial > nt_0).$$

Let us choose $\lambda \in (0, \alpha_1 - \alpha_2)$ (α_1, α_2 defined in Hypothesis (F_2) of Theorem 4.1.3) and let

$$\Psi : (k, x) \in \mathbb{N} \times D \mapsto \mathbb{E}_x \left[\mathrm{e}^{\lambda(\tau_K \wedge (kt_0))} | \tau_\partial > kt_0 \right].$$

Using [20, Assumption (E) p.8], the authors prove that Ψ satisfies [20, Propositions 9.1] and that S satisfies [20, Propositions 9.2]. Then, adapting the proof of [40, Theorem 3.9] with P and V (using the notations of Assumptions (i) and (ii)) defined by: $\mathrm{P} := S^n_{k,k+1}$ and $V := \Psi(n-k-1, \cdot)$ for $n \geq 1$ and $k \in ⟦1, n-1⟧$, they manage to obtain [20, Proposition 9.3] which is recalled below.

Proposition 4.2.2 ([19]). *There exists* $C > 0$, $\rho \in (0,1)$ *such that for all* $n \geq 1$, $x, y \in D$,

$$\left\| S^n_{0,n}(x,\cdot) - S^n_{0,n}(y,\cdot) \right\|_{TV} \leq C\rho^n (2 + \Psi(n,x) + \Psi(n,y)).$$

In pages 65-67 of [20], Champagnat and Villemonais show how to deduce (4.3) for the process $(X_t)_{t\geq 0}$ from the proposition above, using the estimate provided in [20, Lemma 9.4]. Finally, Section 11.5.3 is devoted to the construction of the function ϕ satisfying (ii) and (iii) in Theorem 4.1.3.

4.3 Proof of Theorem 4.1.6

Let us now come back to the setting of Theorem 4.1.6.

For $k \geq 1$, let K_k be the following compact subset of D

$$K_k = \left\{ (q,p) \in D : |p| \leq k, d_\partial(q) \geq \frac{1}{k} \right\} \tag{4.8}$$

where d_∂ is the Euclidean distance to $\partial\mathscr{O}$ from a point in $\mathscr{O}$.

Theorem 4.1.6 is an immediate consequence of the theorem below which is proven in this section.

Theorem 4.3.1. *Under Assumptions (A1) and (A2), there exists* k_0 *large enough such that the diffusion process* $(X_t)_{t\geq 0}$ *satisfies the hypotheses* (F_1), (F_2) *and* (F_3) *on the compact set* K_{k_0} *with* $\psi_1 \in \mathrm{L}^\infty(D)$ *and* $\psi_2 > 0$ *on* D.

The fact that ψ_2, defined in (4.4), is positive on D, is just a consequence of the positivity of u_A stated in Thereom 4.1.5. Therefore, we decompose the proof of Theorem 4.3.1 as follows.

Proposition 4.3.2. *Under Assumptions (A1) and (A2), the process* $(X_t)_{t\geq 0}$ *satisfies* (F_1) *and* (F_3) *on* K_{k_0} *for* k_0 *large enough.*

Proposition 4.3.3. *Under Assumptions (A1) and (A2), the process* $(X_t)_{t\geq 0}$ *satisfies* (F_2) *on* K_{k_0} *for* k_0 *large enough, with a function* $\psi_1 \in \mathrm{L}^\infty(D)$.

Let us start with the proof of Proposition 4.3.2.

Proof of Proposition 4.3.2. **Proof of** (F_1): Let k_0 be large enough such that K_{k_0} has a non-empty interior. Let $x_0 \in K_{k_0}$, $t_0 > 0$, $A \in \mathscr{B}(D)$ and u_A be the function defined in (4.5). Theorem 4.1.5 ensures the existence of $c_1 := C_{K_{k_0},t_0,1} > 0$ such that for all $x \in K_{k_0}$,

$$\begin{aligned}\mathbb{P}_x(X_{t_0+1} \in A, \tau_\partial > t_0+1) &\geq c_1^{-1}\mathbb{P}_{x_0}(X_{t_0} \in A, \tau_\partial > t_0)\\ &\geq c_1^{-1} \underbrace{\mathbb{P}_{x_0}(X_{t_0} \in K_{k_0}, \tau_\partial > t_0)}_{=u_{K_{k_0}}(t_0,x_0)>0 \text{ by Theorem 4.1.5}} \underbrace{\frac{\mathbb{P}_{x_0}(X_{t_0} \in A\cap K_{k_0}, \tau_\partial > t_0)}{\mathbb{P}_{x_0}(X_{t_0} \in K_{k_0}, \tau_\partial > t_0)}}_{:=\widetilde{\nu}(A\cap K_{k_0})},\end{aligned}$$

where $\widetilde{\nu}$ is a probability measure on K_{k_0}, which yields $(F_1)$with $t_1 = t_0 + 1$.
Proof of (F_3): Theorem 4.1.5 applied to u_D ensures the existence of $c_2 > 0$ such that for all $t \geq 1$,

$$\sup_{x\in K_{k_0}} \mathbb{P}_x(\tau_\partial > t) \leq c_2 \inf_{x\in K_{k_0}} \mathbb{P}_x(\tau_\partial > t+1) \leq c_2 \inf_{x\in K_{k_0}} \mathbb{P}_x(\tau_\partial > t),$$

since u_D is a decreasing function of t. Now it remains to prove such an inequality for $t \in [0,1]$.
For all $t \in [0,1]$, $x, y \in K_{k_0}$,

$$\mathbb{P}_x(\tau_\partial > t) \leq 1 \leq \frac{\mathbb{P}_y(\tau_\partial > t)}{\mathbb{P}_y(\tau_\partial > 1)}.$$

Besides, the function $y \in K_{k_0} \mapsto \mathbb{P}_y(\tau_\partial > 1)$ is a positive and continuous function by Theorem 4.1.5, therefore it reaches a minimum $c_3 > 0$. Hence, for all $x, y \in K_{k_0}$ and $t \in [0,1]$,

$$\mathbb{P}_x(\tau_\partial > t) \leq c_3^{-1}\mathbb{P}_y(\tau_\partial > t).$$

Therefore, for all $t \geq 0$,

$$\sup_{x\in K_{k_0}} \mathbb{P}_x(\tau_\partial > t) \leq (c_2 \vee c_3^{-1}) \inf_{x\in K_{k_0}} \mathbb{P}_x(\tau_\partial > t),$$

which concludes the proof of (F_3). □

The proof of Proposition 4.3.3 is a bit more involved and requires the three following lemmata.

Lemma 4.3.4 (Lyapunov function)**.** *Let Assumptions (A1) and (A2) hold. For all* $\lambda > 0$*, there exists a bounded measurable subset* $D_\lambda \subset D$ *closed in* D*, a constant* $c_\lambda > 0$*, and a bounded* $\mathscr{C}^2(D)$ *function* $\phi_\lambda : D \mapsto [1,\infty)$ *such that*

- $\forall \lambda > 0, \qquad \|\nabla\phi_\lambda\|_\infty < \infty,$
- $\sup_{\lambda>0} \|\phi_\lambda\|_\infty < \infty,$
- $\forall x \in D, \qquad \mathscr{L}\phi_\lambda(x) \leq -\lambda\phi_\lambda(x) + c_\lambda \mathbb{1}_{D_\lambda}(x).$

Proof of Lemma 4.3.4. Let us start the proof by defining a non-negative function $g \in \mathscr{C}^2(\mathbb{R}_+^*)$ such that

(i) $\forall \rho \in (0, 1/2), \qquad g(\rho) = \rho,$

(ii) $\forall \rho > 1, \qquad g(\rho) = 1,$

(iii) $\forall \rho > 0, \qquad g(\rho) \leq 1.$

Now let $\lambda > 0$. Let $\beta := 1 + \sup_{q \in \mathscr{O}} |q|$ and $p_a > 0$ be a parameter independent of λ which will be defined later. Let $p_0(\lambda) := 1 + p_a + 4\lambda\beta$ and $D_\lambda \subset D$ be defined as follows:

$$D_\lambda = \{(q,p) \in D : |p| \leq p_0(\lambda)\}.$$

We define ϕ_λ on D by:

$$\phi_\lambda(q,p) := \begin{cases} \beta - \dfrac{q \cdot p}{|p|} g(|p|), & |p| \neq 0 \\ \beta, & p = 0, \end{cases} \tag{4.9}$$

then $\phi_\lambda \in \mathscr{C}^2(D)$. Besides, for $(q,p) \in D \setminus D_\lambda$, $\phi_\lambda(q,p) = \beta - \frac{q \cdot p}{|p|}$ and satisfies

$$\begin{aligned} \mathscr{L}\phi_\lambda &= p \cdot \nabla_q \phi_\lambda + F(q) \cdot \nabla_p - \gamma p \cdot \nabla_p \phi_\lambda + \frac{\sigma^2}{2} \Delta_p \phi_\lambda \\ &= -|p| \left(1 + \frac{q \cdot F(q)}{|p|^2} - \frac{(q \cdot p)(p \cdot F(q))}{|p|^4} - \frac{\sigma^2}{2}(d-1)\frac{q \cdot p}{|p|^4} \right). \end{aligned}$$

Since F is bounded on $\mathscr{O}$, by the Cauchy-Schwarz inequality,

$$\sup_{q \in \mathscr{O}} \left| \frac{q \cdot F(q)}{|p|^2} - \frac{(q \cdot p)(p \cdot F(q))}{|p|^4} - \frac{\sigma^2}{2}(d-1)\frac{q \cdot p}{|p|^4} \right| \underset{|p| \to \infty}{\longrightarrow} 0.$$

As a result, let us define p_a such that for $|p| \geq p_a$

$$\sup_{q \in \mathscr{O}} \left| \frac{q \cdot F(q)}{|p|^2} - \frac{(q \cdot p)(p \cdot F(q))}{|p|^4} - \frac{\sigma^2}{2}(d-1)\frac{q \cdot p}{|p|^4} \right| \leq \frac{1}{2}$$

The triangle inequality ensures that for $|p| \geq p_a$,

$$\mathscr{L}\phi_\lambda \leq -\frac{|p|}{2}.$$

As a result, for $|p| \geq p_0(\lambda)$,

$$\begin{aligned} \mathscr{L}\phi_\lambda &\leq -\frac{|p|}{2} \\ &\leq -2\lambda\beta \\ &\leq -\lambda \left(\beta - \frac{q \cdot p}{|p|} \right) = -\lambda \phi_\lambda(q,p). \end{aligned}$$

Consider now the following function on $\overline{D_\lambda}$:

$$(q,p) \mapsto \mathscr{L}\phi_\lambda(q,p) + \lambda \phi_\lambda(q,p).$$

It is fairly easy to see that this is a continuous function of (q,p) in $\overline{D_\lambda}$. And since $\overline{D_\lambda}$ is a compact set of $\mathbb{R}^{2d}$, it reaches a maximum $c_\lambda < \infty$. Combined with the inequality above this yields that $\mathscr{L}\phi_\lambda \leq -\lambda\phi_\lambda + c_\lambda \mathbb{1}_{D_\lambda}$ on D. Furthermore, by construction of β and g, $1 \leq \phi_\lambda \leq 2\beta - 1$ and it is easy to see that

$$\forall \lambda > 0, \qquad \|\nabla \phi_\lambda\|_\infty < \infty,$$

which concludes the proof of Lemma 4.3.4. □

Lemma 4.3.5. *Let Assumptions (A1) and (A2) hold. Let $\lambda > 0$ and D_λ be the set obtained in Lemma 4.3.4. We have*

$$\sup_{x \in D_\lambda} \mathbb{P}_x(\tau_\partial \wedge \tau_{K_k} > 1) \underset{k\to\infty}{\longrightarrow} 0 \tag{4.10}$$

with $\tau_{K_k} = \inf\{t > 0 : X_t \in K_k\}$.

