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Quelques contributions à l'analyse numérique d'équations stochastiques

Marie Kopec

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THÈSE

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présentée et soutenue publiquement

par

Kopec Marie

Titre:
**Quelques contributions à l'analyse numérique
d'équations stochastiques.**

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Chapter 1

Introduction

Dans cette thèse, on s'intéresse à des équations évolutives modifiées par une force aléatoire, en dimension finie - équations différentielles stochastiques - et en dimension infinie - équations aux dérivées partielles stochastiques. De telles équations permettent d'étudier de nombreux systèmes en neurosciences, physique, biologie, dynamique des populations, dynamique moléculaire,

Dans un premier temps, on étudie deux types d'Equations Différentielles Stochastiques - EDS - qui ont un intérêt en dynamique moléculaire : l'équation de Langevin et l'équation de Langevin amorti. On propose l'analyse en temps long de méthodes numériques d'approximations implicites pour ces deux équations lorsque le terme déterministe est à croissance polynomiale. Le Chapitre 2 traite de l'équation de Langevin amorti. Les preuves y sont moins techniques que dans le Chapitre 3 qui concerne l'équation de Langevin.

Dans un second temps, on s'intéresse à des schémas de discrétisation d'Equation aux Dérivées Partielles Stochastiques - EDPS. Dans le Chapitre 4, on étudie une EDPS non-linéaire avec un bruit blanc additif possédant une unique mesure de probabilité invariante μ et sa discrétisation en temps par un schéma d'Euler semi-implicite et en espace par la méthode des éléments finis. Dans le Chapitre 5, on étudie la convergence faible d'un schéma de splitting approchant la solution d'une EDPS dont le terme non-linéaire est un polynôme.

Après quelques rappels sur certaines notions utiles en analyse numérique d'équations stochastiques, vous trouverez, dans cette introduction, un résumé du contenu des Chapitres 2, 3, 4 et 5. Le Chapitre 2 correspond à un article accepté dans IMA Journal of Numerical Analysis et les Chapitres 3 et 4 correspondent à des articles soumis. Le Chapitre 4 présente un travail réalisé en collaboration avec Charles-Edouard Bréhier.

1 Analyse numérique d'équations stochastiques

1.1 Le cas des équations différentielles stochastiques

De nombreux travaux traitent de la discrétisation des équations différentielles stochastiques - voir [48, 67–70, 81–83]. Soient $m \in \mathbb{N}$, $d \in \mathbb{N}$, $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})$ un espace de probabilité filtré et $W(t) = (W_1(t), \dots, W_m(t))$ un processus de Wiener standard de dimension m et adapté à la filtration $\{\mathcal{F}_t\}_{t \geq 0}$ et $x \in \mathbb{R}^d$. On considère une équation différentielle stochastique sur \mathbb{R}^d de la forme

$$\begin{aligned} dX(t) &= f(X(t))dt + \sigma(X(t))dW(t), \quad t > 0, \\ X(0) &= x, \end{aligned} \tag{1.1}$$

avec $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ et $\sigma : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times m}$. Sous certaines conditions sur f et σ - voir, par exemple, [48] - l'équation (1.1) admet une unique solution intégrale dans \mathbb{R}^d notée $(X_x(t))_{t \geq 0}$ et définie pour $x \in \mathbb{R}^d$ et $t \geq 0$ par

$$X_x(t) = x + \int_0^t f(X_x(s))ds + \int_0^t \sigma(X_x(s))dW(s).$$

Pour discrétiser en temps l'équation (1.1), on introduit un pas de temps δ et pour tout $n \in \mathbb{N}$ des approximations X_n de $X_x(n\delta)$. On peut associer à $(X_n)_{n \in \mathbb{N}}$ deux types de convergence: la convergence forte et la convergence faible. On dit que le schéma $(X_n)_{n \in \mathbb{N}}$ est d'ordre fort γ si pour tout $p \in \mathbb{N}^*$ et $T > 0$ il existe une constante $C(p, T) > 0$ telle que

$$\left(\mathbb{E} \max_{n=0, \dots, [T/\delta]} |X_n - X(n\delta)|^p \right)^{1/p} \leq C(p, T)\delta^\gamma.$$

On dit que le schéma $(X_n)_{n \in \mathbb{N}}$ est d'ordre faible γ si pour toute fonction test $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ et $T > 0$ il existe une constante $C(\phi, T) > 0$ telle que pour tout $n = 0, \dots, [T/\delta]$

$$|\mathbb{E}\phi(X_n) - \mathbb{E}\phi(X(n\delta))| \leq C(\phi, T)\delta^\gamma.$$

L'erreur forte mesure l'écart entre les trajectoires alors que l'erreur faible étudie la convergence en loi de l'approximation vers la solution exacte.

Considérons la discrétisation de l'équation (1.1) par la méthode d'Euler explicite: pour un pas de discrétisation δ fixé, on définit $(X_n)_{n \in \mathbb{N}}$ par $X_0 = x$ et pour $n \in \mathbb{N}$ par

$$X_{n+1} = X_n + \delta f(X_n) + \sigma\left(W((n+1)\delta) - W(n\delta)\right).$$

Il est bien connu que le schéma d'Euler est d'ordre fort $1/2$ et d'ordre faible 1 - pour plus de détails, on peut consulter [48, 69, 83].

Typiquement, un schéma déterministe utilisé sur une équation différentielle stochastique est d'ordre fort $1/2$ et d'ordre faible 1 . Il est possible d'écrire des schémas d'ordre plus élevés mais des termes de correction compliqués apparaissent - voir, entre autres, [69, 81, 82].

La preuve classique pour montrer des résultats de convergence faible consiste à utiliser la solution de l'équation de Kolmogorov associée à l'équation stochastique - voir la partie 1.2 - pour décomposer l'erreur.

1.2 L'équation de Kolmogorov

On note L l'opérateur de Kolmogorov associé à l'équation stochastique (1.1) défini pour $x \in \mathbb{R}^d$ et $\phi \in C^\infty(\mathbb{R}^d)$ par

$$L\phi(x) = \frac{1}{2} \sum_{i,j=1}^d a_{i,j}(x) \frac{\partial^2 \phi}{\partial x_i \partial x_j}(x) + \sum_{i=1}^d f_i(x) \frac{\partial \phi}{\partial x_i}(x),$$

où

$$a_{i,j}(x) = (\sigma(x)\sigma(x)^T)_{ij} = \sum_{\ell=1}^m \sigma_{i\ell}(x)\sigma_{j\ell}(x).$$

Soit $d \in \mathbb{N}$, l'espace $\mathcal{C}_{\text{pol}}^\infty(\mathbb{R}^d)$ désigne l'ensemble des fonctions $C^\infty(\mathbb{R}^d)$ qui sont à croissance polynomiale et telles que toutes leurs dérivées sont à croissance polynomiale. Soit $\phi \in \mathcal{C}_{\text{pol}}^\infty(\mathbb{R}^d)$ fixée, on définit la fonction u pour $x \in \mathbb{R}^d$ and $t \geq 0$ par

$$u(t, x) = \mathbb{E}\phi(X_x(t)),$$

où $(X_x(t))_{t \geq 0}$ est l'unique solution de (1.1)

Sous certaines conditions sur f et σ , on peut montrer que $u \in \mathcal{C}^\infty(\mathbb{R}^+ \times \mathbb{R}^d)$ et que u et ses dérivées sont à croissance polynomiale. De plus, en utilisant la formule d'Itô, il est possible de montrer que u est solution de l'équation de Kolmogorov - voir [10, 31] - définie par

$$\frac{d}{dt}u(t, x) = Lu(t, x), \quad x \in \mathbb{R}^d, \quad t > 0, \quad u(0, x) = \phi(x), \quad x \in \mathbb{R}^d.$$

Ainsi, l'approximation faible $(\mathbb{E}\phi(X_n))_{n \in \mathbb{N}}$ peut aussi permettre de discrétiser les solutions de certaines équations aux dérivées partielles paraboliques. L'utilisation de cette approche est particulièrement adaptée à la simulation en grandes dimensions. En effet, sa simplicité algorithmique permet d'éviter l'inversion de grands systèmes linéaires associés aux méthodes analytiques de différences finies ou éléments finis.

1.3 Le cas des équations aux dérivées partielles stochastiques

1.3.1 Processus de Wiener cylindrique et intégrales stochastiques dans un espace de Hilbert

Soient H un espace de Hilbert séparable muni de la norme $|\cdot|_H$ et du produit scalaire $\langle \cdot, \cdot \rangle_H$, K un espace de Hilbert séparable muni de la norme $|\cdot|_K$ et $(e_i)_{i \in \mathbb{N}}$ un système orthonormé complet de H . On rappelle qu'un opérateur linéaire borné $T \in \mathcal{L}(H, K)$ est Hilbert-Schmidt si

$$\sum_{i=0}^{+\infty} |T(e_i)|_K^2 < +\infty.$$

Il est bien connu qu'une telle somme est indépendante de la base choisie - voir [16]. L'ensemble de tous les opérateurs Hilbert-Schmidt muni de la norme

$$|T|_{\mathcal{L}_2(H, K)} = \left(\sum_{i=0}^{+\infty} |T(e_i)|_K^2 \right)^{1/2}$$

est un espace de Hilbert, noté $\mathcal{L}_2(H, K)$.

Soit $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})$ un espace de probabilité filtré. Un processus de Wiener cylindrique W est défini par:

- Un système orthonormé complet de H , noté $(e_i)_{i \in \mathbb{N}}$;
- Une famille $(\beta_i)_{i \in \mathbb{N}}$ de mouvements browniens mutuellement indépendants et adaptés à la filtration $\{\mathcal{F}_t\}_{t \geq 0}$.

On pose alors pour $t \geq 0$

$$W(t) = \sum_{i \in \mathbb{N}} \beta_i(t) e_i. \tag{1.2}$$

Il est important de remarquer que le processus W ne dépend pas du système orthonormé complet choisi et que la somme (1.2) ne converge pas dans H - cela reflète l'irrégularité en espace d'un tel processus. Cependant, si on considère un opérateur linéaire de Hilbert-Schmidt $T : H \rightarrow K$, alors $TW(t)$ converge dans $L^2(\Omega, H)$ pour tout $t \geq 0$.

On peut aussi caractériser un tel processus gaussien par

$$\mathbb{E}W(t) = 0$$

dans H et

$$\mathbb{E} \left(\langle W(t), v_1 \rangle_H \langle W(s), v_2 \rangle_H \right) = \min(t, s) \langle v_1, v_2 \rangle_H$$

pour tout $v_1 \in H$ et $v_2 \in H$.

Soit Ψ un processus prévisible tel que pour tout $t \geq 0$ $\Psi(t) \in \mathcal{L}_2(H, K)$ et tel que $\int_0^T |\Psi(t)|_{\mathcal{L}_2(H, K)}^2 dt < +\infty$ presque sûrement. Alors on peut définir l'intégrale stochastique $\int_0^T \Psi(s) dW(s)$ dans K : C'est une variable aléatoire à valeurs dans K et

$$\int_0^T \Psi(s) dW(s) = \sum_{i=1}^{+\infty} \int_0^T \Psi(s) e_i d\beta_i(s).$$

De plus, si $\mathbb{E} \left(\int_0^T |\Psi(s)|_{\mathcal{L}_2(H, K)} ds \right) < +\infty$, alors on a

$$\mathbb{E} \int_0^T \Psi(s) dW(s) = 0$$

et

$$\mathbb{E} \left(\left(\int_0^T \Psi(s) dW(s) \right)^2 \right) = \mathbb{E} \left(\int_0^T |\Psi(s)|_{\mathcal{L}_2(H, K)}^2 ds \right).$$

Pour plus de détails sur l'intégrale stochastique, on peut consulter [16].

1.3.2 Convergence faible des équations aux dérivées partielles stochastiques

Comme dans le cas de la dimension finie, il existe deux types de convergence. La convergence forte a été traitée, entre autres, dans [18, 19, 32–35, 40, 41, 66, 75, 79, 88]. La convergence faible pour des équations aux dérivées partielles linéaires stochastiques fait l'objet des articles [19, 25, 52–54, 56] alors que les papiers [2–6, 20, 40, 41, 87] traitent des équations aux dérivées partielles stochastiques semi-linéaires.

Soit H un espace de Hilbert, on considère l'équation parabolique suivante

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t) \\ X(0, x) &= x \end{aligned} \tag{1.3}$$

où $x \in H$, X est un processus à valeurs dans H , A un opérateur linéaire non borné, négatif, auto-adjoint avec un inverse compact et $F : H \rightarrow H$ est supposée globalement Lipschitz. W un processus de Wiener cylindrique sur H défini sur un espace de probabilité filtré $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbb{P})$.

On peut, par exemple, prendre $A = \frac{\partial^2}{\partial x^2}$ sur le domaine $H^2(0, 1) \cap H_0^1(0, 1)$ avec des conditions de Dirichlet homogène au bord.

Sous les conditions ci dessus - voir [16] -, l'équation (1.3) admet une unique solution intégrale dans $L^2(\Omega, \mathcal{C}([0, T], H))$ définie pour $x \in H$ et $t \geq 0$ par

$$X(t, x) = e^{tA}x + \int_0^t e^{(t-s)A}F(X(s, x))ds + \int_0^t e^{(t-s)A}dW(s).$$

Pour discrétiser en temps l'équation (1.3), on introduit, en général, un pas de temps $\delta > 0$, et des approximations $X_n(\delta, x)$ de $X(n\delta, x)$ pour tout $n \in \mathbb{N}$ à l'aide du schéma d'Euler semi-implicite suivant:

$$\begin{aligned} X_{n+1}(\delta, x) &= X_n(\delta, x) + \delta AX_{n+1}(\delta, x) + \delta F(X_n(\delta, x)) + \sqrt{\delta}\chi_{n+1}, \\ X_0(\delta, x) &= x, \end{aligned} \tag{1.4}$$

avec $\chi_{n+1} = \frac{1}{\sqrt{\delta}}(W((n+1)\delta) - W(n\delta))$. Le bruit $\sqrt{\delta}\chi_{n+1}$ représente l'accroissement du processus de Wiener entre les deux instants $n\delta$ et $(n+1)\delta$.

Il s'agit d'un schéma semi-implicite: la partie nonlinéaire est discrétisée de manière explicite, tandis que la partie linéaire l'est de manière implicite. En introduisant l'opérateur $R_\delta = (I - \delta A)^{-1}$, on dispose en fait d'une formule explicite

$$X_{n+1}(\delta, x) = R_\delta X_n(\delta, x) + \delta R_\delta F(X_n(\delta, x)) + \sqrt{\delta} R_\delta \chi_{n+1}.$$

Grâce aux conditions imposées à l'opérateur A , on peut montrer que R_δ est un opérateur de Hilbert-Schmidt; par conséquent le bruit $\sqrt{\delta} \chi_{n+1}$ est bien à valeurs dans H . Ainsi X_n est bien défini pour tout $n \in \mathbb{N}$ et est à valeurs dans H .

Il a été démontré dans [75] que cette approximation à un instant donné est d'ordre 1/4 au sens fort.

La principale difficulté pour adapter la preuve de la convergence faible des EDS aux équations en dimension infinie est que l'équation de Kolmogorov devient une équation aux dérivées partielles avec un nombre infini de variables et des opérateurs non bornés. On doit donc utiliser une discrétisation en espace en plus d'une discrétisation en temps. En général, deux types de discrétisation en espace sont considérés: une discrétisation en espace selon une décomposition spectrale de l'opérateur A - elle permet de justifier tout les calculs dans le cas où l'on ne veut étudier que la discrétisation en temps - ou une discrétisation utilisant la méthode des éléments finis - on étudie alors une discrétisation complète de notre équation.

Dans [20], Debussche adapte la preuve en dimension finie aux EDPS. Il montre que la convergence faible associée à l'approximation (1.4) est d'ordre 1/2 - ce qui est bien le double de l'ordre fort. Les deux principaux outils utilisés dans [20] sont:

- de meilleures estimations sur les dérivées en espace de la solution de l'équation de Kolmogorov, plus précisément, on a besoin que ces dérivées appartiennent aux domaines des puissances fractionnaires de $-A$.
- une formule d'intégration par partie issue du calcul de Malliavin qui nous permet de rendre plus régulier certains termes stochastiques.

Ces deux outils sont fondamentaux pour étudier des équations ayant un terme non-linéaire. Dans le cas d'équations linéaires, on peut ne pas utiliser le deuxième outil, ce qui simplifie les preuves - voir [19, 25], mais on ne peut pas adapter ces méthodes aux équations paraboliques non-linéaires.