Proof of Lemma 4.3.5. Let $\lambda > 0$. Let us prove the following condition, which implies directly (4.10),

$$\sup_{x \in \overline{D_\lambda}} \mathbb{P}_x(X_1 \in D \cap K_k^c) \underset{k\to\infty}{\longrightarrow} 0.$$

By Friedman's uniqueness result [32, Theorem 5.2.1.], the trajectories $(X_t)_{0\leq t\leq\tau_\partial}$ do not depend on the values of F outside of $\mathscr{O}$. Extending F to a function in $\mathscr{C}^\infty(\mathbb{R}^d, \mathbb{R}^d)$ which is bounded and globally Lipschitz continuous, we obtain a strong solution $(X_t)_{t\geq 0}$ to (4.1) defined globally in time, which coincides with our previous solution until τ_∂.

Let us now define the sequence of functions $(f_k)_{k\geq 1}$ on $\mathbb{R}^{2d}$ by

$$\forall x_1 \in \mathbb{R}^{2d}, \quad f_k(x_1) = \mathbb{1}_{D\cap K_k^c}(x_1).$$

By [71, Corollary 7.2], the Langevin process (4.1) admits a smooth transition density. Therefore, for all $k \geq 1$, the function

$$x \in \overline{D_\lambda} \mapsto \mathbb{E}_x[f_k(X_1)] = \mathbb{P}_x(X_1 \in D \cap K_k^c) \tag{4.11}$$

is continuous on $\overline{D_\lambda}$. Furthermore, since $k \mapsto f_k(x_1)$ decreases towards 0 for $x_1 \in \overline{D_\lambda}$, then by the dominated convergence theorem

$$\mathbb{P}_x(X_1 \in D \cap K_k^c) \underset{k\to\infty}{\longrightarrow} 0.$$

Moreover, since 0 is a continuous function, Dini's theorem applied to the decreasing sequence of continuous functions defined in (4.11) ensures that the convergence is uniform and thus

$$\sup_{x \in \overline{D_\lambda}} \mathbb{P}_x(X_1 \in D \cap K_k^c) \underset{k\to\infty}{\longrightarrow} 0,$$

which leads to (4.10). □

Lemma 4.3.6. *Let Assumptions (A1) and (A2) hold. Let $\lambda > 0$. Let ϕ_λ and D_λ be as obtained in Lemma 4.3.4. For $t \geq 0$ and $x \in D \setminus D_\lambda$,*

$$\mathbb{E}_x[\phi_\lambda(X_t)\mathbb{1}_{\tau_\partial\wedge\tau_{D_\lambda}>t}] \leq \mathrm{e}^{-\lambda t}\phi_\lambda(x). \tag{4.12}$$

Proof of Lemma 4.3.6. Let $\lambda > 0$ and $x \in D \setminus D_\lambda$. Let $\tau_{D_\lambda} = \inf\{t > 0 : X_t \in D_\lambda\}$. Applying Itô's formula to the process $(\mathrm{e}^{\lambda(t\wedge\tau_\partial\wedge\tau_{D_\lambda})}\phi_\lambda(X_{t\wedge\tau_\partial\wedge\tau_{D_\lambda}}))_{t\geq 0}$ one has, $\mathbb{P}_x$-almost surely,

$$\begin{aligned}\mathrm{e}^{\lambda(t\wedge\tau_\partial\wedge\tau_{D_\lambda})}\phi_\lambda(X_{t\wedge\tau_\partial\wedge\tau_{D_\lambda}}) = \phi_\lambda(x) + \int_0^t \mathbb{1}_{s\leq\tau_\partial\wedge\tau_{D_\lambda}}\mathrm{e}^{\lambda s}(\mathscr{L}\phi_\lambda(X_s) + \lambda\phi_\lambda(X_s))\mathrm{d}s \\ + \sigma\int_0^t \mathbb{1}_{s\leq\tau_\partial\wedge\tau_{D_\lambda}}\mathrm{e}^{\lambda s}\nabla_p\phi_\lambda(X_s)\cdot\mathrm{d}B_s.\end{aligned}$$

Since $\nabla_p\phi_\lambda$ is bounded on D by Lemma 4.3.4 the last term has zero expectation. Also since ϕ_λ satisfies Lemma 4.3.4, then $\mathscr{L}\phi_\lambda + \lambda\phi_\lambda \leq 0$ on $D \setminus D_\lambda$. Therefore,

$$\mathbb{E}_x\left[\mathrm{e}^{\lambda(t\wedge\tau_\partial\wedge\tau_{D_\lambda})}\phi_\lambda(X_{t\wedge\tau_\partial\wedge\tau_{D_\lambda}})\right] \leq \phi_\lambda(x).$$

As a result, since ϕ_λ is non-negative,

$$\mathbb{E}_x\left[\mathrm{e}^{\lambda t}\phi_\lambda(X_t)\mathbb{1}_{\tau_\partial\wedge\tau_{D_\lambda}>t}\right] \leq \phi_\lambda(x),$$

which yields (4.12). □

Finally we can prove Proposition 4.3.3.

Proof of Proposition 4.3.3. **Proof of** $(F_2)-$(iii): Let $k_0 \geq 1$ large enough such that $K := K_{k_0}$ has a non-empty interior. Let B be an open ball such that $\overline{B}$ is included in the interior of K. Let $t \geq 1$ and $x \in K$, the Markov property at time $\lfloor t \rfloor$ ensures that

$$\begin{aligned}\mathbb{P}_x\left(X_t \in K, \tau_\partial > t\right) &\geq \mathbb{P}_x\left(X_{\lfloor t \rfloor} \in B, X_t \in K, \tau_\partial > t\right)\\ &= \mathbb{E}_x\left(\mathbb{1}_{\tau_\partial > \lfloor t \rfloor, X_{\lfloor t \rfloor} \in B} \mathbb{P}_y\left(X_{t-\lfloor t \rfloor} \in K, \tau_\partial > t - \lfloor t \rfloor\right)|_{y=X_{\lfloor t \rfloor}}\right)\\ &\geq c_1 \mathbb{P}_x\left(X_{\lfloor t \rfloor} \in B, \tau_\partial > \lfloor t \rfloor\right)\end{aligned}$$

where $c_1 := \inf_{y \in \overline{B}, s \in [0,1]} \mathbb{P}_y\left(X_s \in K, \tau_\partial > s\right)$. Besides, for $y \in \overline{B}$, $s \in (0,1]$, $\mathbb{P}_y\left(X_s \in K, \tau_\partial > s\right) > 0$ by Theorem 4.1.5 and it is easy to see that $\mathbb{P}_y\left(X_s \in K, \tau_\partial > s\right)$ converges to 1 when $s \to 0, y \in \overline{B}$. Therefore, $c_1 > 0$. Now let $c_2 := \inf_{x \in K} u_B(1, x) > 0$, then it follows from the Markov property at times $\lfloor t \rfloor - 1, \lfloor t \rfloor - 2, \ldots, 1$ that

$$\mathbb{P}_x\left(X_t \in K, \tau_\partial > t\right) \geq c_1 c_2^{\lfloor t \rfloor}.$$

Taking $\alpha_2 > |\log(c_2)|$, we have $\inf_{x \in K} \mathrm{e}^{\alpha_2 t} \mathbb{P}_x(X_t \in K, \tau_\partial > t) \underset{t \to \infty}{\longrightarrow} \infty$ which yields (iii).
Proof of (F_2)-(i): Let $\epsilon > 0$. Let

$$\overline{\lambda} = \alpha_2 + \log\left(2 \sup_{\lambda > 0} \|\phi_\lambda\|_\infty\right) + \epsilon,$$

since $\sup_{\lambda > 0} \|\phi_\lambda\|_\infty < \infty$ by Lemma 4.3.4. By Lemma 4.3.5, there exists $k_0 \geq 1$ such that for $k \geq k_0$,

$$\sup_{x \in D_{\overline{\lambda}}} \mathbb{P}_x(\tau_\partial \wedge \tau_{K_k} > 1) \leq \mathrm{e}^{-\overline{\lambda}}.$$

Let $K := K_{k_0}$. For $x \in D_{\overline{\lambda}}$ and $t \in [1, 2]$,

$$\begin{aligned}\mathbb{E}_x[\phi_{\overline{\lambda}}(X_t) \mathbb{1}_{\tau_K \wedge \tau_\partial > t}] &\leq \|\phi_{\overline{\lambda}}\|_\infty \sup_{x \in D_{\overline{\lambda}}} \mathbb{P}_x(\tau_\partial \wedge \tau_K > 1)\\ &\leq \mathrm{e}^{-\overline{\lambda}} \|\phi_{\overline{\lambda}}\|_\infty \qquad (4.13)\\ &\leq \mathrm{e}^{-\overline{\lambda}} \|\phi_{\overline{\lambda}}\|_\infty \phi_{\overline{\lambda}}(x) \qquad (4.14)\\ &\leq \mathrm{e}^{-(\alpha_2 + \epsilon)} \phi_{\overline{\lambda}}(x),\end{aligned}$$

since $\phi_{\overline{\lambda}} \geq 1$. For $x \in D \setminus D_{\overline{\lambda}}$, since $D_{\overline{\lambda}}$ is closed in D, it follows from the strong Markov property at $\tau_{D_{\overline{\lambda}}} = \inf\{t > 0 : X_t \in D_{\overline{\lambda}}\}$ that

$$\begin{aligned}\mathbb{E}_x\left[\phi_{\overline{\lambda}}(X_2) \mathbb{1}_{\tau_K \wedge \tau_\partial > 2}\right] &= \mathbb{E}_x\left[\mathbb{1}_{\tau_K \wedge \tau_\partial \wedge \tau_{D_{\overline{\lambda}}} > 1} \mathbb{E}_y\left[\phi_{\overline{\lambda}}(X_1) \mathbb{1}_{\tau_K \wedge \tau_\partial > 1}\right]|_{y=X_1}\right]\\ &+ \mathbb{E}_x\left[\mathbb{1}_{\tau_{D_{\overline{\lambda}}} \leq 1} \mathbb{1}_{\tau_K \wedge \tau_\partial \geq \tau_{D_{\overline{\lambda}}}} \mathbb{E}_y\left(\phi_{\overline{\lambda}}(X_{2-u}) \mathbb{1}_{\tau_K \wedge \tau_\partial > 2-u}\right)|_{u=\tau_{D_{\overline{\lambda}}}, y=X_{\tau_{D_{\overline{\lambda}}}}}\right].\end{aligned} \qquad (4.15)$$

Furthermore, for all $y \in D$,

$$\mathbb{E}_y\left[\phi_{\overline{\lambda}}(X_1) \mathbb{1}_{\tau_K \wedge \tau_\partial > 1}\right] \leq \|\phi_{\overline{\lambda}}\|_\infty \leq \|\phi_{\overline{\lambda}}\|_\infty \phi_{\overline{\lambda}}(y).$$

As a result, the first term in the right hand-side of (4.15) satisfies:

$$\mathbb{E}_x\left[\mathbb{1}_{\tau_K \wedge \tau_\partial \wedge \tau_{D_{\overline{\lambda}}} > 1} \mathbb{E}_y\left[\phi_{\overline{\lambda}}(X_1) \mathbb{1}_{\tau_K \wedge \tau_\partial > 1}\right]|_{y=X_1}\right] \leq \|\phi_{\overline{\lambda}}\|_\infty \mathbb{E}_x\left[\mathbb{1}_{\tau_K \wedge \tau_\partial \wedge \tau_{D_{\overline{\lambda}}} > 1} \phi_{\overline{\lambda}}(X_1)\right].$$

Using Lemma 4.3.6, it follows that

$$\mathbb{E}_x\left[\mathbb{1}_{\tau_K \wedge \tau_\partial \wedge \tau_{D_{\overline{\lambda}}} > 1} \mathbb{E}_y\left[\phi_{\overline{\lambda}}(X_1) \mathbb{1}_{\tau_K \wedge \tau_\partial > 1}\right]|_{y=X_1}\right] \leq \|\phi_{\overline{\lambda}}\|_\infty \mathrm{e}^{-\overline{\lambda}} \phi_{\overline{\lambda}}(x).$$