1.3.3 Méthode des éléments finis pour des EDPS

On considère \mathcal{D} un intervalle ouvert borné de \mathbb{R} et l'espace de Hilbert $H = L^2(\mathcal{D})$ muni du produit scalaire $\langle \cdot, \cdot \rangle_H$ et de la norme $|\cdot|_H$ et on s'intéresse aux équations de la forme

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t), \\ X(0, x) &= x, \end{aligned} \tag{1.5}$$

avec $x \in H$. On suppose que A est un opérateur linéaire non borné, négatif, auto-adjoint avec un inverse compact et que la fonction $F : H \rightarrow H$ est C^2 , lipchitzienne et bornée et que ces deux premières dérivées sont bornées. W est un processus de Wiener cylindrique sur H .

Pour discrétiser en espace l'équation (1.5) par la méthode des éléments finis, on introduit $(V_h)_{h \in (0,1)}$, une famille d'espace de fonctions linéaires continues par morceaux associée à une famille quasi-uniforme de sous intervalles, avec h la taille du plus grand intervalle. On note $P_h : H \rightarrow V_h$ la projection orthogonale de H dans V_h et $A_h \in \mathcal{L}(H)$ la discrétisation

de l'opérateur A . Plus précisément, on définit $A_h : V_h \rightarrow V_h$ comme l'unique opérateur vérifiant pour $x_h \in V_h$ et $y_h \in V_h$

$$\langle A_h x_h, y_h \rangle_H = \langle A x_h, y_h \rangle_H.$$

Pour $h \in (0, 1)$, on peut maintenant définir une discrétisation $(X^h(t))_{t \geq 0}$ de $(X(t))_{t \geq 0}$ par l'équation

$$dX^h(t) = A_h X^h(t) dt + P_h F(X^h(t)) dt + P_h dW(t), \quad X^h(0) = P_h x = P_h X_0.$$

Comme pour tout $h \in (0, 1)$, A_h vérifie les mêmes propriétés de régularité que A , l'équation précédente admet une unique solution intégrale à valeurs dans V_h définie pour tout $0 \leq t \leq T$ par

$$X^h(t) = e^{tA_h} P_h x + \int_0^t e^{(t-s)A_h} F^h(X^h(s)) ds + \int_0^t e^{(t-s)A_h} P_h dW(s).$$

Cette approximation est d'ordre 1/2 au sens fort - voir [56] - et 1 au sens faible - voir [3]: pour tout $T > 0$, pour toute condition initiale $x \in H$, pour toute fonction test $\phi : H \rightarrow H$, \mathcal{C}^2 bornée dont les deux premières dérivées sont bornées et pour tout $0 < \kappa < 1/2$, il existe une constante C telle que pour tout $h \in (0, 1)$ et tout $t \leq T$, on ait

$$\begin{aligned} \mathbb{E}|X^h(t) - X(t)|_H &\leq Ch^{1/2-\kappa} \\ |\mathbb{E}\phi(X^h(t)) - \mathbb{E}\phi(X(t))|_H &\leq Ch^{1-\kappa}. \end{aligned}$$

En dimension supérieure, on peut utiliser la même méthode pour discrétiser (1.5), mais on est obligé de colorer le bruit - voir [3]. On obtient, à nouveau, que l'erreur faible est le double de l'erreur forte.

Pour plus d'information sur la méthode des éléments finis, on pourra regarder [12, 28] pour le cas déterministe et [3, 25] pour le cas stochastique.

1.4 Comportement en temps long

Il est intéressant d'étudier le comportement en temps long de la solution d'une équation stochastique, notamment pour connaître le comportement à l'équilibre de certains systèmes utilisés en biologie ou en physique. Cette étude peut, par exemple, nous permettre d'approcher des quantités macroscopiques utiles en dynamique moléculaire - voir le début de la partie 2 pour plus de détails. On se pose alors les questions suivantes: Existe-t-il une mesure invariante μ ? Si oui, notre processus est-il ergodique - i.e. la loi de notre processus converge-t-elle vers μ , à quelle vitesse et dans quel espace?

Considérons X la solution d'une EDS de la forme (1.1), possédant une mesure invariante μ . Pour étudier la convergence de la loi de X vers la mesure invariante, plusieurs méthodes sont possibles. L'une d'entre elles consiste à utiliser des fonctions de Lyapunov et des résultats issus de la théorie des chaînes de Markov - voir [9, 43, 84]. Il existe aussi des preuves n'utilisant que des outils analytiques - voir [38]. Une dernière approche consiste à utiliser des estimations provenant de la structure elliptique ou hypocoercive de l'équation considérée - voir, entre autres, [42, 64, 84, 86]. L'avantage de cette dernière méthode est de fournir des vitesses de convergence plus précises. Dans le cas où le processus est à valeurs dans \mathbb{R}^d , on a en général besoin de la condition de dissipativité suivante: il existe des constantes $c > 0$ et $C > 0$ telles que pour tout $x \in \mathbb{R}^d$

$$\langle f(x), x \rangle \leq -c|x|^2 + C.$$

Considérons X la solution d'une EDPS de la forme (1.3). On se place sous les mêmes hypothèses que dans la partie sur la convergence faible des EDPS. On impose une condition de dissipativité forte : si λ_0 est la plus petite valeur propre de l'opérateur $-A$ et si L_F désigne un majorant de la constante de Lipschitz de la fonction F , on suppose

$$0 \leq L_F < \lambda_0. \quad (1.6)$$

Dans cette situation les trajectoires issues de deux conditions initiales x_1 et x_2 différentes, et soumises à la même perturbation stochastique $(W(t))_{t \geq 0}$, se rapprochent exponentiellement vite, presque sûrement: pour tout $t \geq 0$

$$|X(t, x_1) - X(t, x_2)|_H \leq e^{\frac{\lambda_0 - L_F}{2}t} |x_1 - x_2|_H.$$

Cette contraction assure l'unicité d'une mesure de probabilité invariante. L'existence d'une telle mesure est une conséquence des propriétés du bruit; notamment la propriété de Feller est vérifiée.

La condition de dissipativité peut être affaiblie, auquel cas la contraction des trajectoires n'est plus valable; en revanche, grâce à des techniques de couplage, on obtient une contraction sur les lois. Plus précisément, on suppose qu'il existe deux constantes $c > 0$ et $C > 0$ telles que pour tout $x \in D(A) \cap H$, avec $D(A)$ le domaine de A , on ait

$$\langle Ax + F(x), x \rangle \leq -c|x|^2 + C. \quad (1.7)$$

La preuve de l'existence d'une mesure de probabilité invariante est la même que dans le cas de dissipativité forte; néanmoins celle de l'unicité devient plus complexe et nécessite des hypothèses sur la nature du bruit. On obtient alors la propriété de contraction suivante: si ϕ est une fonction test bornée alors il existe deux constantes $c > 0$ et $C(\phi) > 0$, telles que toutes conditions initiales x_1 et x_2 et tout $t \geq 0$, on ait

$$|\mathbb{E}\phi(X(t, x_1)) - \mathbb{E}\phi(X(t, x_2))| \leq C(\phi)(1 + |x_1|^2 + |x_2|^2)e^{-ct}.$$

Outre l'unicité de la mesure invariante, on peut aussi déduire de cette inégalité, la convergence en loi, à une vitesse exponentielle, de notre processus vers la mesure invariante: Si ϕ est une fonction test bornée alors il existe des constantes $C(\phi) > 0$ et $c > 0$ telles que pour toute condition initiale x et $t \geq 0$, on ait

$$|\mathbb{E}\phi(X(t, x)) - \int \phi d\mu| \leq C(\phi)(1 + |x|^2)e^{-ct}.$$

Pour plus de détail sur la méthode de couplage, on peut consulter [21, 55, 63, 72]. Cette méthode peut aussi être utilisée pour étudier la convergence en loi de solution d'EDS.

Soit μ la mesure invariante associée à l'équation considérée et ϕ une fonction test, deux des méthodes les plus communes pour approcher $\int \phi d\mu$ consistent à utiliser les trajectoires d'une approximation en temps $(X_n)_{n \in \mathbb{N}}$ de la solution de l'équation pour calculer une moyenne empirique. Plus précisément, on peut utiliser une moyenne en temps le long des trajectoires pour approcher $\int \phi d\mu$: on étudie alors la quantité

$$\left| \frac{1}{N} \sum_{n=0}^{N-1} \phi(X_n) - \int \phi(x) \mu(dx) \right|,$$

lorsque N tend vers l'infini. Une autre méthode consiste à utiliser la moyenne de différentes réalisations de notre approximation. En effet, sous des conditions assurant l'ergodicité du processus $(X(t))_{t \geq 0}$, on a que $\mathbb{E}\phi(X(t))$ converge vers $\int \phi d\mu$ quand t tend vers l'infini,

exponentiellement vite. Dans la situation où l'estimation d'erreur faible est indépendante du temps final, on peut alors utiliser une méthode de Monte-Carlo pour calculer $\mathbb{E}\phi(X_n)$, et approcher $\int \phi d\mu$.

On se pose alors plusieurs questions : Est ce que le schéma numérique possède une mesure invariante? Quelle est la vitesse de convergence? Quelle est l'erreur entre la mesure invariante associée au schéma numérique et celle associée à la solution exacte? Quelle est l'erreur entre l'estimateur construit par l'une des méthodes précédentes et la mesure invariante associée à la solution exacte?

Dans le cas des EDS, de nombreux articles - voir, entre autres, [43, 57, 64, 81–84] et les références citées dedans - ont répondu à ces questions. Dans [22, 58, 64, 84, 85], les auteurs montrent des développements en série entière par rapport au pas de discrétisation de la mesure invariante ou de l'approximation faible. Les articles traitant des EDPS sont moins nombreux. On pourra par exemple consulter [5].

Dans cette thèse, on répond à certaines de ces questions. Dans les Chapitres 2 et 3, on étudie le comportement en temps long de $(\mathbb{E}\phi(X_n))_{n \in \mathbb{N}}$ pour ϕ une fonction test régulière et $(X_n)_{n \in \mathbb{N}}$ un schéma de discrétisation en temps de la solution de l'équation de Langevin amortie ou de l'équation de Langevin. On montre, entre autres, un développement en série entière par rapport au pas de discrétisation de l'approximation faible. Dans le Chapitre 4, on s'intéresse à une EDPS parabolique avec bruit additif possédant une unique mesure de probabilité invariante μ et on étudie la convergence de $\frac{1}{N} \sum_{n=0}^{N-1} \phi(X_n)$ vers $\int \phi(x)\mu(dx)$ pour ϕ une fonction test régulière et $(X_n)_{n \in \mathbb{N}}$ une discrétisation en temps par un schéma d'Euler semi-implicite et en espace par une méthode des éléments finis de la solution de l'EDPS considérée. Dans le Chapitre 5, on s'intéresse à une EDPS parabolique avec bruit additif dont le terme non linéaire est un polynôme et à son approximation en temps par un schéma de splitting implicite. Avant d'étudier le comportement en temps long d'une telle approximation, il est intéressant de connaître la convergence de cette dernière vers la solution exacte sur un intervalle de temps borné. Plus précisément, on montre que ce schéma est d'ordre faible $1/2$.

2 Analyse d'erreur faible rétrograde pour l'équation de Langevin amortie et l'équation de Langevin

Cette partie présente le contenu des Chapitres 2 et 3.

Considérons une fonction V représentant l'énergie potentielle d'un système moléculaire classique et la fonction de densité de Gibbs-Boltzmann défini par

$$\bar{\rho}(x) = Z^{-1}e^{-\beta V(x)},$$

où $\beta^{-1} = k_B T$, k_B est la constante de Boltzmann, T est la température et Z est une constante de renormalisation. Un objectif fondamental de la dynamique moléculaire est de calculer des moyennes par rapport à $\bar{\rho}$. Une des méthodes les plus populaires pour calculer ces quantités utilise l'équation de Langevin amortie et l'équation de Langevin. Plus précisément, on approche ces intégrales en utilisant des propriétés d'ergodicité pour des schémas numériques approchant la solution de l'équation de Langevin ou de l'équation de Langevin amortie - voir [9, 39, 57, 60].

Dans cette partie, on étudie les propriétés asymptotiques de discrétisation par des schémas implicites de l'équation de Langevin amortie - Chapitre 2 - et de l'équation de Langevin - Chapitre 3. L'idée principale est d'adapter aux cas des EDS la méthode d'analyse d'erreur rétrograde utilisée pour étudier le comportement en temps long de schéma numérique discrétisant des équations différentielles ordinaires. En adaptant cette méthode, on montre,

pour chacune des deux équations, un résultat d'analyse d'erreur faible rétrograde: une fonctionnelle de la solution numérique est proche de la solution d'une équation de Kolmogorov modifiée à des ordres arbitrairement élevés par rapport au pas de discrétisation. On étudie aussi les propriétés asymptotiques des schémas implicites considérés: on montre que toute mesure invariante du schéma numérique est proche d'une mesure invariante modifiée obtenue par développement asymptotique.

Après avoir expliqué le principe d'analyse d'erreur rétrograde dans la partie 2.1, on présentera, dans la partie 2.2 les résultats obtenus pour l'équation de Langevin amorti. Enfin, dans la partie 2.3, on exposera le cas de l'équation de Langevin.

La principale différence entre l'équation de Langevin et l'équation de Langevin amortie est que la première équation est elliptique alors que la deuxième est hypoelliptique. Il est donc plus facile d'obtenir certains résultats pour l'équation de Langevin amortie que pour l'équation de Langevin.

2.1 Analyse d'erreur rétrograde

L'analyse d'erreur rétrograde est un outil puissant pour étudier le comportement en temps long de schémas numériques approchant les solutions d'équations d'évolution - voir [36, 37, 59, 71, 76]. L'idée principale peut être décrite de la manière suivante: Considérons une équation différentielle ordinaire de la forme

$$\dot{y}(t) = f(y(t)), \tag{2.1}$$

avec $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ un champ de vecteurs régulier. On note $\psi_t^f(y)$ le flot associé à cette équation. Par définition, une méthode numérique définit pour un pas de temps δ petit, une approximation ϕ_δ du flot exact ψ_δ^f de l'équation (2.1): On a pour $y \in \mathbb{R}^d$ borné,

$$\phi_\delta(y) = \psi_\delta^f(y) + \mathcal{O}(\delta^{r+1}),$$

avec r l'ordre de la méthode.

L'analyse d'erreur rétrograde permet de montrer que l'on peut interpréter ϕ_δ comme le flot exact $\psi_\delta^{f_\delta}$ d'un champ de vecteurs défini par une série en puissance de δ

$$f_\delta = f + \delta^r f_r + \delta^{r+1} f_{r+1} + \dots,$$

avec f_ℓ , $\ell \geq r$, des champs de vecteurs dépendants de la méthode numérique considérée. En général, la série définissant f_δ ne converge pas, mais on peut montrer que pour y borné et $N \in \mathbb{N}^*$ quelconque, on a

$$\phi_\delta(y) = \psi_\delta^{f_\delta^N}(y) + C_N \delta^N,$$

avec f_δ^N la série tronquée définie par

$$f_\delta^N = f + \delta^r f_r + \dots + \delta^N f_N.$$

Sous certaines conditions, la constante $C_N \delta^N$ peut être optimisée en N , ainsi, on peut choisir le terme d'erreur de l'équation précédente exponentiellement petit par rapport à δ .

Il existe de nombreuses applications à ce résultat dans le cas où f possède certaines propriétés géométriques - par exemple, lorsque f est un champ de vecteurs hamiltonien ou possède une structure réversible. Dans ce cas, et sous certaines conditions sur la méthode numérique ϕ_δ , le champ de vecteurs modifié hérite de la structure de f . Par exemple, si ϕ_δ est symplectique et f est un champ de vecteurs hamiltonien, alors f_δ est un champ de vecteurs hamiltonien. Une conséquence de ce résultat est la conservation d'un Hamiltonien

modifié pour le schéma numérique, pour des temps très long - de l'ordre de δ^{-N} . On peut alors en déduire des résultats de stabilité en temps long.

Plus récemment, ces idées ont été étendues à certaines équations aux dérivées partielles Hamiltoniennes : d'abord dans le cas linéaire [23] et ensuite dans le cas semi-linéaire - Schrödinger ou équations des ondes - voir [29, 30]. Dans la suite de cette partie, on étend ces idées aux équations stochastiques de Langevin et de Langevin amorti.

2.2 Analyse d'erreur faible rétrograde pour l'équation de Langevin amorti

Soit $d \in \mathbb{N}^*$, on considère le processus de Langevin amorti $(X(t))_{t \geq 0}$ à valeurs dans \mathbb{R}^d défini par l'EDS:

$$dX(t) = -\nabla V(X(t))dt + dW(t) \quad t > 0, \quad (2.2)$$

avec $V \in C_{pol}^\infty(\mathbb{R}^d)$ et W un mouvement brownien de dimension d .