The second term in the right hand-side of (4.15) satisfies by the inequality (4.13):

$$\begin{aligned}\mathbb{E}_x\left[\mathbb{1}_{\tau_{D_{\overline{\lambda}}}\leq 1}\mathbb{1}_{\tau_K\wedge\tau_\partial\geq\tau_{D_{\overline{\lambda}}}}\mathbb{E}_y\left(\phi_{\overline{\lambda}}(X_{2-u})\mathbb{1}_{\tau_K\wedge\tau_\partial>2-u}\right)|_{u=\tau_{D_{\overline{\lambda}}},y=X_{\tau_{D_{\overline{\lambda}}}}}\right] &\leq \mathrm{e}^{-\overline{\lambda}}\|\phi_{\overline{\lambda}}\|_\infty\mathbb{P}_x(\tau_{D_{\overline{\lambda}}}\leq 1)\\ &\leq \mathrm{e}^{-\overline{\lambda}}\|\phi_{\overline{\lambda}}\|_\infty\phi_{\overline{\lambda}}(x)\end{aligned}$$

Thus for all $x \in D \setminus D_{\overline{\lambda}}$,

$$\begin{aligned}\mathbb{E}_x[\phi_{\overline{\lambda}}(X_2)\mathbb{1}_{\tau_K\wedge\tau_\partial>2}] &\leq 2\mathrm{e}^{-\overline{\lambda}}\|\phi_{\overline{\lambda}}\|_\infty\phi_{\overline{\lambda}}(x)\\ &\leq \mathrm{e}^{-(\alpha_2+\epsilon)}\phi_{\overline{\lambda}}(x).\end{aligned}$$

In conclusion, for all $x \in D$,

$$\mathbb{E}_x[\phi_{\overline{\lambda}}(X_2)\mathbb{1}_{\tau_K\wedge\tau_\partial>2}] \leq \mathrm{e}^{-(\alpha_2+\epsilon)}\phi_{\overline{\lambda}}(x).$$

Therefore, taking $t_2 = 2$, $\alpha_1 = \alpha_2 + \epsilon$ and $\psi_1 = \phi_{\overline{\lambda}}$ concludes the proof of (i). The proof of (ii) is immediate since $\psi_1 = \phi_{\overline{\lambda}}$ is bounded on D by Lemma 4.3.4. □

Part III

Entry, exit points of the Langevin process

CHAPTER 5

ENTRY, EXIT POINTS OF THE LANGEVIN PROCESS

This work focuses on the study of the stationary distribution of the Langevin process crossing the boundary of a smooth domain.

5.1 Introduction and motivation

5.1.1 Objective of this work

Let us consider the Langevin process $(q_t, p_t)_{t\geq 0}$ solution to the stochastic differential equation

$$\begin{cases} \mathrm{d}q_t = M^{-1}p_t\mathrm{d}t, \\ \mathrm{d}p_t = -\nabla V(q_t)\mathrm{d}t - \gamma M^{-1}p_t\mathrm{d}t + \sigma \mathrm{d}B_t, \end{cases} \tag{5.1}$$

where $q_t \in \mathbb{R}^d$ denotes the set of positions, $p_t \in \mathbb{R}^d$ are the associated momenta and $(B_t)_{t\geq 0}$ is a d-dimensional Brownian motion. Such dynamics are typically used to describe the evolution of a molecular system. In this case, $V : \mathbb{R}^d \to \mathbb{R}$ gives the potential energy as a function of the positions, $\gamma > 0$ is the friction parameter and $\sigma = \sqrt{2\gamma\beta^{-1}} > 0$ is the diffusion parameter, with $\beta^{-1} = k_B T$ where T is the temperature. Let us now introduce $A \subset \mathbb{R}^d$ a subset of the position space. The objective of this work is to identify the stationary distribution of the sequence of the entry (and exit) points of the Langevin process in A. This is a measure supported by $\partial A \times \mathbb{R}^d$, which is particularly useful to compute mean reaction times and more generally average quantities over the so-called transition paths from A to another set B. In Section 5.1.2, we give some more details about this motivation, using results from [8]. Notice that Section 5.1.2 is independent from the rest of this work and can be easily skipped.

5.1.2 One motivation: computing the mean reaction time between two states

Let us consider another set $B \subset \mathbb{R}^d$ which does not intersect A, and let us assume that A is a metastable state for the dynamics (5.1), in the sense that when leaving A, the stochastic process q_t has a very small probability to reach B before returning to A. Such a situation is ubiquitous in the context of computational statistical physics, where the sets A and B then describe two macroscopic conformations, and one is interested in the so-called transition paths from entrances in A to entrances in B, and in particular in their mean durations at (called the mean reaction time). More precisely, the mean reaction time is defined as [62, 8]

$$T_{AB} = \lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} (\tau_n^B - \tau_n^A)$$

where $\tau_{n+1}^A = \inf\{t > \tau_n^B,\, q_t \in A\}$ and $\tau_{n+1}^B = \inf\{t > \tau_{n+1}^A,\, q_t \in B\}$ are the so-called reactive entrance times in A and B with $\tau_0^A = \inf\{t \geq 0,\, q_t \in A\}$, $\tau_0^B = \inf\{t \geq 0,\, q_t \in B\}$.

To formalize this question, let us consider the successive entry points in A and B defined by: for $n \geq 0$

$$X_n = (q(\tau_n^E), p(\tau_n^E))$$

where $\tau_{n+1}^E = \inf\{t > \tau_n^E, (q_t, p_t) \in \Gamma_A^- \cup \Gamma_B^-\}$, $\tau_0^E = \inf\{t \geq 0, (q_t, p_t) \in \Gamma_A^- \cup \Gamma_B^-\}$ with $\Gamma_A^- = \{(q,p) \in \partial A \times \mathbb{R}^d,\, p \cdot n_A(q) < 0\}$ and $\Gamma_B^- = \{(q,p) \in \partial B \times \mathbb{R}^d,\, p \cdot n_B(q) < 0\}$. The unit vectors n_A and n_B denote the outward normals to A and B respectively. Starting from a point $X_0 = (q_0, p_0) \in \Gamma_A^- \cup \Gamma_B^-$, the sequence of random vectors $(X_n)_{n\geq 0}$ is a Markov chain with values in $\Gamma_A^- \cup \Gamma_B^-$. It can be shown (see [62, 8]) that the mean reaction time T_{AB} can be rewritten in terms of $(X_n)_{n\geq 0}$ as follows:

$$T_{AB} = \mathbb{E}_{\nu_E}\left[\sum_{n=0}^{N_B-1} \Delta(X_n)\right] \tag{5.2}$$

where $\nu_E = \lim_{N\to\infty} \frac{1}{N}\sum_{n=0}^{N-1} \delta_{(q(\tau_n^A), p(\tau_n^A))}$ is a distribution supported on Γ_A^- called the reactive entrance distribution, $\Delta(x) = \mathbb{E}_x[\tau_1^E]$ is the average time between two entrances in $A \cup B$ for the process $(q_t, p_t)_{t\geq 0}$ and $N_B = \inf\{n \geq 0, X_n \in \Gamma_B^-\}$. Notice that by changing the function Δ, one can have access to any mean quantity over the transition paths from A to B at the stationary regime.

From a computational viewpoint, Equation (5.2) is not very useful for two reasons. First, the reactive entrance distribution is difficult to sample (it does not have in particular a simple analytical expression in terms of the potential energy V, see [62]). Second, when A is metastable (which is the practical case of interest), N_B is very large and thus the sum in (5.2) is not easily sampled. One way to circumvent this difficulty is to use the so-called Hill relation [62, Section 4.2] which yields (for a general function Δ):

$$\begin{aligned}
\mathbb{E}_{\nu_E}\left[\sum_{n=0}^{N_B-1} \Delta(X_n)\right] &= \frac{\mathbb{E}_{\mu_A^-}[\Delta(X_0)]}{\mathbb{P}_{\mu_A^-}(X_1 \in \Gamma_B^-)} \\
&= \mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_A^-]\left(\frac{1}{\mathbb{P}_{\mu_A^-}(X_1 \in \Gamma_B^-)} - 1\right) \\
&\quad + \mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_B^-],
\end{aligned}$$

where μ_A^- is the stationary distribution μ of $(X_n)_{n\geq 0}$ conditioned to Γ_A^-. Starting from this distribution, $\mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_A^-]$ is the mean duration of a loop between two entrances in A, $\mathbb{P}_{\mu_A^-}(X_1 \in \Gamma_B^-)$ is the probability to see a path entering A and then going to B without going back to A, and $\mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_B^-]$ is the mean duration of such a path entering A and then going to B without going back to A. This last formula is much more convenient from a computational viewpoint at least if one is able to sample μ_A^-. Indeed, $\mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_A^-]$ can be computed by brute force simulations since it only requires to simulate loops from A to A. And the two quantities $\mathbb{P}_{\mu_A^-}(X_1 \in \Gamma_B^-)$ and $\mathbb{E}_{\mu_A^-}[\Delta(X_0)|X_1 \in \Gamma_B^-]$ can be estimated using rare event simulation methods such as splitting methods [17, 18, 1], in order to efficiently simulate a path leaving A and going to B without going back to A.

The whole point of this work is to provide an analytical formula for the stationary distribution of the entry points μ_A^-, which can thus be used to sample efficiently this measure.

5.1.3 Outline of this work

The paper is organized as follows. In Section 5.2, we present the general setting and the results we obtain. As will become clear, we actually identify the stationary distribution of the entry (and exit) points in A for the Langevin process in a slightly more general setting than (5.1), namely for general

$\gamma \in \mathbb{R}$ and $\sigma > 0$, and for a force field which may be non conservative ($-\nabla V$ is replaced by a general force field $F : \mathbb{R}^d \to \mathbb{R}^d$ in (5.1)). The proofs of the results are provided in Sections 5.3 and 5.4. The proofs rely on a combination of probabilistic arguments on the Langevin stochastic process, in particular on the notion of Harris recurrence for continous state Markov chains, and of tools from partial differential equations applied to the associated infinitesimal generator which follow from Chapter 2.

5.2 Setting and results

Throughout this paper, we fix $d \geq 1$ and denote by $|u| = \sqrt{u \cdot u}$ the Euclidean norm of $u \in \mathbb{R}^d$.

5.2.1 Langevin process

Let $F : \mathbb{R}^d \to \mathbb{R}^d$ be a $\mathscr{C}^\infty$ vector field, $\gamma \in \mathbb{R}$ and $\sigma > 0$. We consider the *Langevin process* $(q_t, p_t)_{t \geq 0}$ defined by the stochastic differential equation

$$\begin{cases} \mathrm{d}q_t = p_t \mathrm{d}t, \\ \mathrm{d}p_t = F(q_t)\mathrm{d}t - \gamma p_t \mathrm{d}t + \sigma \mathrm{d}B_t, \end{cases} \tag{5.3}$$

where $(B_t)_{t \geq 0}$ is a d-dimensional Brownian motion. We consider the mass M to be identity without loss of generality (see the change of variables in [56, Equation (.117)]). Since F is locally Lipschitz continuous on $\mathbb{R}^d$ then the equation (5.3) admits a unique strong solution $(q_t, p_t)_{0 \leq t < \tau_\infty}$ until some explosion time τ_∞. We make the following assumptions on the process $(q_t, p_t)_{0 \leq t < \tau_\infty}$

(A1) $\tau_\infty = \infty$, almost surely;

(A2) the process $(q_t, p_t)_{t \geq 0}$ is ergodic with respect to its unique stationary distribution $\mu(\mathrm{d}q\mathrm{d}p)$, and this measure has a smooth and positive density $\rho(q, p)$ with respect to the Lebesgue measure on $\mathbb{R}^d \times \mathbb{R}^d$;

(A3) the density $\rho(q, p)$ satisfies

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \left(|p \cdot \nabla_q \rho| + |\nabla_p \cdot (F(q)\rho)| + |\gamma \nabla_p (p\rho)| + \frac{\sigma^2}{2} |\Delta_p \rho| \right) \mathrm{d}q\mathrm{d}p < +\infty.$$