Après avoir présenté certains résultats asymptotiques sur la loi du processus, on introduira les schémas numériques qui nous intéressent. On expliquera ensuite un résultat d'analyse d'erreur faible rétrograde.

Si V vérifie la condition de dissipativité suivante : il existe des constantes $C > 0$ et $c > 0$ telles que pour tout $x \in \mathbb{R}^d$

$$\langle \nabla V(x), x \rangle \geq c|x|^2 - C, \quad (2.3)$$

alors on a existence et unicité de la solution intégrale associée à (2.2) - voir [10, 47].

Sous certaines conditions sur V , la loi de la solution de l'équation de (2.2) va converger exponentiellement vite vers une constante. Plus précisément, on considère $(X_x(t))_{t \geq 0}$ la solution de (2.2) qui vérifie $X_x(0) = x$ et $u(t, x) = \mathbb{E}\phi(X_x(t))$ la solution de l'équation de Kolmogorov associée à (2.2) avec $\phi \in C_{pol}^\infty(\mathbb{R}^{2d})$. De nombreux travaux étudient le comportement en temps long de u , mais, en général, les résultats obtenus sont dans un espace à poids et pas point par point. Dans [43], en utilisant des résultats de la théorie des chaînes de Markov, les auteurs ont montré, sous certaines conditions, le résultat suivant

Proposition 2.1 *En utilisant les notations du paragraphe précédent, on a qu'il existe des constantes $C = C(\phi) > 0$, $r_0 := r(\phi) > 0$ et $\lambda_0 = \lambda_0(\phi) > 0$ telles que pour tout $t \geq 0$ et $x \in \mathbb{R}^d$,*

$$\left| u(t, x) - \int_{\mathbb{R}^d} \phi(y)\rho(y)dy \right| \leq C(1 + |x|^{r_0}) \exp(-\lambda_0 t),$$

où $\rho(y)dy$ est la mesure invariante associée à l'équation de Langevin amortie (2.2) définie pour $x \in \mathbb{R}^d$ par

$$\rho(x) = \frac{1}{Z} e^{-2V(x)}$$

avec Z une constante de renormalisation.

Les dérivées de u se comportent comme u :

Proposition 2.2 *Pour tout entier $m \in \mathbb{N}^*$, il existe des constantes $C := C(m, \phi) > 0$ et $r = r(m, \phi) \geq r_0$ telles que pour tout $t \geq 0$ et $x \in \mathbb{R}^d$*

$$|D^m u(t, x)| \leq C(1 + |x|^r) \exp(-\lambda_0 t),$$

où $D^m u(t)$ représente le vecteur de toutes les dérivées en espace d'ordre m de $u(t)$ et λ_0 est définie dans la proposition 2.1.

Comme l'équation de Langevin amortie est elliptique, on peut utiliser des formules de Bismuth-Elworthy pour obtenir le contrôle des dérivées - voir l'annexe du Chapitre 2 pour plus de détails. On déduit de cette proposition le résultat de régularité suivant:

Corollaire 2.3 Soit $g \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ telle que $\int_{\mathbb{R}^d} g(x)\rho(x)dx = 0$. L'équation de Poisson

$$Lh = g, \quad \int_{\mathbb{R}^d} h(x)\rho(x)dx = 0$$

avec L l'opérateur de Kolmogorov associé à (2.2) admet une unique solution $h \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ définie pour $x \in \mathbb{R}^d$ par $h(x) = -\int_0^\infty \mathbb{E}(g(X_x(t)))dt$.

Comme V est à croissance polynomiale, les schémas explicites peuvent être instables [43]. C'est pourquoi on considère des approximations implicites. Plus précisément, pour un pas de temps δ fixé, on étudie un schéma d'Euler implicite défini par $X_0 = X(0)$ et pour $n \in \mathbb{N}$ par

$$X_{n+1} = X_n - \delta \nabla V(X_{n+1}) + \sqrt{\delta} \eta_n$$

où $\eta_n = (\eta_{n,1}, \dots, \eta_{n,d}) = \frac{1}{\sqrt{\delta}}(W((n+1)\delta) - W(n\delta))$ est une variable aléatoire à valeurs dans \mathbb{R}^d et $\{\eta_{n,i} : n \in \mathbb{N}, i \in \{1, d\}\}$ est une famille de variable aléatoire i.i.d vérifiant $\eta_{1,1} \sim \mathcal{N}(0, 1)$. On étudie aussi un schéma de split-step implicite défini par $X_0 = X(0)$ et pour $n \in \mathbb{N}$ par

$$\begin{cases} X_n^* &= X_n - \delta \nabla V(X_{n+1}) \\ X_{n+1} &= X_n^* + \sqrt{\delta} \eta_n \end{cases}$$

où η_n est défini ci dessus. Pour un pas de temps suffisamment petit, ces schémas sont bien définis via un corollaire du théorème du point fixe de Brouwer et admettent des moments de tout ordre bornés uniformément en temps.

Sous des hypothèses de dissipativité et de semi-convexité sur le potentiel V , on montre une version discrète de la proposition 2.1. Plus précisément, on montre que les deux schémas précédents vont décroître exponentiellement vite à une erreur près en puissance du pas de temps δ :

Théorème 2.4 Soit $N \in \mathbb{N}^*$ fixé. Il existe $\delta_0 > 0$, qui dépend des paramètres de notre équation, tel que si on considère $(X_k)_{k \in \mathbb{N}}$ un des schémas précédents alors pour tout pas de temps $0 < \delta < \delta_0$, on peut construire une mesure de probabilité régulière μ_δ^N tel que pour toute fonction test $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, il existe des constantes $C > 0$ et $0 < \lambda < \lambda_0$, indépendantes de δ , telles que pour tout $n \in \mathbb{N}$

$$\left| \mathbb{E} \phi(X_n) - \int_{\mathbb{R}^d} \phi(y) \mu_\delta^N(dy) \right| \leq C \left(e^{-\lambda n \delta} + \delta^{N+1} \right).$$

A partir de ce résultat, on retrouve que nos deux schémas sont d'ordre faible 1. De plus, on a que toutes les mesures invariantes associées à notre processus de discrétisation sont proches de $\mu^N(y)dy$ à une erreur près d'ordre $C\delta^{N+1}$. D'autres travaux - [22, 58, 64, 82, 83] - montrent le même genre de résultat, mais soit les auteurs travaillent sur le tore, soit leurs conditions sur V sont plus restrictives, soit ils ont besoin d'avoir un pas de temps arbitrairement petit alors que nous, nous avons juste besoin que notre pas de temps soit majoré par une constante dépendant des paramètres de notre équation. On retrouve aussi ici un développement en série entière par rapport au pas de discrétisation de la mesure invariante, comme dans [22, 58, 64, 85].

Pour prouver le théorème 2.7 - dans le Chapitre 3 - on étend la méthode d'analyse d'erreur rétrograde aux équations différentielles stochastiques. Les premiers pas dans cette direction ont été fait par Shardlow dans [80]. Il étudie une équation différentielle stochastique avec un bruit additif et discrétisée par un schéma d'Euler, noté $(X_n)_{n \in \mathbb{N}}$. Il montre qu'on peut lui associer une équation différentielle stochastique, mais seulement pour $N = 2$. Plus précisément, il construit une équation différentielle stochastique modifiée:

$$d\tilde{X} = \tilde{f}(\tilde{X})dt + \tilde{\sigma}(\tilde{X})dW$$

telle que

$$\left| \mathbb{E}(\phi(X_k)) - \mathbb{E}(\phi(\tilde{X}(k\delta))) \right| \leq c(\phi, T)\delta^2, \quad k = 0, \dots, [T/\delta], \quad T > 0.$$

Il explique aussi que pour avoir un ordre plus élevé, il y a trop de conditions à satisfaire pour construire une équation modifiée. Dans [89], Zygalkis a étendu ce résultat aux cas d'EDS avec un bruit multiplicatif.

Ici, on suit l'approche de [22], on construit une équation modifiée en utilisant un développement en série du générateur associé à notre équation au lieu d'utiliser un développement en série des coefficients de l'EDS.

Plus précisément, en notant L l'opérateur de Kolmogorov associé à notre équation, on construit un opérateur de Kolmogorov modifié de la forme

$$\mathcal{L} = L + \delta L_1 + \delta^2 L_2 + \dots,$$

avec L_ℓ , $\ell \in \mathbb{N}^*$ des opérateurs d'ordre $2\ell + 2$ tel que la solution formelle de l'équation de Kolmogorov associée à \mathcal{L} au temps δ coïncide avec $\mathbb{E}\phi(X_1)$. On considère ensuite, comme dans le cas déterministe, les séries tronquées

$$\mathcal{L}^{(N)} = L + \delta L_1 + \dots + \delta^N L_N$$

et on aimerait que la solution de l'équation modifiée

$$\partial_t v^N = \mathcal{L}^{(N)} v^N$$

au temps δ soit une approximation d'ordre $N + 1$ de $\mathbb{E}\phi(X_1)$. Or, il n'est pas évident que l'on puisse correctement définir v^N . Mais, en utilisant les opérateurs L_ℓ , on arrive à construire une fonction $v^{(N)}$ telle que

$$\left| \mathbb{E}(\phi(X_1)) - v^{(N)}(\delta, X_0) \right| \leq c(\phi, N, T, X_0)\delta^{N+1}, \quad T > 0,$$

De plus, en utilisant la proposition 2.1 et son corollaire, on arrive à montrer que la constante précédente ne dépend pas de T et que $v^{(N)}$ converge exponentiellement vite vers l'intégrale de ϕ par rapport à une mesure invariante modifiée pour $\mathcal{L}^{(N)}$. Ceci nous permet d'avoir le résultat pour $k = 1$. On utilise ensuite une propriété de Markov pour avoir le résultat pour tout $k \in \mathbb{N}$.

Une des principales différences entre la preuve faite dans [22], outre le fait que les auteurs travaillent sur le tore, se trouve dans la construction du développement en série entière par rapport au pas de temps de $\mathbb{E}\phi(X_1)$, qui permet de définir les opérateurs L_ℓ . Dans [22], on construit ce développement en utilisant des formules d'Itô. On ne peut pas procéder de la même manière ici car nos schémas sont implicites. En effet, on ne peut pas leur associer un processus continu adapté qui les interpole. On contourne ce problème en utilisant des formules de Taylor avec reste intégrale.

2.3 Analyse d'erreur faible rétrograde pour l'équation de Langevin

Soit $d \in \mathbb{N}^*$, on considère le processus de Langevin $(X(t))_{t \geq 0} := (q(t), p(t))_{t \geq 0}$, à valeurs dans \mathbb{R}^{2d} , défini par l'EDS:

$$\begin{aligned} dq(t) &= p(t)dt \\ dp(t) &= -\nabla V(q(t))dt - \gamma p(t)dt + \sigma dW(t) \quad t > 0, \end{aligned} \tag{2.4}$$

avec $V \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, $\gamma > 0$, $\sigma > 0$ et W un mouvement brownien de dimension d .

Après avoir présenté certains résultats asymptotiques sur la loi du processus, on introduira les schémas numériques qui nous intéressent. Enfin, en utilisant le même raisonnement que pour l'équation de Langevin amorti, on expose un résultat d'analyse d'erreur faible rétrograde.

Si V vérifie la condition de dissipativité (2.3), alors on a existence et unicité de la solution intégrale associée à (2.4) - voir [47].

Sous certaines conditions sur V , on montre le résultat suivant:

Proposition 2.5 *On note $(X_x(t))_{t \geq 0}$ la solution de (2.4) qui vérifie $X_x(0) = x$, $u(t, x) = \mathbb{E}\phi(X_x(t))$ la solution de l'équation de Kolmogorov associée à (2.4) avec $\phi \in C_{pol}^\infty(\mathbb{R}^{2d})$ et $\rho(q, p)dqdp$ la mesure invariante associée à l'équation de Langevin (2.4) définie pour $q \in \mathbb{R}^d$ et $p \in \mathbb{R}^d$ par*

$$\rho(q, p) = \frac{1}{Z} e^{-\frac{\gamma}{\sigma}(|p|^2 + 2V(q))},$$

avec Z une constante de renormalisation. On obtient alors qu'il existe des constantes $\lambda_0 := \lambda_0(\phi) > 0$ et $0 < \lambda < \lambda_0$ telles que pour tout entier $m \in \mathbb{N}$, il existe des constantes $C := C(m, \phi) > 0$ et $r_m := r(m, \phi) > 0$ telles que pour tout $t \geq 0$, $q \in \mathbb{R}^d$ et $p \in \mathbb{R}^d$

$$\left| u(t, q, p) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \phi(x, y) \rho(x, y) dx dy \right| \leq C(1 + |q|^{r_0} + |p|^{r_0}) \exp(-\lambda_0 t),$$

et pour $m \in \mathbb{N}^*$

$$\left| D^m u(t, q, p) \right| \leq C(1 + |q|^{r_m} + |p|^{r_m}) \exp(-\lambda t),$$

où $D^m u(t)$ représente le vecteur de toutes les dérivées en espace d'ordre m de $u(t)$.

Le résultat pour $m = 0$ a été démontré dans [43]. Pour obtenir le contrôle des dérivées, on ne peut pas utiliser la même méthode que pour l'équation de Langevin amorti, car notre équation est hypo-elliptique et non pas elliptique. On utilise une adaptation de la preuve faite par Talay dans [84] qui nous permet de connaître la dépendance de la constante C en fonction de ϕ . On déduit de cette proposition le résultat de régularité suivant:

Corollaire 2.6 *Soit $g \in C_{pol}^\infty(\mathbb{R}^{2d})$ telle que $\int_{\mathbb{R}^d \times \mathbb{R}^d} g(q, p) \rho(q, p) dq dp = 0$. L'équation de Poisson*

$$Lh = g, \quad \int_{\mathbb{R}^d \times \mathbb{R}^d} h(q, p) \rho(q, p) dq dp = 0$$

avec L l'opérateur de Kolmogorov associé à (2.4) admet une unique solution $h \in C_{pol}^\infty(\mathbb{R}^{2d})$ définie pour $x \in \mathbb{R}^{2d}$ par $h(x) = -\int_0^\infty \mathbb{E}(g(X_x(t))) dt$.

Comme V est à croissance polynomiale, les schémas explicites peuvent être instables. C'est pourquoi on considère des approximations implicites. Plus précisément, pour un pas de temps δ fixé, on étudie un schéma d'Euler implicite défini par $q_0 = q(0)$, $p_0 = p(0)$ et pour $n \in \mathbb{N}$ par

$$\begin{cases} q_{n+1} &= q_n + \delta p_{n+1} \\ p_{n+1} &= p_n - \delta \partial_q V(q_{n+1}) - \gamma \delta p_{n+1} + \sqrt{\delta} \sigma \eta_n, \end{cases}$$

où $\eta_n = (\eta_{n,1}, \dots, \eta_{n,d}) = \frac{1}{\sqrt{\delta}}(W((n+1)\delta) - W(n\delta))$ est une variable aléatoire à valeurs dans \mathbb{R}^d et $\{\eta_{n,i} : n \in \mathbb{N}, i \in \{1, d\}\}$ est une famille de variable aléatoire i.i.d vérifiant $\eta_{1,1} \sim \mathcal{N}(0, 1)$. On étudie aussi un schéma de split-step implicite défini par $q_0 = q(0)$, $p_0 = p(0)$ et pour $n \in \mathbb{N}$ par

$$\begin{cases} q_{n+1} &= q_n + \delta p_n^* \\ p_n^* &= p_n - \delta \gamma p_n^* - \delta \partial_q V(q_{n+1}), \\ p_{n+1} &= p_n^* + \sqrt{\delta} \sigma \eta_n, \end{cases}$$

où η_n est définie ci dessus. Ces schémas sont bien définis via un corollaire du théorème du point fixe de Brouwer et admettent des moments de tout ordre bornés uniformément en temps.

Sous des hypothèses de dissipativité et de semi-convexité sur le potentiel V , on montre alors une version discrète de la proposition 2.5. Plus précisément, on montre le même résultat que pour l'équation de Langevin amorti, les deux schémas précédents vont décroître exponentiellement vite à une erreur près en puissance du pas de temps δ :

Théorème 2.7 *Soit $N \in \mathbb{N}^*$ fixé. Il existe $\delta_0 > 0$, qui dépend des paramètres de notre équation, tel que si on considère $(q_k, p_k)_{k \in \mathbb{N}}$ un des schémas précédents alors pour tout pas de temps $0 < \delta < \delta_0$, on peut construire une mesure de probabilité régulière μ_δ^N tel que pour toute fonction test $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$, il existe des constantes $C > 0$ et $0 < \lambda < \lambda_0$, indépendantes de δ , telles que pour tout $n \in \mathbb{N}$*

$$\left| \mathbb{E} \phi(q_n, p_n) - \int_{\mathbb{R}^{2d}} \phi(y) \mu_\delta^N(dy) \right| \leq C \left(e^{-\lambda n \delta} + \delta^{N+1} \right).$$

La preuve du théorème 2.4 est similaire à celui du théorème 2.7, mais elle est plus technique. Ce résultat est similaire à ceux décrits dans [22, 58, 84] mais les hypothèses sont différentes.

3 Approximation de la loi invariante d'EDPS par un schéma de discrétisation en temps et en espace

Cette partie présente le contenu du Chapitre 4.

On s'intéresse dans cette partie à une équation aux dérivées partielles stochastique parabolique, possédant une unique mesure de probabilité invariante μ . On propose d'approcher la loi de la mesure invariante en utilisant une discrétisation de l'EDPS par une méthode des éléments finis en espace et par un schéma d'Euler semi-implicite en temps. Après avoir rappelé les principaux résultats de convergence de cette méthode, on étudie ses propriétés asymptotiques et l'écart entre la moyenne d'une fonction test ϕ évaluée le long de la trajectoire de notre méthode et la quantité qui nous intéresse: $\int \phi d\mu$. On montre que cette convergence est d'ordre $1/2$ par rapport au pas de temps et d'ordre 1 par rapport au maillage.

Le cadre est le même que dans la partie 1.3.3 sur la méthode des éléments finis. Soient $\mathcal{D} \subset \mathbb{R}$, un intervalle ouvert borné et $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})$ un espace de probabilité filtré, on considère l'espace de Hilbert $H = L^2(\mathcal{D})$ et l'EDPS

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t), \\ X(0, x) &= x, \end{aligned} \tag{3.1}$$

avec $x \in H$. On suppose que A est un opérateur linéaire non borné, négatif, auto-adjoint avec un inverse compact et que la fonction $F : H \rightarrow H$ est C^2 , lipchitzienne et bornée et que ses deux premières dérivées sont bornées. W est un processus de Wiener cylindrique sur H . On fait aussi l'hypothèse de dissipativité faible (1.7).

Comme vu dans la partie 1.4, sous l'hypothèse de dissipativité faible, le processus admet une unique mesure de probabilité invariante, notée μ .

Pour discrétiser en temps et en espace l'équation (3.1), on introduit un pas de temps $\delta > 0$, un paramètre de maillage $h \in (0, 1)$ et des approximations $X_k^h(\delta, x)$ de $X(k\delta, x)$

pour tout $k \in \mathbb{N}$ à l'aide de l'algorithme suivant:

$$\begin{aligned} X_{k+1}^h(\delta, x) &= X_k^h(\delta, x) + \delta A_h X_{k+1}^h(\delta, x) + \delta P_h F(X_k^h(\delta, x)) + \sqrt{\delta} P_h \chi_{k+1} \\ X_0^h(\delta, x) &= x, \end{aligned}$$

avec $\chi_{k+1} = \frac{1}{\sqrt{\delta}}(W((k+1)\delta) - W(k\delta))$ et $P_h : H \rightarrow V_h$ et $A_h : V_h \rightarrow V_h$ sont définis dans la partie 1.3.3 sur la méthode des éléments finis.

Il s'agit d'un schéma semi-implicite : la partie nonlinéaire est discrétisée de manière explicite, tandis que la partie linéaire l'est de manière implicite. En introduisant l'opérateur $S_{\delta,h} = (I - \delta A_h)^{-1}$, on dispose en fait d'une formule explicite

$$X_{k+1}^h = S_{\delta,h} X_k^h + \delta S_{\delta,h} P_h F(X_k^h) + \sqrt{\delta} S_{\delta,h} P_h \chi_{k+1}.$$

Grâce aux conditions imposées à l'opérateur A , on peut montrer que $S_{\delta,0} = (I - \delta A)^{-1}$ est un opérateur de Hilbert-Schmidt; par conséquent le bruit $\sqrt{\delta} \chi_{k+1}$ est bien à valeurs dans H , ainsi notre processus est bien défini sur H . De plus, pour $h > 0$, X_k^h est bien défini pour tout $k \in \mathbb{N}$ et est à valeurs dans V_h .

Rappelons que notre approximation à un instant donné est d'ordre $1/4$ en temps et $1/2$ en espace au sens fort - voir [75] et [56] - et $1/2$ en temps et 1 en espace au sens faible - voir [20] et [3].

Toujours d'après la partie 1.4, on a que

$$\mathbb{E}\phi(X(t, x)) \xrightarrow{t \rightarrow +\infty} \int_H \phi(z) \mu(dz),$$

avec une vitesse exponentielle. Pour obtenir un résultat d'approximation de la mesure μ , on peut donc, par exemple, montrer que l'estimation de l'erreur faible est indépendante du temps final. C'est l'approche utilisée dans [5]. Ici, on utilise une autre méthode : celle décrite dans [64] pour approcher la loi de la mesure invariante d'équations différentielles stochastiques définies sur le tore. Les auteurs étudient l'écart entre la moyenne d'une fonction test ϕ , le long d'une trajectoire d'une discrétisation et la moyenne de ϕ par rapport à la mesure invariante. Pour étudier l'erreur ils introduisent la solution d'une équation de Poisson associée à leur équation. En outre, ils donnent un développement en série de l'erreur pour une grande classe de schémas.

En adaptant la méthode décrite dans [64] pour notre équation (3.1), on démontre le résultat suivant:

Théorème 3.1 *Pour tout $0 < \kappa < 1/2$, $\delta_0 > 0$, et pour toute fonction test $\phi : H \rightarrow H$, C^2 , bornée dont les deux premières dérivées sont bornées, il existe une constante $C(\phi) > 0$ telle que pour tout $h \in (0, 1)$, $N \geq 1$, $x \in H$ et $0 < \delta \leq \delta_0$*

$$\left| \frac{1}{N} \sum_{m=0}^{N-1} \mathbb{E}\phi(X_m^h) - \bar{\phi} \right| \leq C(\phi)(1 + |x|^3) \left(\delta^{1/2-\kappa} + h^{1-\kappa} + \frac{1}{N\delta} \right),$$

avec $\bar{\phi} = \int_H \phi(z) \mu(dz)$.

L'erreur se divise en trois parties, la première provient de la discrétisation en temps, la seconde de celle en espace et la dernière tend vers 0 lorsque le temps augmente. L'apparition du dernier terme est due à des problèmes de régularité spécifiques aux EDPS.

Comme vu dans la partie 1.4, le comportement de $\mathbb{E}\phi(X(m\delta, x))$ lorsque m tend vers l'infini dépend de l'hypothèse de dissipativité. En général, on a existence d'une mesure invariante pour le processus $(X_k^h)_{k \in \mathbb{N}}$, tandis que l'unicité n'est assurée que sous l'hypothèse de dissipativité forte (1.6). On obtient le résultat suivant:

Proposition 3.2 *Pour tout $0 < \kappa < 1/2$, $\delta_0 > 0$ et pour toute fonction test $\phi : H \rightarrow H$, \mathcal{C}^2 , bornée dont les deux premières dérivées sont bornées, il existe une constante $C(\phi) > 0$ telle que pour tout $0 < \delta < \delta_0$ et $h \in (0, 1)$, si $\mu^{\delta, h}$ est une mesure de probabilité invariante et ergodique de $(X_k^h(\delta, \cdot))_{k \in \mathbb{N}}$ alors on a*

$$\left| \int_H \phi(z) d\mu(z) - \int_{V_h} \phi(z) d\mu^{\delta, h}(z) \right| \leq C(\phi) (\delta^{1/2-\kappa} + h^{1-\kappa}).$$

Dans le cas où plusieurs mesures invariantes ergodiques existent, le résultat précédent nous fournit une estimation de l'écart entre deux de ces mesures.

Pour prouver le théorème 3.1 - dans le Chapitre 4 - on combine les approches de [20] et [3] pour analyser l'erreur faible pour les EDPS, de [64] pour étudier le comportement en temps long de schémas dans le cas des EDS et de [5] pour approcher la mesure invariante d'EDPS. L'idée principale est de considérer la solution d'une équation de Poisson Ψ , de décomposer $\mathbb{E}\Psi(X_{m+1}^h) - \mathbb{E}\Psi(X_m^h)$ en utilisant des formules d'Itô, puis de sommer les termes pour voir apparaître les quantités qui nous intéressent.

Plus précisément, on commence par utiliser une approximation de Galerkin, afin de se ramener à des quantités appartenant à des sous-espaces de dimension finie de H - construits à partir des éléments propres de A . Cela nous permet de travailler en dimension finie et de bien définir Ψ , la solution de l'équation de Poisson définie par :

$$\begin{aligned} L\Psi &= \phi - \bar{\phi} \\ \int \Psi d\mu &= 0, \end{aligned}$$

avec ϕ notre fonction test et L l'opérateur de Kolmogorov associé à (3.1). Sous nos hypothèses, on a une forme explicite pour Ψ , - elle dépend de la dimension de l'approximation de Galerkin:

$$\Psi(x) = - \int_0^\infty (\mathbb{E}\phi(X(t, x)) - \bar{\phi}) dt.$$

Grâce à des formules d'Itô, l'erreur va dépendre d'un contrôle sur les dérivées de Ψ . Il faut, de plus, que les bornes obtenues permettent un passage à la limite lorsque la dimension de l'approximation de Galerkin augmente. Les difficultés liées à cette exigence sont principalement les mêmes que dans les articles [3, 5, 20], sauf que leurs termes d'erreurs dépendent du contrôle de $u(t, x) = \mathbb{E}\phi(X(t, x))$, la solution de l'équation de Kolmogorov associée à (3.1). En outre, on remarque que dans la décomposition de l'erreur, certains termes sont similaires à ceux décrits dans [3, 5, 20] : l'utilisation de l'équation de Poisson ne simplifie pas vraiment la preuve, elle déplace juste certains problèmes techniques à d'autres endroits.

Donnons les deux idées essentielles utilisées dans la preuve. La première est que le contrôle des dérivées première et seconde de Ψ dans les normes induites par la norme de l'espace de Hilbert H est insuffisant. Pour avoir un ordre de $1/2$ plutôt que de $1/4$, on a besoin que les quantités considérées appartiennent aux domaines des puissances fractionnaires de $-A$. On obtient les bornes sur la solution de l'équation de Poisson en montrant que u et ses dérivées possèdent des bornes qui décroissent exponentiellement vite en temps. L'autre idée essentielle est le contrôle de certaines quantités par une transformation de l'expression en utilisant une formule d'intégration par parties, issue du calcul de Malliavin.

4 Estimation de l'erreur faible pour des EDPS dont le terme non-linéaire est un polynôme

Cette partie présente le contenu du Chapitre 5.

On s'intéresse dans cette partie à une EDPS parabolique dont le terme non-linéaire est un polynôme et à sa discrétisation par un schéma de splitting implicite. On montre que la convergence faible de ce schéma est d'ordre $1/2$ par rapport au pas de temps.

Soient $\mathcal{D} = (0, 1)$ et $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \geq 0}, \mathbb{P})$ un espace de probabilité filtré, on considère l'espace de Hilbert $H = L^2(\mathcal{D})$ et l'EDPS

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t), \\ X(0, x) &= x, \end{aligned} \quad (4.1)$$

avec $x \in \mathcal{C}([0, 1])$, $A = \partial_{xx}^2$ et F un polynôme de la forme $F(x) = -\alpha_{2p-1}x^{2p-1} + \sum_{\ell=0}^{2(p-1)} \alpha_\ell x^\ell$ avec $p \in \mathbb{N}^*$, $\alpha_{2p-1} > 0$ et $\alpha_\ell \in \mathbb{R}$ pour $\ell = 0, \dots, 2(p-1)$. W est un processus de Wiener cylindrique sur H . Il a été démontré dans [10, 16] que cette équation admet une unique solution intégrale dans $L^k(\Omega, \mathcal{C}([0, T] \times [0, 1]))$ pour tout $T > 0$ et $k \in \mathbb{N}^*$.

En général, pour discrétiser en temps une EDPS de la forme (4.1), on utilise le schéma semi-implicite (1.4). Comme notre terme non-linéaire est un polynôme, un tel schéma peut être instable. De plus, on doit avoir des moments de tout ordre dans $L^\infty(\mathcal{D})$, on va donc plutôt considérer un schéma implicite. Plus précisément, on introduit un pas de temps δ et des approximations $X_k(\delta, x)$ de $X(k\delta, x)$ pour tout $k \in \mathbb{N}$ à l'aide du schéma de splitting implicite suivant:

$$\begin{aligned} X_{k+1/2}(\delta, x) &= X_k(\delta, x) + \delta F(X_{k+1/2}(\delta, x)) \\ X_{k+1}(\delta, x) &= X_{k+1/2}(\delta, x) + \delta AX_{k+1}(\delta, x) + \sqrt{\delta} \chi_{k+1} \\ X_0(\delta, x) &= x \end{aligned}$$

avec $\chi_{k+1} = \frac{1}{\delta}(W((k+1)\delta) - W(k\delta))$. En introduisant l'opérateur $R_\delta = (I - \delta A)^{-1}$, on dispose de la formule suivante

$$\begin{aligned} X_{k+1/2}(\delta, x) &= X_k(\delta, x) + \delta F(X_{k+1/2}) \\ X_{k+1}(\delta, x) &= R_\delta X_{k+1/2}(\delta, x) + \sqrt{\delta} R_\delta \chi_{k+1}. \end{aligned}$$

Comme R_δ est un opérateur de Hilbert-Schmidt, le bruit $\sqrt{\delta} R_\delta \chi_{k+1}$ est bien à valeurs dans H . En fait, on a qu'il est dans $L^\infty(\mathcal{D})$ presque sûrement. Notre schéma est donc bien défini et à valeurs dans $L^\infty(\mathcal{D})$.

De plus, dans les cas où il est facile de calculer $X_{k+1/2}$ en fonction de X_k on dispose alors d'une formule explicite pour notre schéma.

Ce schéma est d'ordre faible $1/2$:

Théorème 4.1 *Pour toute condition initiale $x \in \mathcal{C}([0, 1])$, pour toute fonction-test $\phi : H \rightarrow H$, \mathcal{C}^2 , bornée dont les deux premières dérivées sont bornées, pour tout temps final $T > 0$, pour tout $\delta_0 > 0$ et pour tout $0 < \kappa < 1/2$, il existe une constante $C > 0$ telle que pour tout pas de temps $0 < \delta \leq \delta_0$ et pour tout indice $m \in \mathbb{N}$ tel que $m\delta \leq T$, on a*

$$\left| \mathbb{E}\phi(X_m(\delta, x)) - \mathbb{E}\phi(X(m\delta, x)) \right| \leq C\delta^{1/2-\kappa}.$$

Pour prouver le théorème 4.1 - dans le Chapitre 5 - on suit l'approche de [20] pour analyser l'erreur faible dans le cas des EDPS dont le terme non-linéaire est borné. On utilise une approximation de Galerkin pour se ramener à des quantités appartenant à des sous-espaces de dimension finie de H - construits à partir des éléments propres de l'opérateur A . Puis on décompose $\mathbb{E}\phi(X(m\delta, x)) - \mathbb{E}\phi(X_m(\delta, x))$ en utilisant la solution u de l'équation de

Kolmogorov associée à l'approximation de Galerkin de l'équation (4.1) - voir la partie 1.2. Grâce à la formule d'Itô, l'erreur dépend d'un contrôle des dérivées de u - qui doit être indépendant de la dimension de l'approximation de Galerkin.

Comme dans [20], le contrôle de certaines quantités est assuré par une transformation de l'expression en utilisant une formule d'intégration par partie, issue du calcul de Malliavin. De plus, le contrôle des dérivées première et seconde de u dans les normes induites par la norme de l'espace de Hilbert H est insuffisant pour obtenir de l'ordre $1/2$. On montre que les quantités considérées appartiennent aux domaines des puissances fractionnaires de $-A$. Plus précisément, on prouve le résultat suivant:

Proposition 4.2 *Pour tout $0 \leq \alpha < 1/2$, $0 < t \leq T$ et $x \in \mathcal{C}([0, 1])$, il existe une constante $C(T, \phi, x) > 0$ telle que*

$$|Du(t, x)|_\alpha \leq C(T, \phi, x)(1 + t^{-\alpha}).$$

De plus, pour tout $0 \leq \alpha < 1/2$, $0 \leq \beta < 1/2$, $0 < t \leq T$ et $x \in \mathcal{C}([0, 1])$, il existe une constante $C(T, \phi, x > 0)$ telle que

$$|(-A)^\alpha D^2 u(t, x) (-A)^\beta|_{\mathcal{L}(H)} \leq C(T, \phi, x)(1 + t^{-(\alpha+\beta)}).$$

Comme F est un polynôme et que nous n'avons pas de moments exponentiels pour la solution de l'équation (4.1), on ne peut pas utiliser directement les méthodes classiques. On introduit alors un opérateur de Kolmogorov modifié et on utilise les méthodes usuelles sur le semi-groupe associé - voir l'annexe du Chapitre 5.