Remark 5.2.1 (Gradient system)**.** *These assumptions are in particular satisfied if $\gamma > 0$, $\sigma = \sqrt{2\gamma\beta^{-1}}$ for some $\beta > 0$, and $F = -\nabla V$ where $V : \mathbb{R}^d \to \mathbb{R}$ is a smooth function such that*

$$\int_{\mathbb{R}^d} (1 + |\nabla V(q)|) \mathrm{e}^{-\beta V(q)} \mathrm{d}q < +\infty,$$

in which case we have

$$\rho(q, p) = \frac{1}{Z_\beta} \mathrm{e}^{-\beta H(q,p)},$$

with

$$H(q, p) := V(q) + \frac{|p|^2}{2}, \qquad Z_\beta := \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathrm{e}^{-\beta H(q,p)} \mathrm{d}q\mathrm{d}p.$$

Remark 5.2.2 (Hypoellipticity and Assumptions (A1-A2))**.** *Both the infinitesimal generator $\mathscr{L}$ of the process $(q_t, p_t)_{t \geq 0}$, defined by*

$$\mathscr{L}\phi := p \cdot \nabla_q \phi + F(q) \cdot \nabla_p \phi - \gamma p \cdot \nabla_p \phi + \frac{\sigma^2}{2} \Delta_p \phi, \tag{5.4}$$

and its formal $L^2(\mathrm{d}q\mathrm{d}p)$ adjoint $\mathscr{L}^*$ given by

$$\mathscr{L}^*\psi = -p \cdot \nabla_q \psi - \nabla_p \cdot (F(q)\psi) + \gamma \nabla_p \cdot (p\psi) + \frac{\sigma^2}{2}\Delta_p \psi, \tag{5.5}$$

are known to satisfy Hörmander's condition and therefore be hypoelliptic*, see [58, Section 2.3]. This fact implies that the transition density of the process $(q_t, p_t)_{t\geq 0}$ is smooth. Likewise, in Assumption (A2), if a stationary distribution $\mu(\mathrm{d}q\mathrm{d}p)$ exists, then it necessarily possesses a smooth density $\rho(q,p)$, which in addition solves the stationary Fokker–Planck equation*

$$\forall (q,p) \in \mathbb{R}^d \times \mathbb{R}^d, \qquad \mathscr{L}^*\rho(q,p) = 0, \tag{5.6}$$

in the classical sense.

Following the approach discussed in [66, Section 3.1] for uniformly elliptic diffusions, a practical sufficient condition for the positivity of $\rho(q,p)$ is to show that the transition density of the process is positive. This can be proved by suitable Harnack inequalities for the Fokker–Planck equation associated with (5.3), see Theorem 2.2.15. Once $\rho(q,p)$ is shown to be positive, then both the uniqueness of a stationary distribution (which can also be obtained directly by means of the Stroock–Varadhan support theorem, see [71, Example 6.4]) and the ergodicity of the process $(q_t, p_t)_{t\geq 0}$ follow from [66, Théorème 1].

Throughout this paper, we shall use the notation $\mathbb{P}_\nu$, $\mathbb{E}_\nu$, ... (respectively $\mathbb{P}_{(q,p)}$, $\mathbb{E}_{(q,p)}$, ...) to keep track of the fact that (q_0, p_0) is distributed according to the probability measure ν on $\mathbb{R}^d \times \mathbb{R}^d$ (respectively equal to $(q,p) \in \mathbb{R}^d \times \mathbb{R}^d$).

5.2.2 The sequence of entry and exit points

Let $A \subset \mathbb{R}^d$ satisfy the following conditions.

(B1) The set A is a $\mathscr{C}^2$ open and connected subset of $\mathbb{R}^d$.

(B2) Both A and $\mathbb{R}^d \setminus A$ have positive Lebesgue measure.

As a consequence of Assumption (B1), the boundary Σ of A is $\mathscr{C}^2$ and orientable, that is to say that there exists a $\mathscr{C}^1$ function $n : \Sigma \to \mathbb{R}^d$ such that, for any $q \in \Sigma$, $|n(q)| = 1$ and $n(q)$ is orthogonal to the tangent space $\mathsf{T}_q\Sigma$ at q. We define the orientation such that $n(q)$ points toward the exterior of A.

We also introduce

$$\begin{aligned}
\Gamma^+ &:= \{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d : q \in \Sigma, p \cdot n(q) > 0\},\\
\Gamma^- &:= \{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d : q \in \Sigma, p \cdot n(q) < 0\},\\
\Gamma^0 &:= \{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d : q \in \Sigma, p \cdot n(q) = 0\}.
\end{aligned}$$

Our purpose is to study the sequences $(Y_n^\pm)_{n\geq 0}$ of the successive crossings of $\Gamma^\pm$ by the process $(q_t, p_t)_{t\geq 0}$. To this aim, we introduce the notation $A^+ := A$, $A^- := \mathbb{R}^d \setminus \overline{A}$ and first state the following result.

Lemma 5.2.3 (Return time to Σ)**.** *Under Assumptions (A1-A2) and (B1-B2), let $\tau := \inf\{t > 0 : q_t \in \Sigma\}$. For any $(q,p) \in (\mathbb{R}^d \times \mathbb{R}^d) \setminus \Gamma^0$, we have $0 < \tau < +\infty$, $\mathbb{P}_{(q,p)}$-almost surely. Besides:*

(i) if $q \in A^\pm$, then $(q_\tau, p_\tau) \in \Gamma^\pm$;

(ii) if $(q,p) \in \Gamma^\pm$ then $(q_\tau, p_\tau) \in \Gamma^\mp$.

This allows us to define, for any starting point $(q, p) \in (\mathbb{R}^d \times \mathbb{R}^d) \setminus \Gamma^0$, the following sequences of stopping times $(\tau_n^{\pm})_{n\geq 0}$:

$$\tau_0^{\pm} := \inf\{t \geq 0 : (q_t, p_t) \in \Gamma^{\pm}\},$$
$$\tau_{n+1}^{\pm} := \inf\{t > \tau_n^{\pm} : (q_t, p_t) \in \Gamma^{\pm}\},$$

which are increasing sequences. Furthermore, these sequences of entry and exit times related to A do not accumulate.

Lemma 5.2.4 (Nonaccumulation of $(\tau_n^{\pm})_{n\geq 0}$)**.** *Under the assumptions of Lemma 5.2.3, for any* $(q, p) \in (\mathbb{R}^d \times \mathbb{R}^d) \setminus \Gamma^0$*, we have*

$$\lim_{n\to+\infty} \tau_n^- = \lim_{n\to+\infty} \tau_n^+ = +\infty, \qquad \mathbb{P}_{(q,p)}\text{-almost surely.}$$

The proofs of Lemmata 5.2.3 and 5.2.4 are postponed to Section 5.4.

Remark 5.2.5 (Intertwining between the sequences $(\tau_n^{\pm})_{n\geq 0}$)**.** *The sequences $(\tau_n^{\pm})_{n\geq 0}$ are intertwined in the following sense:*

- *if* $(q, p) \in (A^+ \times \mathbb{R}^d) \cup \Gamma^+$*, then* $\tau_0^+ < \tau_0^- < \tau_1^+ < \cdots$*,*
- *if* $(q, p) \in (A^- \times \mathbb{R}^d) \cup \Gamma^-$*, then* $\tau_0^- < \tau_0^+ < \tau_1^- < \cdots$*.*

By the strong Markov property, which is a consequence of Assumption (A1) (see [14, Theorem 16.21]), the random sequences $(Y_n^{\pm})_{n\geq 0}$ defined by

$$Y_n^{\pm} := (q_{\tau_n^{\pm}}, p_{\tau_n^{\pm}})$$

are homogeneous Markov chains respectively taking their values in $\Gamma^{\pm}$ and correspond to the successive entry and exit points from A. Our purpose is to describe their ergodic behavior.

5.2.3 Statement of the results

We denote by $\mathrm{d}\sigma_\Sigma(q)$ the surface measure on Σ. In addition to Assumptions (A1-A2-A3) and (B1-B2), we suppose that

(C) the function $(q, p) \in \Sigma \times \mathbb{R}^d \mapsto |p \cdot n(q)|\rho(q, p)$ is in $L^1(\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p)$,

and introduce the notation

$$z_\Sigma^{\pm} := \int_{\Gamma^{\pm}} |p \cdot n(q)|\rho(q, p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p.$$

Notice that by Assumption (A2), $\rho(q, p) > 0$ on $\Sigma \times \mathbb{R}^d$ and therefore $z_\Sigma^{\pm} > 0$.

Theorem 5.2.6 (Stationary distribution for $(Y_n^{\pm})_{n\geq 0}$)**.** *Under Assumptions (A1-A2-A3), (B1-B2) and (C), the Markov chain $(Y_n^{\pm})_{n\geq 0}$ has a unique stationary distribution $\mu_\Sigma^{\pm}$, and this probability measure has density*

$$\rho_\Sigma^{\pm}(q, p) := \frac{1}{z_\Sigma^{\pm}} \mathbb{1}_{(q,p)\in\Gamma^{\pm}} |p \cdot n(q)|\rho(q, p)$$

with respect to the measure $\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p$ on $\Sigma \times \mathbb{R}^d$.

Remark 5.2.7. *We shall see in the proof of Theorem 5.2.6 that $z_\Sigma^+ = z_\Sigma^-$. In the case of Remark 5.2.1, this fact is actually obvious since it can be checked directly that $\rho(q, p) = \rho(q, -p)$, which then implies $z_\Sigma^+ = z_\Sigma^-$.*

One may also be interested in the Markov chain $(\overline{Y}_m)_{m\geq 0}$ defined as the sequence of the successive crossings of the surface Σ by the process $(q_t, p_t)_{t\geq 0}$. Following Remark 5.2.5, this sequence writes either $(Y_0^+, Y_0^-, Y_1^+, \dots)$ or $(Y_0^-, Y_0^+, Y_1^-, \dots)$ depending on whether $\tau_0^- < \tau_0^+$ or $\tau_0^+ < \tau_0^-$. In this perspective, the corresponding statement of Theorem 5.2.6 for the Markov chain $(\overline{Y}_m)_{m\geq 0}$ reads as follows.

Theorem 5.2.8 (Stationary distribution for $(\overline{Y}_m)_{m\geq 0}$)**.** *Under the assumptions of Theorem 5.2.6, the probability measure*

$$\overline{\mu}_\Sigma := \frac{1}{2}\left(\mu_\Sigma^+ + \mu_\Sigma^-\right)$$

is the unique stationary distribution of the Markov chain $(\overline{Y}_m)_{m\geq 0}$.

5.2.4 Discussion of the result

5.2.4.1 Trace processes

Let $(X_t)_{t\geq 0}$ be a continuous-time Markov process taking its values in some state space E. For $S \subset E$, define the *trace of* $(X_t)_{t\geq 0}$ *on* S as the process $(Y_t)_{t\geq 0}$ given by

$$Y_t = X(\tau_S(t)), \qquad \tau_S(t) := \sup\left\{r \geq 0 : \int_0^r \mathbb{1}_{X(s)\in S}\mathrm{d}s \leq t\right\},$$

see for instance [9] for continuous-time Markov chains, [54] for diffusion processes, also [7] for an example in the context of discrete-time Markov chains. If the process $(X_t)_{t\geq 0}$ is ergodic with respect to its stationary distribution μ and $\mu(S) > 0$, then it is a folklore result that the process $(Y_t)_{t\geq 0}$ should be ergodic with respect to the conditional distribution $\mu_S(\cdot) := \mu(\cdot|S)$, see for instance [9, Section 6.1].

In our context, Lemma 5.2.3 shows that the time spent on $\Gamma^\pm$ by the continuous-time process $(q_t, p_t)_{t\geq 0}$ is always 0, and consequently $\mu(\Gamma^\pm) = 0$, so that it is not clear whether the sequence $(Y_n^\pm)_{n\geq 0}$ can be considered as the *trace* of $(q_t, p_t)_{t\geq 0}$ on $\Gamma^\pm$.