Chapter 2

Weak backward error analysis for overdamped Langevin processes

1 Introduction

In [22], the authors give a weak backward error analysis for SDEs defined on the d -dimensional torus. The aim of this chapter is to extend the result of [22] to the overdamped Langevin process on \mathbb{R}^d .

In the last decades, backward error analysis has become a powerful tool to analyze the long time behavior of numerical schemes applied to evolution equations (see [37, 59, 76]). The main idea can be described as follows: Let us consider an ordinary differential equation of the form

$$\dot{y}(t) = f(y(t)),$$

where $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a smooth vector field, and denote by $\phi_t^f(y)$ the associated flow. By definition, a numerical method defines for a small time step δ an approximation Φ_δ of the exact flow ϕ_δ^f : We have for bounded $y \in \mathbb{R}^d$, $\Phi_\delta(y) = \phi_\delta^f(y) + \mathcal{O}(\delta^{r+1})$ where r is the order of the method.

The idea of backward error analysis is to show that Φ_δ can be interpreted as the exact flow $\phi_\delta^{f_\delta}$ of a modified vector field defined as a series in powers of δ

$$f_\delta = f + \delta^r f_r + \delta^{r+1} f_{r+1} + \dots,$$

where f_l , $l \geq r$ are vector fields depending on the numerical method. In general, the series defining f_δ does not converge, but it can be shown that for bounded y , we have for arbitrary N

$$\Phi_\delta(y) = \phi_\delta^{f_\delta^N}(y) + C_N \delta^{N+1},$$

where f_δ^N is the truncated series:

$$f_\delta^N = f + \delta^r f_r + \dots + \delta^N f_N.$$

Under some analytic assumptions, the constant $C_N \delta^{N+1}$ can be optimized in N , so that the error term in the previous equation can be made exponentially small with respect to δ .

Such a result is very important and has many applications in the case where f has some strong geometric properties, such as Hamiltonian (see [36, 37, 59, 71, 76]). In this situation, and under some compatibility conditions on the numerical method Φ_δ , the modified vector field f_δ inherits the structure of f .

More recently, these ideas have been extended in some situations to Hamiltonian PDEs : First in the linear case [23] and then in the semi linear case (nonlinear Schrödinger or

wave equations), see [29, 30].

We want to use this approach to have weak error behavior for long times for the stochastic differential equation:

$$dX(t) = -\nabla V(X(t))dt + dW(t), \quad (1.1)$$

where V and all its derivatives have at most polynomial growth at infinity. This equation is studied a lot in molecular dynamics: it describes the evolution of particles in a potential such that the corresponding canonical measure has several regions of high probability separated by low probability regions (see [60]) and the invariant measure associated to (1.1) represents the positions of the particles at equilibrium. This equation can also describe the blood clotting dynamics [48].

Error estimates on long times for elliptic and hypoelliptic SDEs have already been proved, especially in the case of explicit scheme. In [82,83], it is shown that for a sufficiently small time step the explicit Euler scheme defines an ergodic process and that the invariant measure of the Euler scheme is close to the invariant measure of the SDE. In [85], under the assumption of the existence of a unique invariant measure associated to the SDE, Talay and Tubaro have shown that the weak error and the invariant measure associated to the Euler scheme can be expanded in powers of the time step δ . Unfortunately, the assumptions on f and g used in [82,83,85] are restrictive and the results described in these papers are only valid for explicit schemes.

In [43,84], Higham, Mattingly, Stuart and Talay work with implicit schemes, but they need the time step to be small enough. In [43], under certain assumptions and in particular in the case of the overdamped Langevin equation, it is shown that for sufficiently small time step, two kinds of implicit schemes are ergodic processes. They also show that the invariant measures associated with these schemes converge to the invariant measure of the overdamped Langevin equation. In [84], Talay studies stochastic Hamiltonian system. He shows the exponential convergence of the solution associated to the Kolmogorov equation and, for a sufficiently small time step δ , an expansion with respect to δ of the invariant measure to the implicit scheme which is close to the invariant measure of the SDE.

In [64], a larger class of schemes is studied. It is shown that given an elliptic or hypoelliptic SDE defined on the d -dimensional torus, the ergodic averages provided by a class of implicit and explicit schemes are asymptotically close to the average of the invariant measure of the SDE. The authors also show an expansion in expectation of the invariant measure for any time-step.

In this chapter, we work on \mathbb{R}^d . Moreover, in our case V and all its derivatives are not bounded but have polynomial growth. If the coefficients of the SDEs are not globally Lipschitz continuous, it is known that classical explicit methods of weak approximation may result in unbounded solutions (see [45,46]). However, there exist weak explicit schemes and strong explicit schemes which give a good approximation for some SDEs with not globally Lipschitz continuous coefficients (see [46,70]). Also, in practice, people use explicit methods in computing averages (see [57]). However, since it is not possible in general to control the growth of the numerical solutions, we decide to work with implicit schemes.

The aim of this paper is, under assumptions on V , to show a weak backward error analysis result: We show an expansion with respect to the time step δ of $\mathbb{E}\phi(X_p)$ where X_p is an implicit scheme. The idea to extend the backward error analysis to SDEs has already been developed in [1, 22, 80, 89]. In [1], the authors use this approach to construct new methods of weak order two to approximate stochastic differential equations. In [22], the authors study SDEs defined on the d -dimensional torus and its approximation by the explicit Euler scheme. They show, without any restriction on the time step, an expansion

of $\mathbb{E}\phi(X_p)$ where X_p is the explicit Euler scheme. In [80], Shardlow considers SDEs with additive noise (g does not depend on X). He shows that it is possible to build a modified SDE associated with the Euler scheme, but only at the first step, i.e. for $N = 2$. In this case, he is able to write down a modified SDE:

$$d\tilde{X} = \tilde{f}(\tilde{X})dt + \tilde{g}(\tilde{X})dW,$$

such that

$$|\mathbb{E}(\phi(X_p)) - \mathbb{E}(\phi(\tilde{X}(p\delta)))| \leq c_1(\phi, T)\delta^2, \quad p = 0, \dots, \lfloor T/\delta \rfloor, \quad T > 0.$$

In [89], Zygalkis describes modified equations for SDEs with respect to weak convergence and gives applications of modified equations in the numerical study of some SDEs.

In this paper, we take the approach described in [22]. We show that the generator associated with the solution of the SDE (1.1) coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. It is known (see [10, 31]) that given $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ and denoting by $X_x(t)$ the solution of the SDE (1.1) satisfying $X(0) = x$, the function u defined for $t \geq 0$ and $x \in \mathbb{R}^d$ by $u(t, x) = \mathbb{E}(\phi(X_x(t)))$ satisfies the Kolmogorov equation

$$\partial_t u(t, x) = L(x)u(t, x), \quad x \in \mathbb{R}^d, \quad t \geq 0,$$

where $L := L(x)$ is the Kolmogorov operator associated with the SDE (1.1).

We show that with a numerical solution, we can associate a modified Kolmogorov operator of the form

$$\mathcal{L}(\delta, x) = L(x) + \delta L_1(x) + \delta^2 L_2(x) + \dots,$$

where L_l , $l \geq 1$ are some modified operators of order $2l + 2$. The series does not converge but we consider truncated series:

$$\mathcal{L}^{(N)}(\delta, x) = L(x) + \delta L_1(x) + \delta^2 L_2(x) + \dots + \delta^N L_N(x).$$

Note that this operator is no longer of order 2 and we can not define easily a solution to the modified equation

$$\partial_t v^N(t, x) = \mathcal{L}^{(N)}(\delta, x)v^N(t, x).$$

However, in our case, we can build a function $v^{(N)}$ such that

$$\| \mathbb{E}(\phi(X_p(\cdot))) - v^{(N)}(p\delta, \cdot) \|_{\mathcal{C}} \leq c_2(\phi, N)\delta^{N+1}, \quad p = 0, \dots, \lfloor T/\delta \rfloor, \quad T > 0,$$

where \mathcal{C} is an appropriate space and $X_p(x)$ is the p^{th} step of a scheme with initial condition x . As the constant c_2 does not depend on T , we have an approximation result also valid for long times. We also show that $v^{(N)}$ will converge exponentially fast in time to a constant.

The two main tools are the exponential convergence to equilibrium and the ellipticity of the Poisson equation, i.e. the equation $L(x)g = h$. The second tool is also used in [64].

In Section 2, we first introduce the SDE which we are interested in, state our assumptions and introduce the numerical schemes that we use. Then, we give some results on the Kolmogorov operator and on the solution of the Kolmogorov equation. In Section 3, we give an asymptotic expansion of the weak error over one step. In Section 4, we study the modified operator \mathcal{L} and its approximation. In Section 5, we analyze the long time behavior of $v^{(N)}$.

2 Preliminaries

2.1 Presentation of the SDE

Throughout this chapter, we use the following notation. We denote by $\mathbb{N} = \{0, 1, 2, \dots\}$ the set of nonnegative integers and $\mathbb{N}^* = \mathbb{N} \setminus \{0\}$. We write the scalar product of two vectors $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ and $y = (y_1, \dots, y_d) \in \mathbb{R}^d$ as

$$\langle x, y \rangle = \sum_{i=1}^d x_i y_i.$$

We identify the gradient of a function with its differential D . For $k \in \mathbb{N}$, $h = (h_1, \dots, h_k) \in \mathbb{R}^{k_d}$, $x \in \mathbb{R}^d$ and ϕ a function, we denote the differential of order k of ϕ at the point x and in the direction (h_1, \dots, h_k) by $D^k \phi(x) \cdot (h_1, \dots, h_k)$. For a multi-index $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d$, we set $|\mathbf{k}| = k_1 + \dots + k_d$ and for a function $\phi \in C^\infty(\mathbb{R}^d)$

$$\partial_{\mathbf{k}} \phi(x) = \frac{\partial^{|\mathbf{k}|} \phi(x)}{\partial^{k_1} x_1 \dots \partial^{k_d} x_d}, \quad x \in \mathbb{R}^d.$$

We also use the following notation

$$\begin{aligned} \mathcal{C}_{pol}^\infty(\mathbb{R}^d) &= \{f \in C^\infty(\mathbb{R}^d) \text{ such that } f \text{ and all its derivatives have polynomial growth}\} \\ &= \{f \in C^\infty(\mathbb{R}^d) \text{ such that for all } \mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d, \exists C_{\mathbf{k}} > 0, n_{\mathbf{k}} \in \mathbb{N}^* \\ &\quad \text{such that for all } x \in \mathbb{R}^d, |\partial_{\mathbf{k}} f(x)| \leq C_{\mathbf{k}}(1 + |x|^{n_{\mathbf{k}}})\}. \end{aligned}$$

Let $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbf{P})$, $t \geq 0$, be a filtered probability space and $W(t) = (W_1(t), \dots, W_d(t))$ be a d -dimensional $\{\mathcal{F}_t\}_{t \geq 0}$ -adapted standard Wiener process. We want to give a similar result to the result described in [22] for a process $X(t)$ on \mathbb{R}^d which solves the stochastic differential equation

$$dX(t) = -DV(X(t))dt + dW(t) \quad t > 0, \quad (2.1)$$

where the function V verifies the following conditions, called Assumptions **B**:

B-1: $V \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$.

B-2: *The function V is semi-convex: There exist a bounded function $V_1 \in C^\infty(\mathbb{R}^d)$ with bounded derivatives and a convex function $V_2 \in C^\infty(\mathbb{R}^d)$ such that $V = V_1 + V_2$.*

B-3: *There exist strictly positive real numbers β and κ such that*

$$\langle x, DV(x) \rangle \geq \beta|x|^2 - \kappa \quad \text{for all } x \in \mathbb{R}^d.$$

B-4: *For all $k \in \mathbb{N}$,*

$$\int_{\mathbb{R}^d} |x|^{2k} e^{-2V(x)} dx < \infty.$$

Remark 2.1 *Under these assumptions, the process $X(t)$ is well-defined for all $t > 0$ (see [10, 47, 77]).*

As a consequence of the semi-convexity of V (assumption B-2), we obtain the existence of a positive constant α , usually called the constant of semi-convexity, such that for all $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$

$$D^2V(x) \cdot (h, h) \geq -\alpha|h|^2. \quad (2.2)$$

We denote by $L := L(x)$ the Kolmogorov generator associated with the stochastic differential equation (2.1): for $\phi \in C^\infty$ and $x \in \mathbb{R}^d$

$$L(x)\phi(x) = \frac{1}{2} \sum_{i=1}^d \partial_{ii}\phi(x) - \sum_{i=1}^d \partial_i V(x) \partial_i \phi(x),$$

where we use the notation $\partial_i = \frac{\partial}{\partial x_i}$ and $\partial_{ij} = \frac{\partial^2}{\partial x_i \partial x_j}$ for $i, j \in \{1, \dots, d\}$.

We have the following result:

Proposition 2.2 *Let $x_0 \in \mathbb{R}^d$ and $(X(t))_{t \geq 0}$ satisfying (2.1) with $X(0) = x_0$. Under assumption B-3, for each $p \geq 1$ and $0 < \gamma < 2\beta$, there exists a positive constant C_p such that*

$$\forall t > 0, \quad \mathbb{E}|X(t)|^{2p} \leq C_p(|x_0|^{2p} \exp(-\gamma t) + 1) \quad (2.3)$$

Proof. Let $N \in \mathbb{N}^*$ be fixed. Let $x_0 \in \mathbb{R}^d$ be fixed such that $X(0) = x_0$. We consider $\tau_N = \inf\{t, \text{ such that } |X(t)| \geq N\}$.

Using dissipativity assumption B-3, we get for $x \in \mathbb{R}^d$

$$L(x)|x|^2 = -2\langle x, DV(x) \rangle + d \leq -2\beta|x|^2 + 2\kappa + d. \quad (2.4)$$

Now, we have all in hand to prove (2.3) and the following result by recursion: For $p \in \mathbb{N}^*$ and $0 < \gamma < 2\beta$, there exists a positive constant C_p such that for all $t \geq 0$

$$\mathbb{E}\left(\int_0^{t \wedge \tau_N} |X(s)|^{2p} \exp(\gamma s) ds\right) \leq C_p\left(|x_0|^{2p} + 1 + \mathbb{E}(\exp(\gamma(t \wedge \tau_N)))\right). \quad (2.5)$$

Let $0 < \gamma_1 < 2\beta$. We apply Itô's lemma to $|X(t)|^2 \exp(\gamma_1 t)$. Then we obtain for all $t \geq 0$

$$\begin{aligned} |X(t \wedge \tau_N)|^2 \exp(\gamma_1(t \wedge \tau_N)) &= |X(0)|^2 + \gamma_1 \int_0^{t \wedge \tau_N} |X(s)|^2 \exp(\gamma_1 s) ds \\ &\quad + \int_0^{t \wedge \tau_N} L(X(s))(|X(s)|^2) \exp(\gamma_1 s) ds + \int_0^{t \wedge \tau_N} 2X(s) \exp(\gamma_1 s) dW(s) \end{aligned}$$

since the Brownian motions W^1, \dots, W^d are independent.

Since $X(\cdot)$ is bounded on $[0, t \wedge \tau_N]$, the stochastic integral is a square integrable martingale. Thus, its average vanishes. Using (2.4), we get for all $t \geq 0$

$$\begin{aligned} \mathbb{E}\left(|X(t \wedge \tau_N)|^2 \exp(\gamma_1(t \wedge \tau_N))\right) &\leq |x_0|^2 + (\gamma_1 - 2\beta) \mathbb{E}\left(\int_0^{t \wedge \tau_N} |X(s)|^2 \exp(\gamma_1 s) ds\right) \\ &\quad + \mathbb{E}\left(\int_0^{t \wedge \tau_N} (2\kappa + d) \exp(\gamma_1 s) ds\right). \end{aligned} \quad (2.6)$$

Using $\gamma_1 < 2\beta$, we get for all $t \geq 0$

$$\mathbb{E}\left(|X(t \wedge \tau_N)|^2 \exp(\gamma_1(t \wedge \tau_N))\right) \leq |x_0|^2 + \frac{2\kappa + d}{\gamma_1} \mathbb{E}(\exp(\gamma_1(t \wedge \tau_N))).$$

Using Fatou's lemma on the left hand side and Monotone convergence theorem on the right hand side, we obtain for $t \geq 0$

$$\mathbb{E}\left(|X(t)|^2\right) \exp(\gamma_1 t) \leq |x_0|^2 + \frac{2\kappa + d}{\gamma_1} \exp(\gamma_1 t).$$

Thus, the result (2.3) is proved for $p = 1$. Using (2.6) and $\gamma_1 < 2\beta$, we get for $t \geq 0$

$$(2\beta - \gamma_1)\mathbb{E}\left(\int_0^{t \wedge \tau_N} (|X(s)|^2) \exp(\gamma_1 s) ds\right) \leq |x_0|^2 + \frac{2\kappa + d}{\gamma_1} \mathbb{E}\left(\exp(\gamma_1(t \wedge \tau_N))\right).$$

Hence, the result (2.5) follows in case of $p = 1$.