5.2.4.2 Conditional distribution of μ given $\Gamma^\pm$

Following the approach of [56, Section 3.2.1], let us assume that $\Gamma^\pm$ rewrites under the form $\{(q,p) \in \mathbb{R}^d \times \mathbb{R}^d : \xi^\pm(q,p) = 0\}$ for some measurable function $\xi^\pm : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. Then [14, Theorem 4.34] shows that μ admits a regular conditional distribution given $\xi^\pm$. Under stronger regularity assumptions on $\xi^\pm$, the co-area formula [56, Corollary 3.3, p. 157] then allows to define the conditional distribution of μ given $\Gamma^\pm$ by letting

$$\begin{aligned}\mu(\mathrm{d}q\mathrm{d}p|\Gamma^\pm) &:= \mu(\mathrm{d}q\mathrm{d}p|\xi^\pm = 0)\\ &\propto \rho(q,p)\delta_{\xi^\pm(q,p)}(\mathrm{d}q\mathrm{d}p)\\ &= \rho(q,p)\frac{\mathbb{1}_{\pm p\cdot n(q)>0}\mathrm{d}\sigma_\Sigma(\mathrm{d}q)\mathrm{d}p}{\sqrt{\det G(q,p)}},\end{aligned}$$

where G is the Gram matrix $(\nabla\xi^\pm)^\top(\nabla\xi^\pm)$. This measure depends on the choice of $\xi^\pm$, which is not the case of the probability measure $\mu_\Sigma^\pm$ introduced in Theorem 5.2.6. This shows that, unlike for trace processes such as introduced above, the interpretation of the stationary distribution of our crossing sequences $(Y_n^\pm)_{n\geq 0}$ in terms of conditional distribution of μ is not straightforward.

5.2.4.3 Sampling from $\mu_\Sigma^\pm$

In the gradient case of Remark 5.2.1, the measure μ has the product structure

$$\mu(\mathrm{d}q\mathrm{d}p) \propto \mathrm{e}^{-\beta V(q)}\mathrm{d}q\mathrm{e}^{-\beta|p|^2/2}\mathrm{d}p,$$

which implies that

$$\mu_\Sigma^\pm(\mathrm{d}q\mathrm{d}p) \propto \mathrm{e}^{-\beta V(q)}\mathrm{d}\sigma_\Sigma(q)\mathbb{1}_{(q,p)\in\Gamma^\pm}|p\cdot n(q)|\mathrm{e}^{-\beta|p|^2/2}\mathrm{d}p.$$

From a numerical point of view, sampling from $\mu_\Sigma^\pm$ can therefore be achieved through the following two-step procedure:

1. draw q according to the probability measure with density proportional to $\mathrm{e}^{-\beta V(q)}$ with respect to the surface measure $\mathrm{d}\sigma_\Sigma(q)$;
2. conditionally on $n(q)$, draw p according to the density proportional to $\mathbb{1}_{\pm p\cdot n(q)>0}|p\cdot n(q)|\mathrm{e}^{-\beta|p|^2/2}$ with respect to the Lebesgue measure on $\mathbb{R}^d$.

For Step 1, we refer to the methods developed for example in [26, 57]. Step (2) only requires to draw $d+1$ independent $N(0,1)$ random variables $Z_1, Z_1', Z_2, \dots, Z_d$, and set

$$p = \frac{1}{\sqrt{\beta}}\left(\pm\sqrt{Z_1^2 + Z_1'^2}n(q) + Z_2 e_2 + \cdots + Z_d e_d\right),$$

where $(e_2, \dots, e_d)$ an orthonormal basis of the hyperplane $n(q)^\perp$. Then it is an easy exercise to check that, conditionally on q, p has the correct distribution.

5.3 Proof of Theorem 5.2.6

In Section 5.3.1 we show that the measure $\mu_\Sigma^\pm$ is stationary for the Markov chain $(Y_n^\pm)_{n\geq 0}$. Section 5.3.2 is devoted to the proof of the uniqueness of such stationary distribution. Note that part of these proofs rely on further results which are proven in the Section 5.4. Finally, we prove Lemmata 5.2.3 and 5.2.4 in Section 5.3.3.

5.3.1 Existence and identification

The fact that the measure $\mu_\Sigma^\pm$ is stationary for the Markov chain $(Y_n^\pm)_{n\geq 0}$ is a straightforward consequence of the following result combined with the strong Markov property.

Lemma 5.3.1 (Stationarity of $\mu_\Sigma^\pm$)**.** *Under the assumptions of Theorem 5.2.6, if (q_0, p_0) is distributed according to $\mu_\Sigma^\pm$, then $(q_{\tau_0^\mp}, p_{\tau_0^\mp})$ is distributed according to $\mu_\Sigma^\mp$.*

The proof of Lemma 5.3.1 relies on the following proposition, in which we recall that the infinitesimal generator $\mathscr{L}$ of the Langevin process is defined in (5.4). Its proof is postponed to Section 5.4.

Proposition 5.3.2. *Let the assumptions of Theorem 5.2.6 hold. Let $f : \Gamma^c up\Gamma^0 \to \mathbb{R}$ be a continuous and bounded function. Let*

$$u : (q,p) \in \mathbb{R}^{2d}\setminus\Gamma^0 \mapsto \mathbb{E}_{(q,p)}\left[f(q_{\tau_0^-}, p_{\tau_0^-})\right]. \tag{5.7}$$

Then,

(i) u is continuous on $(A^-\times\mathbb{R}^d)\cup\Gamma^-$ and $\mathscr{C}^\infty$ on the open set $A^-\times\mathbb{R}^d$ and satisfies

$$\begin{cases} \mathscr{L}u = 0 & \text{in } A^-\times\mathbb{R}^d, \\ u = f & \text{on } \Gamma^-, \end{cases}$$

(ii) $u \in \mathscr{C}^\infty(\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0))$, and satisfies $\mathscr{L}u = 0$ on $\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$.

We now detail the proof of Lemma 5.3.1.

Proof of Lemma 5.3.1. For the sake of legibility we assume that (q_0, p_0) is distributed according to μ_Σ^+, so that $\tau_0^+ = 0$, and show that $(q_{\tau_0^-}, p_{\tau_0^-})$ is distributed according to μ_Σ^-. The symmetric case can be addressed with the same arguments.

Let $f : \Gamma^- \cup \Gamma^0 \to \mathbb{R}$ be a continuous and bounded function and let u be defined by (5.7). By the definition of u, μ_Σ^+ and Γ^+, we have

$$\begin{aligned}
&\mathbb{E}_{\mu_\Sigma^+}\left[f\left(q_{\tau_0^-}, p_{\tau_0^-}\right)\right] \\
&= \int_{\Sigma\times\mathbb{R}^d} \mathbb{E}_{(q,p)}\left[f\left(q_{\tau_0^-}, p_{\tau_0^-}\right)\right]\mu_\Sigma^+(\mathrm{d}q\mathrm{d}p) \\
&= \frac{1}{z_\Sigma^+}\int_{\Gamma^+} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p.
\end{aligned} \tag{5.8}$$

On the other hand, since u is bounded, Assumptions (A3), (C) and the definition (5.5) of $\mathscr{L}^*$ allow to write the integration by part formula

$$\begin{aligned}
\int_{A^-\times\mathbb{R}^d} u(q,p)\mathscr{L}^*\rho(q,p)\mathrm{d}q\mathrm{d}p &= \int_{\Sigma\times\mathbb{R}^d} -p\cdot(-n(q))u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p \\
&\quad + \int_{A^-\times\mathbb{R}^d} \mathscr{L}u(q,p)\rho(q,p)\mathrm{d}q\mathrm{d}p.
\end{aligned}$$

On $A^-\times\mathbb{R}^d$, (i) in Proposition 5.3.2 shows that $\mathscr{L}u = 0$ while by (5.6), $\mathscr{L}^*\rho = 0$. Therefore, we deduce that

$$\begin{aligned}
0 &= \int_{\Sigma\times\mathbb{R}^d} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p \\
&= \int_{\Gamma^-} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p + \int_{\Gamma^+} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p.
\end{aligned}$$

By (5.8), we have

$$\int_{\Gamma^+} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p = z_\Sigma^+\mathbb{E}_{\mu_\Sigma^+}\left[f\left(q_{\tau_0^-}, p_{\tau_0^-}\right)\right],$$

while by (i) in Proposition 5.3.2,

$$\begin{aligned}
\int_{\Gamma^-} p\cdot n(q)u(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p &= \int_{\Gamma^-} p\cdot n(q)f(q,p)\rho(q,p)\mathrm{d}\sigma_\Sigma(q)\mathrm{d}p \\
&= -z_\Sigma^-\int_{\Sigma\times\mathbb{R}^d} f(q,p)\mu_\Sigma^-(\mathrm{d}q\mathrm{d}p).
\end{aligned}$$

Letting $f \equiv 1$ shows that $z_\Sigma^- = z_\Sigma^+$, and we finally conclude that

$$\mathbb{E}_{\mu_\Sigma^+}\left[f\left(q_{\tau_0^-}, p_{\tau_0^-}\right)\right] = \int_{\Sigma\times\mathbb{R}^d} f(q,p)\mu_\Sigma^-(\mathrm{d}q\mathrm{d}p),$$

which is the claimed result. □

5.3.2 Uniqueness

We now proceed to show the uniqueness of a stationary distribution for $(Y_n^\pm)_{n\geq 0}$. To this aim, we first recall that a homogeneous Markov chain $(Y_m)_{m\geq 0}$ with values in some Polish state space Γ, endowed with its Borel σ-field, is called *Harris recurrent* [5, Section VII.3] whenever there exist $R\subset\Gamma$, $r\geq 1$, $C>0$ and a probability measure λ on Γ such that:

(i) for any $y\in R$, for any measurable subset $B\subset\Gamma$, $\mathbb{P}(Y_r\in B|Y_0 = y)\geq C\lambda(B)$;

(ii) for any $y \in \Gamma$, $\mathbb{P}(\exists m \geq 1 : Y_m \in R | Y_0 = y) = 1$.

Then a Harris recurrent chain has a σ-finite stationary distribution which is unique up to a multiplicative constant [5, Theorem 3.2, p. 200 and Theorem 3.5, p. 201]. When this measure has finite mass and can therefore be normalised to a (unique) probability distribution, the chain is called *positive* Harris recurrent.

As an intermediary step, it is convenient to prove that the Markov chain $(\overline{Y}_m)_{m\geq 0}$ from Theorem 5.2.8 is Harris recurrent.

Lemma 5.3.3 (Harris recurrence of $(\overline{Y}_m)_{m\ \geq 0}$). *Under the assumptions of Lemma 5.2.3, the Markov chain $(\overline{Y}_m)_{m\geq 0}$ is Harris recurrent.*

The proof of this lemma is provided in Section 5.4. Besides, under the assumptions of Lemma 5.3.1, using Remark 5.2.5 it is easy to show that the probability measure $\overline{\mu}_\Sigma$ defined in Theorem 5.2.8 is stationary for the Markov chain $(\overline{Y}_m)_{m\geq 0}$. Combined with Lemma 5.3.3, this proves that the Markov chain $(\overline{Y}_m)_{m\geq 0}$ is positive Harris recurrent and therefore implies Theorem 5.2.8. We now complete the proof of Theorem 5.2.6 by showing that $\mu_\Sigma^\pm$ is the unique stationary distribution for $(Y_n^\pm)_{n\geq 0}$.