Let us now proceed inductively. We assume that (2.3) and (2.5) hold true for $p - 1$. We use the same ideas as above in order to prove (2.3) and (2.5) for p .

Let $0 < \gamma_1 < 2\beta$. We apply the Itô's lemma to $\exp(\gamma_1 t)|X(t)|^{2p}$. The average of the stochastic integral vanishes. Using (2.4) and the two following relations: for all $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$,

$$D|x|^{2p} \cdot h = 2p\langle x, h \rangle |x|^{2(p-1)}$$

and

$$D^2|x|^{2p} \cdot (h, h) = 2|x|^{2(p-1)}|h|^2 + 4p(p-1)|\langle x, h \rangle|^2 |x|^{2(p-2)},$$

we obtain for $t \geq 0$

$$\mathbb{E}\left(\exp(\gamma_1(t \wedge \tau_N))|X(t \wedge \tau_N)|^{2p}\right) \tag{2.7}$$

$$\begin{aligned} &= \mathbb{E}\left(|X(0)|^{2p}\right) + \gamma_1 \mathbb{E}\left(\int_0^{t \wedge \tau_N} \exp(\gamma_1 s) |X(s)|^{2p} ds\right) \\ &\quad + p \mathbb{E}\left(\int_0^{t \wedge \tau_N} \exp(\gamma_1 s) L(X(s)) \left(|X(s)|^2\right) |X(s)|^{2(p-1)} ds\right) \\ &\quad + 2p(p-1) \mathbb{E}\left(\int_0^{t \wedge \tau_N} \exp(\gamma_1 s) |X(s)|^{2(p-1)} ds\right) \\ &\leq |x_0|^{2p} + (\gamma_1 - 2\beta p) \mathbb{E}\left(\int_0^{t \wedge \tau_N} \exp(\gamma_1 s) |X(s)|^{2p} ds\right) \\ &\quad + p(2(p-1) + 2\kappa + d) \mathbb{E}\left(\int_0^{t \wedge \tau_N} \exp(\gamma_1 s) |X(s)|^{2(p-1)} ds\right). \end{aligned} \tag{2.8}$$

Thus, by induction, we get for $t \geq 0$

$$\begin{aligned} &\mathbb{E}\left(\exp(\gamma_1(t \wedge \tau_N))|X(t \wedge \tau_N)|^{2p}\right) \\ &\leq |x_0|^{2p} + p(2(p-1) + 2\kappa + d)C_{p-1} \left(|x_0|^{2(p-1)} + 1 + \mathbb{E}\left(\exp(\gamma_1(t \wedge \tau_N))\right)\right) \end{aligned}$$

Using Fatou's lemma on the left hand side and Monotone convergence theorem on the right hand side, we obtain for $t \geq 0$

$$\begin{aligned} \mathbb{E}\left(|X(t)|^{2p}\right) \exp(\gamma_1 t) &\leq |x_0|^{2p} + p(2(p-1) + 2\kappa + d)C_{p-1} \left(|x_0|^{2(p-1)} + 1 + \exp(\gamma_1 t)\right) \\ &\leq C_p \left(|x_0|^{2p} + 1 + \exp(\gamma_1 t)\right). \end{aligned}$$

Thus, we have shown (2.3) for p .

Using (2.7) and the induction hypothesis, we get for $t \geq 0$

$$\mathbb{E}\left(\int_0^{t \wedge \tau_N} |X(s)|^{2p} \exp(\gamma_1 s) ds\right) \leq C \left(|x_0|^{2p} + 1 + \mathbb{E}\left(\exp(\gamma_1(t \wedge \tau_N))\right)\right).$$

The result (2.5) follows for p which completes the proof. \blacklozenge

Remark 2.3 Another proof of Proposition 2.2 can be found in [43] or [44].

2.2 Numerical schemes

The ordinary Euler scheme may be unstable when the coefficients of the differential equation (2.1) are unbounded (see [43]). We are led to avoid explicit schemes. In fact, we study two different implicit schemes. For a small time step $\delta > 0$ and $x \in \mathbb{R}^d$, we consider an implicit split-step scheme defined by $X_0 = x$ and for $n \in \mathbb{N}$

$$\begin{cases} X_n^* &= X_n - \delta DV(X_n^*), \\ X_{n+1} &= X_n^* + W((n+1)\delta) - W(n\delta) = X_n^* + \sqrt{\delta}\eta_n, \end{cases} \quad (2.9)$$

where $\eta_n = {}^t(\eta_{n,1}, \dots, \eta_{n,d})$ is a \mathbb{R}^d -valued random variable and $\{\eta_{n,i} : n \in \mathbb{N}, i \in \{1, \dots, d\}\}$ is a collection of i.i.d. real-valued random variables satisfying $\eta_{1,1} \sim \mathcal{N}(0, 1)$. The strong convergence of the implicit split-step scheme in our case has already been studied (see [44]). We also consider the implicit Euler scheme defined by $X_0 = x$ and for $n \in \mathbb{N}$

$$X_{n+1} = X_n - DV(X_{n+1})\delta + \sqrt{\delta}\eta_n, \quad (2.10)$$

where $\eta_n = {}^t(\eta_{n,1}, \dots, \eta_{n,d})$ is as above.

The following Lemma shows that these two schemes are well-defined for $\delta < \delta_0 = \frac{1}{\alpha}$, where α is the constant of semi-convexity of V .

Lemma 2.4 *Let $x \in \mathbb{R}^d$ and $\delta < \delta_0 = \frac{1}{\alpha}$. Under assumptions B, there exists a unique $y \in \mathbb{R}^d$ such that $y = x - \delta DV(y)$.*

Proof. Let $x \in \mathbb{R}^d$. Let $P : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be defined for $z \in \mathbb{R}^d$ by $P(z) = z - x + \delta DV(z)$. We have that $P \in C^\infty$. Using dissipativity assumption B-3, we obtain

$$\langle P(z), z \rangle = |z|^2 - \langle x, z \rangle + \delta \langle DV(z), z \rangle \geq (1 + \beta\delta)|z|^2 - \kappa\delta - \langle x, z \rangle.$$

Thus, for $|z|^2$ large enough, we conclude that $\langle P(z), z \rangle > 0$. Then, using a Corollary of Brouwer fixed-point Theorem (see for instance [62]), we have that there exists $y \in \mathbb{R}^d$ such that $P(y) = 0$. Therefore, we have shown the existence of $y \in \mathbb{R}^d$ such that $y = x - \delta DV(y)$. Let us show the uniqueness.

Let $\delta < \delta_0 = \frac{1}{\alpha}$, $y \in \mathbb{R}^d$ and $z \in \mathbb{R}^d$ such that $P(z) = P(y) = 0$ and $y \neq z$. We have

$$y - z = -\delta(DV(y) - DV(z)).$$

Due to assumption of semi-convexity (B-2), we get

$$|y - z|^2 = -\delta \int_0^1 D^2V(y + t(z - y)) \cdot (y - z, y - z) dt \leq \delta\alpha|y - z|^2 < |y - z|^2$$

and as a consequence $y = z$. ♦

Remark 2.5 *The condition $\delta < \frac{1}{\alpha}$ is necessary only in the uniqueness part of the proof. We have the existence for all $\delta > 0$. Moreover, in the case where V is convex, the inequality on the second derivative (2.2) hold true for all $\alpha \geq 0$ and therefore we can show the uniqueness for all $\delta > 0$. Another proof can be found in [44].*

Proposition 2.6 *Let $\delta < \delta_0 := \frac{1}{\alpha}$, where α is the constant of semi-convexity of V . Under assumptions B, the implicit split-step scheme (2.9) and the implicit Euler scheme (2.10) satisfy:*

$$\forall p \in \mathbb{N}, \quad \exists C_p(\delta_0) \text{ such that } \forall n \in \mathbb{N}, \quad \mathbb{E}(|X_n|^{2p}) < C_p(\delta_0)(1 + |x|^{2p}). \quad (2.11)$$

Proof. We start by showing that the implicit split-step scheme has moments of all order. The proof in the case of the implicit Euler scheme (2.10) is similar.

Let $p \in \mathbb{N}^*$ and $n \in \mathbb{N}^*$ be fixed. As $x \mapsto |x|^{2p}$ is convex, it holds for all $x \in \mathbb{R}^d$ and $y \in \mathbb{R}^d$

$$|x + y|^{2p} \geq |x|^{2p} + 2p|x|^{2(p-1)}\langle x, y \rangle$$

so

$$|X_n|^{2p} = |X_n^* + \delta DV(X_n^*)|^{2p} \geq |X_n^*|^{2p} + 2p\delta\langle X_n^*, DV(X_n^*) \rangle |X_n^*|^{2(p-1)}.$$

Using dissipativity assumption B-3, we get

$$|X_n|^{2p} \geq (1 + 2p\delta\beta)|X_n^*|^{2p} - 2p\kappa\delta|X_n^*|^{2(p-1)}.$$

Let $\ell \in \mathbb{N}^*$ and $\varepsilon > 0$, then there exists $C_\varepsilon > 0$ such that for any $x \in \mathbb{R}^d$

$$|x|^{2(\ell-1)} \leq \varepsilon|x|^{2\ell} + C_\varepsilon. \quad (2.12)$$

Using (2.12) for $\ell = p$ and $\varepsilon = \frac{\beta}{2\kappa}$, we get

$$|X_n|^{2p} \geq (1 + p\beta\delta)|X_n^*|^{2p} - \delta C. \quad (2.13)$$

Moreover, we have

$$\begin{aligned} |X_{n+1}|^{2p} &= \left(|X_n^*|^2 + 2\sqrt{\delta}\langle X_n^*, \eta_n \rangle + \delta|\eta_n|^2 \right)^p \\ &= \sum_{i+j+k=p} \frac{2^j p!}{i!j!k!} |X_n^*|^{2i} \langle X_n^*, \eta_n \rangle^j |\eta_n|^{2k} \delta^{k+j/2} \\ &= |X_n^*|^{2p} + \sum_{\substack{i+2j+k=p \\ i \neq p}} \frac{2^{2j} p!}{i!(2j)!k!} |X_n^*|^{2i} \langle X_n^*, \eta_n \rangle^{2j} |\eta_n|^{2k} \delta^{k+j} \\ &\quad + \sum_{\substack{i+2j+1+k=p \\ i \neq p}} \frac{2^{2j+1} p!}{i!(2j+1)!k!} |X_n^*|^{2i} \langle X_n^*, \eta_n \rangle^{2j} |\eta_n|^{2k} \langle X_n^*, \eta_n \rangle \delta^{k+j+1/2} \\ &:= |X_n^*|^{2p} + A + B. \end{aligned}$$

Note that each term in B is a product of an odd number of $\eta_{n,i}$. Hence, using the fact that for $i \in \{1, \dots, d\}$ $\eta_{n,i}$ is independent of X_n^* and $\eta_{n,j}$ for $i \neq j$ and that the moments of odd order of $\eta_{n,i}$ vanish, we have $\mathbb{E}(B) = 0$.

Let $i, j, k \in \mathbb{N}^*$, if $i + 2j + k = p$ and $i \neq p$ then $i + j < p$ and $j \neq 0$ or $k \neq 0$. Let $\varepsilon > 0$, using properties of η_n and (2.12), we also have for $i + 2j + k = p$ and $i \neq p$

$$\begin{aligned} \mathbb{E}\left(|X_n^*|^{2i} \langle X_n^*, \eta_n \rangle^{2j} |\eta_n|^{2k}\right) &\leq C\mathbb{E}\left(|X_n^*|^{2(j+i)}\right) \\ &\leq \varepsilon\mathbb{E}\left(|X_n^*|^{2p}\right) + C_\varepsilon \end{aligned}$$

and

$$\mathbb{E}(A) \leq \delta C_{p,d}(\delta_0)(\varepsilon\mathbb{E}|X_n^*|^{2p} + C_\varepsilon).$$

Then, using (2.13), we get

$$\begin{aligned} \mathbb{E}|X_{n+1}|^{2p} &\leq \mathbb{E}|X_n^*|^{2p} + \delta C_{p,d}(\delta_0)\varepsilon\mathbb{E}|X_n^*|^{2p} + \delta C_{p,d}(\delta_0)C_\varepsilon \\ &\leq \frac{1 + \delta C_{p,d}(\delta_0)\varepsilon}{1 + p\delta\beta}\mathbb{E}|X_n|^{2p} + \delta C. \end{aligned}$$

If $\varepsilon < \frac{p\beta}{C_{p,d}(\delta_0)}$, we obtain by induction on n

$$\begin{aligned} \mathbb{E}|X_n|^{2p} &\leq \left(\frac{1 + \delta C_{p,d}(\delta_0)\varepsilon}{1 + 2p\delta\beta} \right)^n |x|^{2p} + \delta \sum_{i=0}^{n-1} \left(\frac{1 + \delta C_{p,d}(\delta_0)\varepsilon}{1 + 2p\delta\beta} \right)^i C \\ &\leq |x|^{2p} + C(1 + |x|^{2(p-1)}) \\ &\leq C_p(\delta_0)(1 + |x|^{2p}). \end{aligned}$$

◆

2.3 Main result

Before giving the main result, we will introduce some notations and give some results on the Kolmogorov generator L . In particular, we will describe the two important properties that we need to prove our main result.

We will use the following notation for $k \in \mathbb{N}$ and $l \in \mathbb{N}$

$$\begin{aligned} \mathcal{C}_k^l(\mathbb{R}^d) := \{ \phi \in C^l(\mathbb{R}^d) \text{ such that } \exists C_{l,k} > 0 \text{ such that for all } x \in \mathbb{R}^d \text{ and } \mathbf{j} \in \mathbb{N}^d, |\mathbf{j}| \leq l, \\ |\partial_{\mathbf{j}}\phi(x)| \leq C_{l,k}(1 + |x|^k) \}. \end{aligned}$$

Let $\psi \in \mathcal{C}_k^l(\mathbb{R}^d)$, we define the following norm

$$\|\psi\|_{l,k} := \sup_{\substack{\mathbf{j}=(j_1,\dots,j_d), |\mathbf{j}|\leq l \\ x \in \mathbb{R}^d}} (|\partial_{\mathbf{j}}\psi(x)|(1 + |x|^k)^{-1}),$$

and the semi-norm

$$|\psi|_{l,k} := \sup_{\substack{\mathbf{j}=(j_1,\dots,j_d), 1 \leq |\mathbf{j}| \leq l \\ x \in \mathbb{R}^d}} (|\partial_{\mathbf{j}}\psi(x)|(1 + |x|^k)^{-1}).$$

We recall that we denoted by L the Kolmogorov generator associated with the stochastic differential equation (2.1): it is defined for $\phi \in C^\infty(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$ by

$$L(x)\phi(x) = \frac{1}{2} \sum_{i=1}^d \partial_{ii}\phi(x) - \sum_{i=1}^d \partial_i V(x) \partial_i \phi(x) = \frac{1}{2} e^{2V(x)} \sum_{i=1}^d \partial_i (e^{-2V(x)} \partial_i \phi(x)). \quad (2.14)$$

Moreover, its formal adjoint in $L^2(\mathbb{R}^d)$ is given for $\phi \in C^\infty(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$ by

$$L^\top(x)\phi(x) = \sum_{i=1}^d \partial_{ii}V(x)\phi(x) + \frac{1}{2} \sum_{i=1}^d \partial_{ii}\phi(x) + \sum_{i=1}^d \partial_i V(x) \partial_i \phi(x).$$

We consider $\rho = \frac{1}{Z} e^{-2V}$ where $Z = \int_{\mathbb{R}^d} e^{-2V(x)} dx$. It is classical to prove that the measure $\rho(x)dx =: d\rho$ is invariant by P_t and that for any $x \in \mathbb{R}^d$, $L^\top(x)\rho(x) = 0$.

We also define the formal adjoint L^* of L in $L^2(\rho)$. We have the useful equality:

$$L^* = L.$$

Indeed, let ψ and ϕ be two C^∞ -functions with compact support. Using (2.14), we have by integration by parts:

$$\begin{aligned} \int_{\mathbb{R}^d} \phi(x)L(x)\psi(x)\rho(x)dx &= -\frac{1}{2Z} \int_{\mathbb{R}^d} e^{-2V(x)}(D\phi(x), D\psi(x))dx \\ &= \int_{\mathbb{R}^d} \psi(x)L(x)\phi(x)\rho(x)dx, \end{aligned} \quad (2.15)$$

which can be easily extended to ψ and ϕ in $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$.

We will now establish two preliminary results which are necessary in order to prove our main result.

For $x \in \mathbb{R}^d$, we denote by $(X_x(t))_{t \geq 0}$ a process which solves (2.1) with $X_x(0) = x$ (see Remark 2.1). From now on, $(P_t)_{t \geq 0}$ is the transition semigroup associated with the Markov process $(X_x(t))_{t \geq 0}$. We consider a function $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and we set, for all $x \in \mathbb{R}^d$ and $t \geq 0$,

$$u(t, x) = \mathbb{E}(\phi(X_x(t))) = P_t\phi(x). \quad (2.16)$$

This is well defined thanks to Proposition 2.2. It is a classical result that u is a C^∞ function of $(t, x) \in \mathbb{R}^+ \times \mathbb{R}^d$. Moreover, one can show that $u \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ (see Appendix). Using this result and Itô's formula, it is possible to show that u is the unique solution of the Kolmogorov equation (see [10] for more details):

$$\frac{d}{dt}u(t, x) = L(x)u(t, x), \quad x \in \mathbb{R}^d, \quad t > 0, \quad u(0, x) = \phi(x), \quad x \in \mathbb{R}^d. \quad (2.17)$$

Note that we use the standard identification $u(t) = u(t, \cdot)$.

The first property is the existence of a solution to the Poisson equation associated with the operator L . Under assumptions B, the following Lemma holds true (see e.g. [74]).

Lemma 2.7 *Let $h \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that $\int_{\mathbb{R}^d} h(x)\rho(x)dx = 0$. Then, there exists a unique function $g \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that*

$$Lg = h \quad \text{and} \quad \int_{\mathbb{R}^d} g(x)\rho(x)dx = 0. \quad (2.18)$$

The second property is the exponential convergence to 0 of u , the solution of (2.17), and its derivatives in an appropriate space:

Proposition 2.8 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that $\int_{\mathbb{R}^d} \phi(x)\rho(x)dx = 0$. Let u be the solution of (2.17). There exists a constant $\lambda > 0$ such that for each $k \in \mathbb{N}$, there exist integers n_k and $m_k \geq n_k$ and $C_k > 0$ such that $\phi \in \mathcal{C}_{n_k}^k(\mathbb{R}^d)$ and we have the following estimate: for all $t \geq 0$ and $x \in \mathbb{R}^d$*

$$|D^k u(t, x)| \leq C_k \|\phi\|_{k, n_k} e^{-\lambda t} (1 + |x|^{m_k}). \quad (2.19)$$

The proof of this proposition can be found in the appendix.

Remark 2.9 *Lemma 2.7 is a consequence of Proposition 2.8. Indeed, it is known that the unique solution of (2.18) is defined by*

$$g(x) = \int_0^\infty \mathbb{E}(h(X_x(t)))dt.$$

Our main result can be stated as follows:

Theorem 2.10 *Let X_p be the discrete process defined by the implicit Euler scheme (2.10) or the implicit split-step scheme (2.9). Let N and n_N be fixed. Let $\delta_0 = \frac{1}{\alpha}$ where α is the constant of semi-convexity of V . Then, for all $\delta < \delta_0$, there exists a modified function*

$$\mu^N = 1 + \sum_{n=1}^N \delta^n \mu_n$$

such that $\mu^N \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and

$$\int_{\mathbb{R}^d} \mu^N(x) \rho(x) dx = 1.$$

Moreover, for all functions $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d) \cap \mathcal{C}_{n_N}^{6N+8}(\mathbb{R}^d)$, there exist $C_N > 0$, $k_N \in \mathbb{N}^*$ and a positive polynomial function P_N satisfying the following: For all $p \in \mathbb{N}$ and $x \in \mathbb{R}^d$,

$$|\mathbb{E}\phi(X_p) - \int_{\mathbb{R}^d} \phi(y) \mu^N(y) \rho(y) dy| \leq \left(e^{-\lambda t_p} P_N(t_p) + C_N \delta^{N+1} \right) (1 + |x|^{k_N}) \|\phi - \langle \phi \rangle\|_{6N+8, n_N},$$

where $t_p = p\delta$, $\langle \phi \rangle = \int \phi d\rho$, $X_0 = x$ and $\lambda > 0$ is defined in Proposition 2.8.

The constant C_N appearing in the above estimate depends on N , the semi-convexity constant α , the polynomial growth of V and all its derivatives.

This result can be viewed as a discrete version of the Proposition 2.8 in the case $k = 0$. We have for X_p , the discrete process defined by (2.10) or (2.9), that $\mathbb{E}\phi(X_p)$ which is an approximation of u , has the same property as u : $\mathbb{E}\phi(X_p)$ converges exponentially fast to a constant in $\mathcal{C}_{k_N}^0(\mathbb{R}^d)$ up to an error $\delta^{N+1} C_N$ with the same rate as u . At a fixed p and a fixed $\delta < \delta_0 := \frac{1}{\alpha}$, where α is the constant of semi-convexity of V , fixed, we can optimize this error with a good choice of N .

Our result can be compared with [22, 64, 82, 83]. As in [22, 64], the only assumption made on δ is that $\delta < \delta_0$. In the case of V convex, we do not need to choose δ smaller than δ_0 , it is only necessary that $\delta < \delta_1$ where δ_1 is any fixed number. We also recover an expansion of the invariant measure as in [85]. Although our result is similar to the one established in [22] for the case of SDEs on the torus, we point out that the proofs of [22] are not all applicable in our case and hence our methods are different.

To prove Theorem 2.10, we will proceed in several steps. In Section 3, we give an asymptotic expansion of the weak error for the first step. Then, we use this expansion to build a modified operator $\mathcal{L}^{(N)}$ and a function $v^{(N)}$ such that the weak error at the first step and $v^{(N)}$ are close to an error δ^{N+1} (Section 4). In Section 5, using Lemma 2.7, we build the modified function μ^N and, using Proposition 2.8, we show the exponential convergence of $v^{(N)}$ to a constant depending of μ^N . Finally, using Markov property and Proposition 2.6, we complete the proof of Theorem 2.10.

3 Asymptotic expansion of the weak error

We now examine in detail the first time step and its approximation properties in terms of the law. By the Markov property, it is sufficient to obtain information for all the steps. It is easy to have an expansion of u . Indeed, by Taylor expansion in time, we have the formal expansion for small t and $x \in \mathbb{R}^d$:

$$u(t, x) = \phi(x) + tL(x)\phi(x) + \frac{t^2}{2}L^2(x)\phi(x) + \dots + \frac{t^n}{n!}L^n(x)\phi(x) + \dots$$

Since the solution $u(t)$ of the Kolmogorov equation is in $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, the above formal expansion can be justified in $L^2(\rho) = \{f : \mathbb{R}^d \rightarrow \mathbb{R}, \int |f|^2 d\rho < \infty\}$. Indeed, we have the following easy result whose proof is left to the reader.

Proposition 3.1 *Let $\delta_1 > 0$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$. Then, for all N , there exist a constant $C(N, \phi)$ and an integer n_1 which depends of N and of the polynomial growth of V , ϕ and their derivatives such that for all $\delta < \delta_1$,*

$$\left| u(\delta, x) - \sum_{n=0}^N \frac{\delta^n}{n!} L^n(x) \phi(x) \right| \leq C(N, \phi) \delta^{N+1} (1 + |x|^{n_1}).$$

We would like to have an expansion similar to the last Proposition in case of process defined by the implicit Euler scheme (2.10) or the implicit split-step scheme (2.9). Towards this end, we first need an asymptotic expansion for X_1 and then, using Taylor expansions, we get the following Proposition:

Proposition 3.2 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, $\delta < \delta_0$ and $x_0 \in \mathbb{R}^d$ such that $X_0 = x_0$. For all $n \geq 1$, there exist differential operators A_n of order $2n$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that for all integer $N \geq 1$, there exist $C_N > 0$ and $k \in \mathbb{N}$ such that for any $x \in \mathbb{R}^d$*

$$\left| \mathbb{E} \phi(X_1) - \sum_{n=0}^N \delta^n A_n(x_0) \phi(x_0) \right| \leq C_N \delta^{N+1} (1 + |x_0|^k) |\phi|_{2N+2, \ell_{2N+2}}, \quad (3.1)$$

where ℓ_{2N+2} is such that $\phi \in \mathcal{C}_{\ell_{2N+2}}^{2N+2}(\mathbb{R}^d)$. Moreover $A_0 = I$ and $A_1 = L$.

Remark 3.3 *The integer k depends on N , ℓ_{2N+2} and the polynomial growth of V and its derivatives such that $\forall \delta < \delta_0 := \frac{1}{\alpha}$, where α is the semi-convexity constant of V . This result is similar to the asymptotic expansion of the weak error described in [22], however, we cannot use the same proof. Indeed, we cannot use Itô's formula because the schemes considered here are implicit.*

First, we consider the implicit split-step scheme (2.9). Let $\delta < \frac{1}{\alpha}$ be fixed and $x \in \mathbb{R}^d$ be fixed such that $X_0 = X(0) = x$.

Before proving Proposition 3.2, we need an asymptotic expansion for $X_0^* = x - \delta DV(X_0^*)$. We define the function Ψ_δ which associates to $z \in \mathbb{R}^d$ the solution $y \in \mathbb{R}^d$ of $y = z - \delta DV(y)$. The function Ψ_δ is well defined (see Lemma 2.4). Then, by definition of x , we have $X_0^* = \Psi_\delta(x)$. Moreover, we have that $(\delta, z) \mapsto \Psi_\delta(z)$ is C^∞ on $]0, \frac{1}{\alpha}[\times \mathbb{R}^d$. Indeed, let the function f defined on $\Omega_1 =]0, \frac{1}{\alpha}[\times \mathbb{R}^d \times \mathbb{R}^d$ by

$$f(\delta, z, y) = z - \delta DV(y) - y,$$

using the assumption of semi-convexity B-2, we have, for all $(\delta, z, y) \in \Omega_1$, that $D_y f(\delta, z, y)$ is invertible. Then, by implicit function Theorem, we have that $(\delta, z) \mapsto \Psi_\delta(z)$ is C^∞ on a neighborhood of each $(\delta, z) \in]0, \frac{1}{\alpha}[\times \mathbb{R}^d$.

We have the following lemma:

Lemma 3.4 *Let $x \in \mathbb{R}^d$ such that $X_0 = x$. We have, for $\delta < \frac{1}{\alpha}$,*

$$\forall N_0 \in \mathbb{N}, \quad X_0^* = y = \Psi_\delta(x) = x + \sum_{k=1}^{N_0} \delta^k d_k(x) + \delta^{N_0+1} R_{N_0+1}(x, \delta), \quad (3.2)$$

where $\forall k \geq 1$, $d_k \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ is defined for all $z \in \mathbb{R}^d$ by

$$d_1(z) = -DV(z), \quad \forall k \geq 2, \quad d_k(z) = - \sum_{i=1}^{k-1} \frac{1}{i!} \sum_{\substack{k_1 + \dots + k_i = k-1, \\ k_j \geq 1}} D^{i+1} V(z) \cdot (d_{k_1}(z), \dots, d_{k_i}(z))$$

and, for any $N \in \mathbb{N}$, R_{N+1} verifies: There exist $C > 0$ and $\ell_N \in \mathbb{N}$ such that for any $z \in \mathbb{R}^d$ and $\delta < \frac{1}{\alpha}$,

$$|R_{N+1}(z, \delta)| \leq C(1 + |z|^{\ell_N}). \quad (3.3)$$

Proof. We previously showed that $(\delta, x) \mapsto \Psi_\delta(x)$ is C^∞ on $]0, \frac{1}{\alpha}[\times \mathbb{R}^d$. Then, let $x \in \mathbb{R}^d$ fixed, we have that $d_k(x)$ is the k^{th} term of the Taylor expansion of $\delta \mapsto \Psi_\delta(x)$ and we can write (3.2). We now search an expression for d_k .

Let $x \in \mathbb{R}^d$ such that $X_0 = x$ and $y = X_0^*$. Let N_0 and $\delta < \frac{1}{\alpha}$ be fixed. We use the temporary notation, for all $1 \leq k \leq N_0$, $g_k = d_k$ and $g_{N_0+1} = R_{N_0+1}$. Using Taylor expansion and

$$y = x + \delta R_1(x, \delta) = x + \sum_{k=1}^{N_0+1} \delta^k g_k(x),$$

we obtain

$$\begin{aligned} DV(y) &= DV(x + \delta R_1(x, \delta)) \\ &= DV(x) + \sum_{n=1}^{N_0-1} \frac{1}{n!} D^{n+1}V(x) \cdot (\delta R_1(x, \delta), \dots, \delta R_1(x, \delta)) + \Theta_{N_0}(x) \\ &= DV(x) + \sum_{n=1}^{N_0-1} \frac{1}{n!} D^{n+1}V(x) \cdot \left(\sum_{k=1}^{N_0+1} \delta^k g_k(x), \dots, \sum_{k=1}^{N_0+1} \delta^k g_k(x) \right) + \Theta_{N_0}(x) \\ &= DV(x) + \sum_{n=1}^{N_0-1} \frac{1}{n!} \sum_{m=n}^{n(N_0+1)} \delta^m \sum_{\substack{k_1+\dots+k_n=m, \\ 1 \leq k_i \leq N_0+1}} D^{n+1}V(x) \cdot (g_{k_1}(x), \dots, g_{k_n}(x)) + \Theta_{N_0}(x) \\ &= DV(x) + I_1(x) + I_2(x) + \Theta_{N_0}(x), \end{aligned}$$

where

$$\begin{aligned} \Theta_{N_0}(x) &= \delta^{N_0} \int_0^1 \frac{(1-t)^{N_0-1}}{(N_0-1)!} D^{N_0+1}V(x + t\delta R_1(x, \delta)) \cdot (R_1(x, \delta), \dots, R_1(x, \delta)) dt, \\ I_1(x) &= \sum_{n=1}^{N_0-1} \frac{1}{n!} \sum_{m=n}^{N_0-1} \delta^m \sum_{\substack{k_1+\dots+k_n=m, \\ 1 \leq k_i \leq N_0}} D^{n+1}V(x) \cdot (d_{k_1}(x), \dots, d_{k_n}(x)) \\ &= \sum_{m=1}^{N_0-1} \delta^m \sum_{n=1}^m \frac{1}{n!} \sum_{\substack{k_1+\dots+k_n=m, \\ 1 \leq k_i \leq N_0}} D^{n+1}V(x) \cdot (d_{k_1}(x), \dots, d_{k_n}(x)), \\ I_2(x) &= \sum_{n=1}^{N_0-1} \frac{1}{n!} \sum_{m=N_0}^{n(N_0+1)} \delta^m \sum_{\substack{k_1+\dots+k_n=m, \\ 1 \leq k_i \leq N_0+1}} D^{n+1}V(x) \cdot (g_{k_1}(x), \dots, g_{k_n}(x)). \end{aligned}$$

Hence, we get

$$DV(y) = DV(x) + I_1(x) + \delta^{N_0} g(\delta, x),$$

and

$$y = x - \delta DV(y) = x - \delta DV(x) - \delta I_1(x) - \delta^{N_0+1} g(\delta, x), \quad (3.4)$$

where

$$g(\delta, x) = \int_0^1 \frac{(1-t)^{N_0-1}}{(N_0-1)!} D^{N_0+1} V(x+t\delta R_1(x, \delta)) \cdot (R_1(x, \delta), \dots, R_1(x, \delta)) dt \\ + \sum_{n=1}^{N_0-1} \frac{1}{n!} \sum_{m=N_0}^{n(N_0+1)} \delta^{m-N_0} \sum_{\substack{k_1+\dots+k_n=m, \\ 1 \leq k_i \leq N_0+1}} D^{n+1} V(x) \cdot (g_{k_1}(x), \dots, g_{k_n}(x)).$$

Thus, by identifying (3.2) and (3.4) and using the expression of I_1 above, we obtain for all $x \in \mathbb{R}^d$,

$$d_1(x) = -DV(x), \quad \forall k \geq 2, \quad d_k(x) = - \sum_{i=1}^{k-1} \frac{1}{i!} \sum_{k_1+\dots+k_i=k-1, k_j \geq 1} D^{i+1} V(x) \cdot (d_{k_1}(x), \dots, d_{k_i}(x)).$$

Moreover, by induction, we have for all $k \geq 1$, $d_k \in C_{pol}^\infty(\mathbb{R}^d)$ and $\int d_k d\rho < \infty$. The above identifying does not give an easy expression of R_{N_0+1} , then we have not immediately (3.3). To show this result, we will use that, for N fixed, R_N is the remainder of order N of $\delta \mapsto \Psi_\delta(x)$. Therefore, if we show that for $n \in \mathbb{N}$, there exist $C > 0$ and $p_n \in \mathbb{N}$ such that for $\delta < \frac{1}{\alpha}$ and $x \in \mathbb{R}^d$,

$$|\partial_\delta^n \Psi_\delta(x)|^2 \leq C(1 + |x|^{p_n}), \quad (3.5)$$

then we show (3.3) and Lemma 3.4 is shown.