Corollary 5.3.4 (Uniqueness of the stationary distribution for $(Y_n^\pm)_{n\geq 0}$). *Under the assumptions of Theorem 5.2.6, the probability measure $\mu_\Sigma^\pm$ is the unique stationary distribution for $(Y_n^\pm)_{n\geq 0}$.*

Proof. We let $\widetilde{\mu}_\Sigma^+$ be a stationary probability distribution for the Markov chain $(Y_n^+)_{n\geq 0}$ and work under $\mathbb{P}_{\widetilde{\mu}_\Sigma^+}$, so that $\tau_0^+ = 0$ and, for all $n \geq 0$, $Y_n^+ = \overline{Y}_{2n}$ is distributed according to $\widetilde{\mu}_\Sigma^+$. As a consequence, for any measurable and bounded function $f : \Gamma^+ \to \mathbb{R}$,

$$\mathbb{E}_{\widetilde{\mu}_\Sigma^+}\left[\frac{1}{n}\sum_{k=0}^{n-1} f(\overline{Y}_{2k})\right] = \int_{\Gamma^+} f(q,p)\widetilde{\mu}_\Sigma^+(\mathrm{d}q\mathrm{d}p)$$

on the one hand, while on the other hand Remark 5.2.5 allows to rewrite

$$\frac{1}{n}\sum_{k=0}^{n-1} f(\overline{Y}_{2k}) = \frac{2}{2n}\sum_{\ell=0}^{2n-1} f(\overline{Y}_\ell)\mathbb{1}_{\overline{Y}_\ell\in\Gamma^+},$$

which by Lemma 5.3.3 and the ergodic theorem for positive Harris recurrent Markov chains [5, Proposition 3.7, p. 203] implies that, $\mathbb{P}_{\widetilde{\mu}_\Sigma^+}$-almost surely,

$$\lim_{n\to+\infty}\frac{1}{n}\sum_{k=0}^{n-1} f(\overline{Y}_{2k}) = 2\int_{\Sigma\times\mathbb{R}^d} f(q,p)\mathbb{1}_{(q,p)\in\Gamma^+}\overline{\mu}_\Sigma(\mathrm{d}q\mathrm{d}p).$$

Since f is bounded, the dominated convergence theorem allows to conclude that

$$\widetilde{\mu}_\Sigma^+(\mathrm{d}q\mathrm{d}p) = 2\mathbb{1}_{(q,p)\in\Gamma^+}\overline{\mu}_\Sigma(\mathrm{d}q\mathrm{d}p) = \mu_\Sigma^+(\mathrm{d}q\mathrm{d}p),$$

and the same arguments similarly show that any stationary distribution $\widetilde{\mu}_\Sigma^-$ for $(Y_n^-)_{n\geq 0}$ actually coincides with μ_Σ^-, which completes the proof. □

5.3.3 Proofs of Lemmata 5.2.3 and 5.2.4

Proof of Lemma 5.2.3. Let $(q,p) \in \mathbb{R}^{2d} \setminus \Gamma^0$ and $\tau := \inf\{t > 0 : q_t \in \Sigma\}$. Following the reasoning in Paragraph 2.3.4.1.1, we obtain that $\tau > 0$, $\mathbb{P}_{(q,p)}$-almost surely and

(i) if $q \in A^\pm$, then $(q_\tau, p_\tau) \in \Gamma^\pm \cup \Gamma^0$;

(ii) if $(q,p) \in \Gamma^\pm$ then $(q_\tau, p_\tau) \in \Gamma^\mp \cup \Gamma^0$.

Besides, since A and $\mathbb{R}^d \setminus A$ satisfy Assumption B2, the ergodicity of the process $(q_t, p_t)_{t\geq 0}$, stated in Assumption (A2), ensures that $\tau < \infty$, $\mathbb{P}_{(q,p)}$-almost surely. It is left to prove that (q_τ, p_τ) does not attain Γ^0 almost surely, which follows from Lemma 5.3.5 proven below. □

Lemma 5.3.5. *Under the assumptions of Lemma 5.2.3, for all* $x \in \mathbb{R}^{2d} \setminus \Gamma^0$,

$$\mathbb{P}_x \left(\exists t > 0 : X_t \in \Gamma^0 \right) = 0.$$

Proof. Let $\tau_0 := \inf\{t > 0 : X_t \in \Gamma^0\}$. It is sufficient to prove that for all $T > 0$, $x \in \mathbb{R}^{2d} \setminus \Gamma^0$,

$$\mathbb{P}_x \left(\tau_0 \leq T \right) = 0. \tag{5.9}$$

If A is bounded and F is globally bounded and Lipschitz continuous, the result follows from Proposition 2.2.7 in Chapter 2. Assume now that A is not bounded and F is such that Assumption (A1) holds. Let $(F_k)_{k\geq 1}$ be a sequence of smooth compactly supported functions on $\mathbb{R}^d$ such that $F_k = F$ on $\mathrm{B}(0,k)$. Let $(A_k)_{k\geq 1}$ be a sequence of $\mathscr{C}^2$ bounded sets of $\mathbb{R}^d$ such that $A_k \cap \mathrm{B}(0,k) = A \cap \mathrm{B}(0,k)$. Let $\Gamma^0_k := \{(q,p) \in \partial A_k \times \mathbb{R}^d : p \cdot n_k(q) = 0\}$ where n_k is the outward unitary vector to A_k. Notice that $\Gamma^0_k \cap \mathrm{B}(0,k) = \Gamma^0 \cap \mathrm{B}(0,k)$.

Consider the process $(X^k_t = (q^k_t, p^k_t))_{t\geq 0}$ solution of (5.3) with F_k instead of F. Let

$$\tau^k_0 := \inf\{t \geq 0 : X^k_t \in \Gamma^0_k\}.$$

By Proposition 2.2.7, one has that for all $x \in \mathbb{R}^{2d} \setminus \Gamma^0$, for all $T > 0$,

$$\mathbb{P}_x(\tau^k_0 \leq T) = 0,$$

since A_k is a $\mathscr{C}^2$ bounded set of $\mathbb{R}^d$ and F_k is bounded and globally Lipschitz continuous.

Let $x \in \mathbb{R}^{2d} \setminus \Gamma^0$, $T > 0$. For $k \geq 1$,

$$\mathbb{P}_x \left(\tau_0 \leq T \right) = \mathbb{P}_x \left(\tau_0 \leq T, q_{\tau_0} \in \mathrm{B}(0,k) \right) + \mathbb{P}_x \left(\tau_0 \leq T, q_{\tau_0} \notin \mathrm{B}(0,k) \right). \tag{5.10}$$

Besides,

$$\mathbb{P}_x \left(\tau_0 \leq T, q_{\tau_0} \in \mathrm{B}(0,k) \right) \leq \mathbb{P}_x(\tau^k_0 \leq T) = 0,$$

since $\Gamma^0_k \cap \mathrm{B}(0,k) = \Gamma^0 \cap \mathrm{B}(0,k)$, and $(X^k_t)_{t\geq 0}$ and $(X_t)_{t\geq 0}$ coincide until the first time they exit $\mathrm{B}(0,k)$. Moreover,

$$\mathbb{P}_x \left(\tau_0 \leq T, q_{\tau_0} \notin \mathrm{B}(0,k) \right) \leq \mathbb{P}_x \left(\sup_{t\in[0,T]} |q_t| \geq k \right) \underset{k\to\infty}{\longrightarrow} 0.$$

Therefore, taking k to infinity in (5.10), we obtain (5.9), which concludes the proof. □

Let us now prove Lemma 5.2.4.

Proof of Lemma 5.2.4. Assume that $\sup_{n\geq 0} \tau^-_n = T < +\infty$ or $\sup_{n\geq 0} \tau^+_n = T < +\infty$. Then Remark 5.2.5 shows that both sequences accumulate at T. By the continuity of the trajectory of $(q_t, p_t)_{t\geq 0}$, we deduce that

$$\lim_{n\to+\infty} Y^\pm_n = (q_T, p_T).$$

Since, by Assumption (B1), the mapping $q \mapsto n(q)$ is continuous on Σ, we then obtain

$$\lim_{n\to+\infty} p_{\tau^-_n} \cdot n(q_{\tau^-_n}) = \lim_{n\to+\infty} p_{\tau^+_n} \cdot n(q_{\tau^+_n}) = p_T \cdot n(q_T).$$

But $p(\tau^-_n) \cdot n(q(\tau^-_n)) < 0$ while $p(\tau^+_n) \cdot n(q(\tau^+_n)) > 0$, as a consequence $p_T \cdot n(q_T) = 0$. In other words, there exists $T < +\infty$ such that $(q_T, p_T) \in \Gamma^0$, which by Lemma 5.3.5 has probability 0 under $\mathbb{P}_{(q,p)}$, for $(q,p) \in \mathbb{R}^{2d} \setminus \Gamma^0$. □

5.4 Proofs of auxiliary results

We prove Proposition 5.3.2 in Section 5.4.1 and in Section 5.4.2 we prove the Harris recurrence of the Markov chain $(\overline{Y}_m)_{m\geq 0}$.

5.4.1 Proof of Proposition 5.3.2

Let us define $(\widetilde{B}_t)_{t\geq 0}$ a $d-$dimensional Brownian motion independent of $(B_t)_{t\geq 0}$ and let $(F_m)_{m\geq 1}$ be a sequence of smooth compactly supported functions on $\mathbb{R}^d$ which coincide with F on the open ball $\mathrm{B}(0,m)$ and such that $|F_m(q)|\leq |F(q)|$ for any $q\in\mathbb{R}^d$. Let $(X_t^{\epsilon,m}=(q_t^{\epsilon,m},p_t^{\epsilon,m}))_{t\geq 0}$ be the following perturbed Langevin process for $\epsilon>0$,

$$\begin{cases} \mathrm{d}q_t^{\epsilon,m} = p_t^{\epsilon,m}\mathrm{d}t + \sqrt{2\epsilon}\mathrm{d}\widetilde{B}_t, \\ \mathrm{d}p_t^{\epsilon,m} = F_m(q_t^{\epsilon,m})\mathrm{d}t - \gamma p_t^{\epsilon,m}\mathrm{d}t + \sigma\mathrm{d}B_t, \end{cases} \tag{5.11}$$

with infinitesimal generator $\mathscr{L}_{\epsilon,m} := p\cdot\nabla_q + F_m(q)\cdot\nabla_p - \gamma p\cdot\nabla_p + \frac{\sigma^2}{2}\Delta_p + \epsilon\Delta_q$. We also define the process $(X_t^m)_{t\geq 0}$ as in (5.3) with F_m instead of F and its infinitesimal generator is denoted by $\mathscr{L}_m$.

Let $(V_k)_{k\geq 1}$ be an increasing sequence of $\mathscr{C}^2$ open bounded subsets of $\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$ such that $\cup_{k\geq 1}V_k = \mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$. For $k\geq 1$ and $\epsilon>0$, let us define the stopping times

$$\begin{aligned} \tau^{\epsilon,m,k} &:= \inf\{t>0 : X_t^{\epsilon,m}\notin V_k\}, \\ \tau^{\epsilon,m} &:= \inf\{t>0 : X_t^{\epsilon,m}\in\Gamma^-\cup\Gamma^0\}, \\ \tau^{m} &:= \inf\{t>0 : X_t^{m}\in\Gamma^-\cup\Gamma^0\}. \end{aligned}$$

We start with the proof of the two following lemmata.

Lemma 5.4.1. *For all $x\in\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$, one has $\mathbb{P}_x$-almost surely,*

(i) $\lim_{k\to\infty}\tau^{\epsilon,m,k} = \tau^{\epsilon,m}$,

(ii) $\forall t>0,\qquad \lim_{\epsilon\to 0}\mathbb{1}_{\tau^{\epsilon,m}\leq t} = \mathbb{1}_{\tau^m\leq t}$,

(iii) on the event $\{\tau^m<\infty\}$, $\lim_{m\to\infty}X^{\epsilon,m}_{\tau^{\epsilon,m}} = X^m_{\tau^m}$.

Proof of Lemma 5.4.1. In this proof we fix $m\geq 1$ and $x\in\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$. Let $\epsilon>0$, since $(V_k)_{k\geq 1}$ is an increasing sequence of subsets of $\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$, then $(\tau^{\epsilon,m,k})_{k\geq 1}$ is an increasing sequence of stopping times, therefore it converges $\mathbb{P}_x$-almost surely towards $\sup_{k\geq 1}\tau^{\epsilon,m,k}$. Besides, it follows from the equality $\cup_{k\geq 1}V_k=\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$ that $\mathbb{P}_x$-almost surely, for all $s\geq 0$,

$$\mathbb{1}_{\sup_{k\geq 1}\tau^{\epsilon,m,k}>s} = \mathbb{1}_{\tau^{\epsilon,m}>s}.$$

One easily deduces from this equality that $\sup_{k\geq 1}\tau^{\epsilon,m,k}=\tau^{\epsilon,m}$, $\mathbb{P}_x$-almost surely, hence (i).

Now let us fix $t>0$. In order to prove (ii) it is sufficient to show the convergence on the partition of events $\{\tau^m<t\}$, $\{\tau^m>t\}$ and $\{\tau^m=t\}$. Since $\mathbb{P}_x(\tau^m=t)\leq\mathbb{P}_x(X_t^m\in\partial A)=0$, one only needs to prove the convergence almost surely on the events $\{\tau^m<t\}$ and $\{\tau^m>t\}$.

Since F_m is globally Lipschitz continuous on $\mathbb{R}^d$, using Gronwall's lemma one obtains the existence of a constant $C_m>0$ such that for all $x\in\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)$, $\mathbb{P}_x$-almost surely, for all $t\geq 0$,

$$\sup_{s\in[0,t]}|X_s^{\epsilon,m}-X_s^m| \leq \sqrt{2\epsilon}\sup_{s\in[0,t]}|\widetilde{B}_s|\mathrm{e}^{C_m t}. \tag{5.12}$$

For a fixed $t>0$, we consider the event $\{\tau^m<t\}$. By Lemma 5.3.5, $X^m_{\tau^m}\in\Gamma^-$, $\mathbb{P}_x$-almost surely. Besides, the process $(X_t^m)_{t\geq 0}$ visits A, $\mathbb{P}_x$-almost surely on $[\tau^m,\tau^m+\alpha]$ for any $\alpha>0$. Therefore, for α small enough so that $\tau^m+\alpha<t$ and for ϵ small enough, one has, using (5.12), that $\tau^{\epsilon,m}<t$.

This ensures the convergence (ii) on the event $\{\tau^m < t\}$. Assume now that $\{\tau^m > t\}$. It follows from (5.12) that for ϵ small enough, the process $(X_s^{\epsilon,m})_{s\in[0,t]}$ is at a positive distance of the boundary Γ^-. Therefore, one has that $\tau^{\epsilon,m} > t$ which ensures the convergence (ii) on the event $\{\tau^m > t\}$.

Using the monotonicity of the function $t \mapsto \mathbb{1}_{\tau^{\epsilon,m}\le t}$ we deduce that $\mathbb{P}_x$-almost surely, for any $t > 0$ such that $t \neq \tau^{\epsilon,m}$, $\mathbb{1}_{\tau^{\epsilon,m}\le t}$ converges $\mathbb{P}_x$-almost surely to $\mathbb{1}_{\tau^m\le t}$ when $\epsilon \to 0$, hence (ii). Furthermore, integrating in time, one concludes that $\tau^{\epsilon,m}$ $\mathbb{P}_x$-converges almost surely when $\epsilon \to 0$ to τ^m.

On the event $\{\tau^m < \infty\}$ we have $\tau^{\epsilon,m} < \infty$ for ϵ small enough, thus we deduce from (5.12) and the continuity of the trajectory of $(X_t^m)_{t\ge0}$ that $X^{\epsilon,m}_{\tau^{\epsilon,m}}$ converges to $X^m_{\tau^m}$. □

Let us now prove Proposition 5.3.2

Proof of Proposition 5.3.2. Let $f \in \mathscr{C}^b(\Gamma^- \cup \Gamma^0)$. We extend f on $\mathbb{R}^{2d}$ so that $f \in \mathscr{C}^b(\mathbb{R}^{2d})$ using Tietze-Urysohn's extension theorem [27, Theorem 4.5.1]. For $\epsilon > 0$, $k \ge 1$ and $m \ge 1$, let us define the function

$$u_{\epsilon,m,k} : x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0) \mapsto \mathbb{E}_x\left[f(X^{\epsilon,m}_{\tau^{\epsilon,m,k}})\right].$$

By [32, Theorem 5.1 in Chapter 6], $\tau^{\epsilon,m,k} < \infty$ almost surely and $u_{\epsilon,m,k}$ is a classical solution on V_k of $\mathscr{L}_{\epsilon,m}u_{\epsilon,m,k} = 0$. Therefore, it is also a distributional solution of $\mathscr{L}_{\epsilon,m}u_{\epsilon,m,k} = 0$ on V_k. Now let Φ be a compactly supported $\mathscr{C}^\infty$ function on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$, then there exists k_0 such that for all $k \ge k_0$, $\mathrm{Supp}(\Phi) \subset V_k$. As a result, for all $k \ge k_0$,

$$\int_{\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)} u_{\epsilon,m,k}(x)\mathscr{L}^*_{\epsilon,m}\Phi(x)\mathrm{d}x = 0. \tag{5.13}$$

Step 1: Let us prove that for all $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$,

$$\lim_{m\to\infty}\lim_{\epsilon\to0}\lim_{k\to\infty} u_{\epsilon,m,k}(x) = u(x),$$

where u is defined in (5.7).

In order to do that, we consider the limits of the two following functions. For $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ and $t > 0$, let

$$u^{(1)}_{t,\epsilon,m,k}(x) := \mathbb{E}_x\left[f(X^{\epsilon,m}_{\tau^{\epsilon,m,k}})\mathbb{1}_{\tau^{\epsilon,m,k}\le t}\right], \qquad u^{(2)}_{t,\epsilon,m,k}(x) := \mathbb{E}_x\left[f(X^{\epsilon,m}_{\tau^{\epsilon,m,k}})\mathbb{1}_{\tau^{\epsilon,m,k}> t}\right],$$

so that $u_{\epsilon,m,k} = u^{(1)}_{t,\epsilon,m,k} + u^{(2)}_{t,\epsilon,m,k}$. As a result, it is enough to prove that

$$\lim_{t\to\infty}\lim_{m\to\infty}\lim_{\epsilon\to0}\lim_{k\to\infty} u^{(1)}_{t,\epsilon,m,k}(x) = u(x), \qquad \lim_{t\to\infty}\limsup_{m\to\infty}\lim_{\epsilon\to0}\lim_{k\to\infty} u^{(2)}_{t,\epsilon,m,k}(x) = 0. \tag{5.14}$$

Since $k \mapsto \tau^{\epsilon,m,k}$ is increasing and $s \mapsto \mathbb{1}_{s\le t}$ is left-continuous, one has using (i) in Lemma 5.4.1 that $\mathbb{P}_x$-almost surely, for all $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ and $t > 0$,

$$\mathbb{1}_{\tau^{\epsilon,m,k}\le t} \underset{k\to\infty}{\longrightarrow} \mathbb{1}_{\tau^{\epsilon,m}\le t},$$

hence

$$u^{(1)}_{t,\epsilon,m,k}(x) \underset{k\to\infty}{\longrightarrow} \mathbb{E}_x\left[f(X^{\epsilon,m}_{\tau^{\epsilon,m}})\mathbb{1}_{\tau^{\epsilon,m}\le t}\right].$$

Furthermore, by (ii) and (iii)

$$\begin{aligned}&\left|\mathbb{E}_x\left[f(X^{\epsilon,m}_{\tau^{\epsilon,m}})\mathbb{1}_{\tau^{\epsilon,m}\le t}\right] - \mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m\le t}\right]\right| \\ &\le \|f\|_\infty\mathbb{E}_x\left[|\mathbb{1}_{\tau^{\epsilon,m}\le t} - \mathbb{1}_{\tau^m\le t}|\right] + \mathbb{E}_x\left[\mathbb{1}_{\tau^m\le t}|f(X^{\epsilon,m}_{\tau^{\epsilon,m}}) - f(X^m_{\tau^m})|\right] \underset{\epsilon\to0}{\longrightarrow} 0.\end{aligned}$$

For $m \geq 1$, let $B_m := \mathrm{B}(0, m)$, $\tau^m_{B^c_m} := \inf\{t > 0 : X^m_t \notin B_m\}$ and $\tau_{B^c_m} := \inf\{t > 0 : X_t \notin B_m\}$. One has for $m \geq 1$, $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$, $t > 0$,

$$\mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m \leq t}\right] = \mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m \leq \tau^m_{B^c_m} \wedge t}\right] + \mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m > \tau^m_{B^c_m}}\mathbb{1}_{\tau^m \leq t}\right]. \tag{5.15}$$

Besides, since F_m and F coincide on B_m, the existence of a unique strong solution to (5.3) ensures that the trajectories of $(X^m_t)_{t\geq 0}$ and $(X_t)_{t\geq 0}$ coincide until $\tau^m_{B^c_m}$ and that $\tau^m_{B^c_m} = \tau_{B^c_m}$, $\mathbb{P}_x$-almost surely. Therefore, for all $m \geq 1$,

$$\mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m \leq \tau^m_{B^c_m} \wedge t}\right] = \mathbb{E}_x\left[f(X_{\tau^-_0})\mathbb{1}_{\tau^-_0 \leq \tau_{B^c_m} \wedge t}\right] \underset{m\to\infty}{\longrightarrow} \mathbb{E}_x\left[f(X_{\tau^-_0})\mathbb{1}_{\tau^-_0 \leq t}\right], \tag{5.16}$$

since $\tau^-_0 < \infty$ by Lemma 5.2.3 and $\tau_{B^c_m} \underset{m\to\infty}{\longrightarrow} \infty$ by Assumption (A1), $\mathbb{P}_x$-almost surely. Moreover,

$$\begin{aligned}\mathbb{E}_x\left[f(X^m_{\tau^m})\mathbb{1}_{\tau^m > \tau^m_{B^c_m}}\mathbb{1}_{\tau^m \leq t}\right] &\leq \|f\|_\infty \mathbb{P}(\tau^m \geq \tau^m_{B^c_m}) \\ &\leq \|f\|_\infty \mathbb{P}(\tau^-_0 \geq \tau_{B^c_m}) \underset{m\to\infty}{\longrightarrow} 0,\end{aligned} \tag{5.17}$$

by Assumption (A1). Again, using that $\tau^-_0 < \infty$, one deduces that $\mathbb{E}_x\left[f(X_{\tau^-_0})\mathbb{1}_{\tau^-_0 \leq t}\right] \underset{t\to\infty}{\longrightarrow} u(x)$, which ensures the first convergence in (5.14).

Consider now the convergence of $u^{(2)}_{t,\epsilon,m,k}$. For $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ and $t > 0$,

$$|u^{(2)}_{t,\epsilon,m,k}(x)| \leq \|f\|_\infty \mathbb{P}_x(\tau^{\epsilon,m,k} > t) \underset{k\to\infty}{\longrightarrow} \mathbb{P}_x(\tau^{\epsilon,m} > t),$$

by (i). Besides, $\mathbb{P}_x(\tau^{\epsilon,m} > t) \underset{\epsilon\to 0}{\longrightarrow} \mathbb{P}_x(\tau^m > t)$ by (ii). In addition,

$$\begin{aligned}\mathbb{P}_x(\tau^m > t) &= \mathbb{P}_x(\tau^m > t, \tau^m > \tau^m_{B^c_m}) + \mathbb{P}_x(\tau^m > t, \tau^m \leq \tau^m_{B^c_m}) \\ &\leq \mathbb{P}_x(\tau^-_0 > \tau_{B^c_m}) + \mathbb{P}_x(\tau^-_0 > t) \underset{m\to\infty}{\longrightarrow} \mathbb{P}_x(\tau^-_0 > t),\end{aligned}$$

since $\tau^-_0 < \infty$, $\mathbb{P}_x$-almost surely. Finally, since $\mathbb{P}_x(\tau^-_0 > t) \underset{t\to\infty}{\longrightarrow} 0$, one obtains the second convergence in (5.14).

Step 2: Let us prove that

$$\lim_{m\to\infty}\lim_{\epsilon\to 0}\lim_{k\to\infty}\int_{\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)} u_{\epsilon,m,k}(x)\mathscr{L}^*_{\epsilon,m}\Phi(x)\mathrm{d}x = \int_{\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)} u(x)\mathscr{L}^*\Phi(x)\mathrm{d}x. \tag{5.18}$$

Using (5.13), one then deduces that u is a distributional solution of $\mathscr{L}u = 0$ on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ and since $\mathscr{L}$ is hypoelliptic, u is in $\mathscr{C}^\infty(\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0))$, hence (ii) in Proposition 5.3.2.

In order to obtain the convergence above, we notice that it is sufficient to prove

$$\begin{aligned}&\lim_{t\to\infty}\lim_{m\to\infty}\lim_{\epsilon\to 0}\lim_{k\to\infty}\int_{\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)} (u^{(1)}_{t,\epsilon,m,k}(x) + u^{(2)}_{t,\epsilon,m,k}(x))\mathscr{L}^*_{\epsilon,m}\Phi(x)\mathrm{d}x \\ &= \int_{\mathbb{R}^{2d}\setminus(\Gamma^-\cup\Gamma^0)} u(x)\mathscr{L}^*\Phi(x)\mathrm{d}x.\end{aligned}$$

Since for all $x \in \mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$, $\epsilon\Delta_q\Phi(x) \underset{\epsilon\to 0}{\longrightarrow} 0$ and $F_m(x) \cdot \nabla_p\Phi(x) \underset{m\to\infty}{\longrightarrow} F(x) \cdot \nabla_p\Phi(x)$, then $\lim_{m\to\infty}\lim_{\epsilon\to 0}\mathscr{L}^*_{\epsilon,m}\Phi(x) = \mathscr{L}^*\Phi(x)$. Moreover, Φ is $\mathscr{C}^\infty$ and compactly supported on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ and $|F_m(q)| \leq |F(q)|$ for any q belonging to the support of Φ. Therefore, using the dominated convergence theorem and **Step 1**, one gets the convergence (5.18). It remains to prove in Proposition 2.2.8 the continuity of u on Γ^- starting from points in $\mathbb{R}^{2d} \setminus A$. This is done following the exact same proof of Assertion (i) of Proposition 2.2.8. □

5.4.2 Harris recurrence

Let us prove here the Harris recurrence of the Markov chain $(\overline{Y}_m)_{m\geq 0}$. In order to do that one needs to prove Assertions (i) and (ii) in Section 5.3.2 for some $R \subset \partial D$, $r \geq 1$, $C > 0$ and some probability measure λ on ∂D. Let us start with the proof of Assertion (i) stated in Proposition 5.4.2 below. We first explicit our choice of the subset $R \subset \partial D$.

Let $x^* := (q^*, p^*) \in \Gamma^+$ and let $\beta > 0$ sufficiently small such that for all $x = (q,p) \in \mathrm{B}(x^*, \beta)$ we have $p \cdot \nabla \mathrm{d}_\partial(q) \geq \frac{p^* \cdot n(q^*)}{2}$. We define hereafter R as the following compact set of Γ^+

$$R := \overline{\mathrm{B}(x^*, \beta) \cap \Gamma^+}.$$

Proposition 5.4.2 (First criterion for Harris recurrence)**.** *There exist $C > 0$, a probability measure λ on ∂D such that for any $y \in R$, for any measurable subset $B \subset \partial D$, $\mathbb{P}_y(\overline{Y}_1 \in B) \geq C\lambda(B)$.*

Proof of Proposition 5.4.2. Let u be the function defined in (5.7) with $f \in \mathscr{C}^b(\Gamma^- \cup \Gamma^0)$. Then, by Proposition 5.3.2, u is a smooth solution of $\mathscr{L}u = 0$ on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$, in particular it is also a distributional solution of $\mathscr{L}u = 0$ on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$. Using an elementary regularization argument and noticing that $\overline{Y}_1 \in \Gamma^- \cup \Gamma^0$, $\mathbb{P}_y$−almost surely for $y \in R$, one gets that u is still a distributional solution of $\mathscr{L}u = 0$ on $\mathbb{R}^{2d} \setminus (\Gamma^- \cup \Gamma^0)$ if $f \in \mathrm{L}^\infty(\partial D)$.

Now let $B \subset \partial D$ be a measurable set. Applying the Harnack inequality in Theorem 2.2.15 to the function u with $f = \mathbb{1}_B$, (u has no time dependency therefore u also satisfies $\partial_t u - \mathscr{L}u = 0$), we deduce the existence of a constant $C > 0$ such that for all $y \in R$,

$$u(y) = \mathbb{P}_y(\overline{Y}_1 \in B) \geq C \underbrace{\mathbb{P}_{x^*}(\overline{Y}_1 \in B)}_{=\lambda(B)},$$

and λ is a probability measure on ∂D, hence the proof. □

Let us now prove the second criterion for Harris recurrence.

Proposition 5.4.3 (Second criterion for Harris recurrence)**.** *For any $y \in \partial D$,*

$$\mathbb{P}_y(\exists m \geq 1 : \overline{Y}_m \in R) = 1.$$

Proof. Let $y \in \partial D$ and let $\tau_R := \inf\{t > 0 : (q_t, p_t) \in R\}$. Since the sequence $(\tau_n^\pm)_{n\geq 0}$ does not accumulate, see Lemma 5.2.4, it is sufficient to prove that

$$\mathbb{P}_y(\tau_R = \infty) = 0. \tag{5.19}$$

For $n \geq 1$, let us define the set E_n by

$$E_n := \mathrm{B}\left(x^*, 1/n\right) \cap (A \times \mathbb{R}^d).$$

Let $\tau_{E_n} := \inf\{t > 0 : (q_t, p_t) \in E_n\}$. Since the process $(q_t, p_t)_{t\geq 0}$ is ergodic and $|E_n| > 0$, then for all $n \geq 1$,

$$\mathbb{P}_y(\tau_{E_n} < \infty) = 1.$$

Therefore,

$$\mathbb{P}_y\left(\bigcap_{n\geq 1}\{\tau_{E_n} < \infty\}\right) = 1.$$

Thus, the condition (5.19) is equivalent to the equality

$$\mathbb{P}_y\left(\bigcap_{n\geq 1}\{\tau_{E_n} < \infty, \tau_R = \infty\}\right) = 0.$$

Since the intersection $\bigcap_{n\geq 1}\{\tau_{E_n} < \infty, \tau_R = \infty\}$ is decreasing then

$$\mathbb{P}_y\Big(\bigcap_{n\geq 1}\{\tau_{E_n} < \infty, \tau_R = \infty\}\Big) = \lim_{n\to\infty} \mathbb{P}_y\big(\tau_{E_n} < \infty, \tau_R = \infty\big).$$

Furthermore, for $n \geq 1$, the strong Markov property at the stopping time τ_{E_n} ensures that

$$\mathbb{P}_y\big(\tau_{E_n} < \infty, \tau_R = \infty\big) = \mathbb{E}_y\Big[\mathbb{1}_{\tau_{E_n}<\infty}\mathbb{P}_{X_{\tau_{E_n}}}(\tau_R = \infty)\Big].$$

If one proves that

$$\sup_{x\in\overline{E_n}} \mathbb{P}_x(\tau_R = \infty) \underset{n\to\infty}{\longrightarrow} 0,$$

the convergence of the expectation above easily follows from the application of the dominated convergence theorem. Let $\alpha \in (0, 1/2)$, $t_n := \frac{1}{n^{\frac{1}{1+\alpha}}}$. We prove here the following stronger convergence

$$\sup_{x\in\overline{E_n}} \mathbb{P}_x(\tau_R > t_n) \underset{n\to\infty}{\longrightarrow} 0.$$

Let $n \geq 1$, $x = (q, p) \in \overline{E_n}$, and let

$$\tau_\beta := \inf\{t > 0 : (q_t, p_t) \notin \mathrm{B}(x^*, \beta)\}.$$

For $s \in [0, t_n]$, on the event $\{\tau_\beta > t_n\}$,

$$p_s = p + \int_0^s F(q_r)\mathrm{d}r - \gamma\int_0^s p_r\mathrm{d}r + \sigma B_s.$$

Let $\widetilde{C} := \sup_{0<s\leq 1}\frac{B_s}{s^\alpha}$, then one has that

$$|p_s - p| \leq c_1 s + \sigma\widetilde{C}s^\alpha,$$

where $c_1 := \sup\{|F(q') - \gamma p'| : x' = (q', p') \in \mathrm{B}(x^*, \beta)\}$.

As a result, since for all $s \in [0, t_n]$,

$$q_s = q + \int_0^s p_r\mathrm{d}r, \tag{5.20}$$

one has for $n \geq 1$,

$$\begin{aligned}|q_{t_n} - q^* - t_n p^*| &\leq |q - q^*| + \frac{c_1}{2}t_n^2 + \frac{\sigma\widetilde{C}}{1+\alpha}t_n^{1+\alpha} + t_n|p - p^*| \\ &\leq \frac{1}{n} + \frac{c_1}{2}t_n^2 + \frac{\sigma\widetilde{C}}{1+\alpha}t_n^{1+\alpha} + \frac{t_n}{n}.\end{aligned} \tag{5.21}$$

By the expression of t_n, there exists $n_0 \geq 1$ such that for all $n \geq n_0$,

$$\frac{1}{n} + \frac{c_1}{2}t_n^2 + \frac{t_n}{n} \leq \frac{p^*\cdot n(q^*)}{6}t_n. \tag{5.22}$$

Therefore, on the event $\Big\{\tau_\beta > t_n, \frac{\sigma\widetilde{C}}{1+\alpha}t_n^{1+\alpha} \leq \frac{p^*\cdot n(q^*)}{6}t_n\Big\}$, one has by (5.21) and (5.22) for $n \geq n_0$,

$$|q_{t_n} - q^*| \leq \left(\frac{p^*\cdot n(q^*)}{3} + |p^*|\right)t_n. \tag{5.23}$$

In addition, using Cauchy-Schwarz inequality one has also that,

$$(q_{t_n} - q^* - t_n p^*) \cdot n(q^*) \geq -\frac{p^* \cdot n(q^*)}{3} t_n.$$

As a result, for all $n \geq n_0$,

$$\frac{(q_{t_n} - q^*) \cdot n(q^*)}{|q_{t_n} - q^*|} \geq \frac{2p^* \cdot n(q^*)}{p^* \cdot n(q^*) + 3|p^*|} > 0. \tag{5.24}$$

Consequently, on the event $\left\{\tau_\beta > t_n, \frac{\sigma\widetilde{C}}{1+\alpha} t_n^{1+\alpha} \leq \frac{p^* \cdot n(q^*)}{6} t_n\right\}$, (5.23) and (5.24) ensure by the exterior sphere condition satisfied by A, the existence of $n_1 \geq n_0$ large enough such that for $n \geq n_1$, $q_{t_n} \notin A$. Besides, since we place ourselves on the event $\{\tau_\beta > t_n\}$, then necessarily $\tau_R < t_n$, $\mathbb{P}_x$-almost surely. As a result, for $n \geq n_1$, $x \in \overline{E_n}$,

$$\mathbb{P}_x\left(\tau_R > t_n\right) \leq \mathbb{P}_x\left(\tau_\beta \leq t_n\right) + \mathbb{P}_x\left(\frac{\sigma\widetilde{C}}{1+\alpha} t_n^{1+\alpha} > \frac{p^* \cdot n(q^*)}{6} t_n\right).$$

Let $n_2 \geq n_1$ such that $\frac{1}{n_2} \leq \frac{\beta}{2}$, then one has for $n \geq n_2$,

$$\mathbb{P}_{x_n}\left(\tau_R > t_n\right) \leq \sup_{x \in \mathrm{B}(x^*, \beta/2)} \mathbb{P}_x\left(\tau_\beta \leq t_n\right) + \underbrace{\mathbb{P}\left(\widetilde{C} > (1+\alpha)\frac{p^* \cdot n(q^*)}{6\sigma} t_n^{-\alpha}\right)}_{\underset{n\to\infty}{\longrightarrow} 0},$$

since $t_n^{-\alpha} \underset{n\to\infty}{\longrightarrow} \infty$ and $\widetilde{C} < \infty$ almost surely.

Moreover, for $x \in \mathrm{B}(x^*, \beta/2)$, $\tau_\beta > 0$, $\mathbb{P}_x$-almost surely. Therefore, $\mathbb{P}_x\left(\tau_\beta \leq t_n\right) \underset{n\to\infty}{\longrightarrow} 0$. Since $x \in \mathrm{B}(x^*, \beta/2) \mapsto \mathbb{P}_x\left(\tau_\beta \leq t_n\right)$ is continuous and is a decreasing function of n, then using Dini's theorem it follows that

$$\sup_{x \in \mathrm{B}(x^*, \beta/2)} \mathbb{P}_x\left(\tau_\beta \leq t_n\right) \underset{n\to\infty}{\longrightarrow} 0.$$

Consequently,

$$\sup_{x \in \overline{E_n}} \mathbb{P}_x\left(\tau_R > t_n\right) \underset{n\to\infty}{\longrightarrow} 0,$$

which concludes the proof. □

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