Let $x \in \mathbb{R}^d$ and $\delta < \frac{1}{\alpha}$ be fixed. Let us show (3.5) by induction on n . We have, by definition of $\Psi_\delta(x)$,

$$x = \Psi_\delta(x) + \delta DV(\Psi_\delta(x)).$$

Then, multiplying by $\Psi_\delta(x)$ and using dissipativity assumption B-3, we get

$$\langle x, \Psi_\delta(x) \rangle = |\Psi_\delta(x)|^2 + \delta \langle DV(\Psi_\delta(x)), \Psi_\delta(x) \rangle \geq (1 + \beta\delta) |\Psi_\delta(x)|^2 - \kappa\delta.$$

Using

$$2\langle a, b \rangle \leq \varepsilon |a|^2 + \frac{1}{\varepsilon} |b|^2, \quad \text{for } a \in \mathbb{R}^d, b \in \mathbb{R}^d, \varepsilon > 0, \quad (3.6)$$

we have

$$|\Psi_\delta(x)|^2 (1 + \beta\delta - \frac{\varepsilon}{2}) \leq \frac{1}{2\varepsilon} |x|^2 + \kappa\delta.$$

Taking $\varepsilon = 1$, this shows (3.5) for $n = 0$ and $p_0 = 2$.

Let us assume the result (3.5) is true for all $j < n$ and let us show it for n .

We have

$$\partial_\delta^n \Psi_\delta(x) = -\delta \partial_\delta^n (DV(\Psi_\delta(x))) - n \partial_\delta^{n-1} (DV(\Psi_\delta(x))) \\ = -B_1(x, \delta) - n B_2(x, \delta).$$

Using Faà di Bruno's formula, we get

$$B_1(x, \delta) = \delta \sum \frac{n!}{m_1! m_2! (2!)^{m_2} \dots m_n! (n!)^{m_n}} D^{m_1+\dots+m_n+1} V(\Psi_\delta(x)) \cdot \prod_{j=1}^n (\partial_\delta^j \Psi_\delta(x))^{m_j}, \\ B_2(x, \delta) = \sum \frac{(n-1)!}{m_1! m_2! (2!)^{m_2} \dots m_{n-1}! ((n-1)!)^{m_{n-1}}} D^{m_1+\dots+m_{n-1}+1} V(\Psi_\delta(x)) \cdot \prod_{j=1}^{n-1} (\partial_\delta^j \Psi_\delta(x))^{m_j},$$

where $m_1 + 2m_2 + \dots + nm_n = n$ in B_1 and $m_1 + 2m_2 + \dots + (n-1)m_{n-1} = n-1$ in B_2 . Multiplying by $\partial_\delta^n \Psi_\delta(x)$, we get

$$|\partial_\delta^n \Psi_\delta(x)|^2 = -\delta D^2 V(\Psi_\delta(x)) \cdot (\partial_\delta^n \Psi_\delta(x), \partial_\delta^n \Psi_\delta(x)) - \langle B_3(x, \delta), \partial_\delta^n \Psi_\delta(x) \rangle - n \langle B_2(x, \delta), \partial_\delta^n \Psi_\delta(x) \rangle,$$

where

$$\begin{aligned} B_3(x, \delta) &= B_1(x, \delta) - \delta D^2 V(\Psi_\delta(x)) \cdot \partial_\delta^n \Psi_\delta(x) \\ &= \delta \sum \frac{n!}{m_1! m_2! (2!)^{m_2} \dots m_n! (n!)^{m_n}} D^{m_1 + \dots + m_n + 1} V(\Psi_\delta(x)) \cdot \prod_{j=1}^n (\partial_\delta^j \Psi_\delta(x))^{m_j}, \end{aligned}$$

where $m_1 + 2m_2 + \dots + (n-1)m_{n-1} = n$ and $m_n = 0$ in B_3 .

Then, in B_2 and B_3 , we have that the order of each derivative of Ψ_δ is less than $n-1$. Hence, using polynomial growth assumption B-1 and induction assumption, we have that B_2 and B_3 have polynomial growth in x . Using (3.6), we have for $\varepsilon > 0$

$$|\partial_\delta^n \Psi_\delta(x)|^2 + \delta D^2 V(\Psi_\delta(x)) \cdot (\partial_\delta^n \Psi_\delta(x), \partial_\delta^n \Psi_\delta(x)) \leq \frac{1}{2\varepsilon} B(x) + \frac{\varepsilon}{2} |\partial_\delta^n \Psi_\delta(x)|^2,$$

where B has polynomial growth. Using semi-convexity assumption B-2 and choosing ε small enough, we have (3.5). \blacklozenge

Proof of Proposition 3.2 in the case of the implicit split-step scheme (2.9). Let $x \in \mathbb{R}^d$ such that $X_0 = x$ and $\delta < \frac{1}{\alpha}$. We define ε_δ by $\varepsilon_\delta(x) = \Psi_\delta(x) - x$. Let N fixed. We have

$$X_1 = X_0^* + \sqrt{\delta} \eta_0 = x + \varepsilon_\delta(x) + \sqrt{\delta} \eta_0.$$

Using (3.2) and its proof, we have for each $N_0 \in \mathbb{N}^*$,

$$\varepsilon_\delta(x) = \sum_{j=1}^{N_0} \delta^j d_j(x) + \delta^{N_0+1} R_{N_0+1}(x, \delta) = \delta R_1(x, \delta),$$

where R_{N_0+1} and R_1 have polynomial growth. Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that $\phi \in \mathcal{C}_{n_0}^{2N+2}(\mathbb{R}^d)$. We have

$$\begin{aligned} \phi(X_1) &= \phi(x + \varepsilon_\delta(x) + \sqrt{\delta} \eta_0) \\ &= \sum_{k=0}^{2N+1} \frac{1}{k!} \delta^{k/2} D^k \phi(x + \varepsilon_\delta(x)) \cdot (\eta_0, \dots, \eta_0) \\ &\quad + \int_0^1 \frac{(1-t)^{2N+1}}{(2N+1)!} \delta^{N+1} D^{2N+2} \phi(x + \varepsilon_\delta(x) + t\sqrt{\delta} \eta_0) \cdot (\eta_0, \dots, \eta_0) dt. \end{aligned}$$

Let $[\cdot]$ denotes the integer part. Using Taylor expansion on $D^k \phi(x + \varepsilon_\delta(x))$ at the order $N_k = N - [(k+1)/2]$ and the computations done in the proof of the previous Lemma, we obtain

$$\phi(X_1) = I_1(x, \eta_0) + I_2(x, \eta_0) + I_3(x, \eta_0) + I_4(x, \eta_0),$$

where

$$\begin{aligned}
 I_1(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \delta^{k/2} D^k \phi(x) \cdot (\eta_0, \dots, \eta_0) \\
 &\quad + \sum_{k=0}^{2N+1} \frac{1}{k!} \delta^{k/2} \sum_{j=1}^{N_k} \frac{1}{j!} \sum_{m=j}^{N_k} \delta^m \sum_{k_1+\dots+k_j=m, k_s \geq 1} D^{j+k} \phi(x) \cdot (d_{k_1}(x), \dots, d_{k_j}(x), \eta_0, \dots, \eta_0), \\
 I_2(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \delta^{k/2} \sum_{j=1}^{N_k} \frac{1}{j!} \sum_{m=N_k+1}^{jN_k} \delta^m B_{m,j,k}(x, \eta_0), \\
 I_3(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \delta^{k/2} \int_0^1 \frac{(1-t)^{N_k}}{N_k!} D^{N_k+1+k} \phi(x + t\varepsilon_\delta(x)) \cdot (\varepsilon_\delta(x), \dots, \varepsilon_\delta(x), \eta_0, \dots, \eta_0) dt, \\
 I_4(x, \eta_0) &= \delta^{N+1} \int_0^1 \frac{(1-t)^{2N+1}}{(2N+1)!} D^{2N+2} \phi(x + \varepsilon_\delta(x) + t\sqrt{\delta}\eta_0) \cdot (\eta_0, \dots, \eta_0) dt,
 \end{aligned}$$

and, with the temporary notation, for all $0 \leq k \leq 2N+1$ and $1 \leq i \leq N_k$, $g_{k,i} = d_i$ and $g_{k, N_k+1} = R_{N_k+1}$,

$$B_{m,j,k}(x, \eta_0) = \sum_{k_1+\dots+k_j=m, k_s \geq 1} D^{j+k} \phi(x) \cdot (g_{k,k_1}(x), \dots, g_{k,k_j}(x), \eta_0, \dots, \eta_0).$$

We have, for all $p \in \mathbb{N}$ and $i \in \{1, \dots, d\}$, $\mathbb{E}(\eta_{0,i}^{2p+1}) = 0$ and $\eta_{0,i}$ is independent with x and $\eta_{0,j}$ for $j \neq i$. Then, the expectation of all the odd term in k in I_1 , I_2 and I_3 vanish. Hence, we have

$$\begin{aligned}
 \mathbb{E}(I_1(x, \eta_0)) &= \sum_{k=0}^N \frac{1}{(2k)!} \delta^k \mathbb{E} \left(D^{2k} \phi(x) \cdot (\eta_0, \dots, \eta_0) \right) \\
 &\quad + \sum_{k=0}^N \frac{1}{(2k)!} \delta^k \sum_{j=1}^{N-k} \frac{1}{j!} \sum_{m=j}^{N-k} \delta^m \sum_{k_1+\dots+k_j=m, k_s \geq 1} \mathbb{E} \left(D^{j+2k} \phi(x) \cdot (d_{k_1}(x), \dots, d_{k_j}(x), \eta_0, \dots, \eta_0) \right), \\
 \mathbb{E}(I_2(x, \eta_0)) &= \sum_{k=0}^N \frac{1}{(2k)!} \delta^k \sum_{j=1}^{N-k} \frac{1}{j!} \sum_{m=N+1-k}^{j(N-k)} \delta^m \mathbb{E}(B_{m,j,2k}(x, \eta_0)) \\
 &= \delta^{N+1} \sum_{k=0}^N \frac{1}{(2k)!} \sum_{j=1}^{N-k} \frac{1}{j!} \sum_{m=N+1-k}^{j(N-k)} \delta^{m+k-N-1} \mathbb{E}(B_{m,j,2k}(x, \eta_0)), \\
 \mathbb{E}(I_3(x, \eta_0)) &= \sum_{k=0}^N \frac{1}{(2k)!} \delta^k \int_0^1 \frac{(1-t)^{N-k}}{(N-k)!} \mathbb{E} \left(D^{N+1+k} \phi(x + t\varepsilon_\delta(x)) \cdot (\varepsilon_\delta(x), \dots, \varepsilon_\delta(x), \eta_0, \dots, \eta_0) \right) dt, \\
 \mathbb{E}(I_4(x, \eta_0)) &= \delta^{N+1} \int_0^1 \frac{(1-t)^{2N+1}}{(2N+1)!} \mathbb{E} \left(D^{2N+2} \phi(x + \varepsilon_\delta(x) + t\sqrt{\delta}\eta_0) \cdot (\eta_0, \dots, \eta_0) \right) dt.
 \end{aligned}$$

Using the polynomial growth of d_i and R_i for all i and $\phi \in \mathcal{C}_{\ell_{2N+2}}^{2N+2}(\mathbb{R}^d)$, we have that there exists an integer n_1 which depends of N , ℓ_{2N+2} and the polynomial growth of V and its derivatives such that

$$|\mathbb{E}(I_2(x, \eta_0))| \leq C_N \delta^{N+1} (1 + |x|^{n_1}) |\phi|_{2N, \ell_{2N+2}}.$$

Similarly, we have that there exists an integer n_2 which depends of N , ℓ_{2N+2} and the polynomial growth of V and its derivatives such that

$$|\mathbb{E}(I_4(x, \eta_0))| \leq C_N \delta^{N+1} (1 + |x|^{n_2}) \|D^{2N+2} \phi\|_{0, \ell_{2N+2}}.$$

Using $\varepsilon_\delta(x) = \delta R_1(x, \delta)$ and similar computations, we have that there exists an integer n_3 which depends of N , ℓ_{2N+2} and the polynomial growth of V and its derivatives such that

$$|\mathbb{E}(I_3(x, \eta_0))| \leq C_N \delta^{N+1} (1 + |x|^{n_3}) \|D^{N+1}\phi\|_{N, \ell_{2N+2}}.$$

Moreover, we have

$$\mathbb{E}(I_1(x, \eta_0)) = \sum_{n=0}^N \delta^n A_n(x) \phi(x),$$

where $A_0 = I$ and, for all $n \in \mathbb{N}^*$ and $x \in \mathbb{R}^d$,

$$\begin{aligned} A_n(x) \phi(x) = & \sum_{\substack{m+k=n, \\ m \geq 1, k \geq 0}} \left(\sum_{j=1}^m \frac{1}{j!(2k)!} \sum_{k_1 + \dots + k_j = m, k_s \geq 1} \mathbb{E}(D^{j+2k} \phi(x) \cdot (d_{k_1}(x), \dots, d_{k_j}(x), \eta_0, \dots, \eta_0)) \right) \\ & + \frac{1}{(2n)!} \mathbb{E}(D^{2n} \phi(x) \cdot (\eta_0, \dots, \eta_0)). \end{aligned}$$

For $n = 1$, we have only one possibility: $m = 1$ and $k = 0$, then $j = 1$, $k_1 = 1$ and

$$A_1(x) \phi(x) = \mathbb{E}(D\phi(x) \cdot d_1(x)) + \frac{1}{2} \mathbb{E}(D^2\phi(x) \cdot (\eta_0, \eta_0)).$$

Using properties of η_0 and the definition of d_1 , we get $A_1 = L$.

We have that there exists an integer k which depends of N , ℓ_{2N+2} and the polynomial growth of V and their derivatives such that

$$|\mathbb{E}\phi(X_1) - \sum_{n=0}^N \delta^n A_n(x) \phi(x)| \leq C_N \delta^{N+1} (1 + |x|^k) |\phi|_{2N+2, \ell_{2N+2}}.$$

Finally, we have proved (3.1) for the implicit split-step scheme (2.9). ◆

Let now consider the case of the implicit Euler scheme (2.10).

Let $x \in \mathbb{R}^d$ such that $X_0 = x$ and $\delta < \frac{1}{\alpha}$. We need an asymptotic expansion for $X_1 = x - DV(X_1)\delta + \sqrt{\delta}\eta_0$. We use the local notation $\theta = \sqrt{\delta}$. We define the function ψ_θ which associate to y the solution z of $z = x - \theta^2 DV(z) + \theta\eta_0$. This function is well defined (see Lemma 2.4) and we have $X_1 = \psi_\theta(x)$. If we consider the function f_1 defined on $]0, \frac{1}{\sqrt{\alpha}}[\times \mathbb{R}^d \times \mathbb{R}^d$ by

$$f_1(\theta, y, z) = -z + y - \theta^2 DV(z) + \theta\eta_0,$$

we can show, as previously, that $(\theta, y) \mapsto \psi_\theta(y)$ is C^∞ on $]0, \frac{1}{\sqrt{\alpha}}[\times \mathbb{R}^d$.

We have the following lemma:

Lemma 3.5 *Let $x \in \mathbb{R}^d$ such that $X_0 = x$. For $\delta < \frac{1}{\alpha}$, with the local notation $\theta = \sqrt{\delta}$*

$$\forall N_0 \in \mathbb{N}, \quad X_1 = \psi_\theta(x) = x + \sum_{k=1}^{N_0} \delta^{\frac{k}{2}} d_k(x, \eta_0) + \delta^{\frac{N_0+1}{2}} R_{N_0}(x, \delta, \eta_0)$$

where $\forall k \geq 1$, d_k is defined for all $z \in \mathbb{R}^d$ by

$$\begin{aligned} d_1(z, \eta_0) &= \eta_0, \quad d_2(z, \eta_0) = -DV(z), \\ \forall k \geq 3, \quad d_k(z, \eta_0) &= \sum_{i=1}^{k-2} \frac{1}{i!} \sum_{k_1 + \dots + k_i = k-2, k_j \geq 1} -D^{i+1}V(z) \cdot (d_{k_1}(z, \eta_0), \dots, d_{k_i}(z, \eta_0)). \end{aligned}$$

Moreover, we have that $\mathbb{E}(d_k) \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, for all $z \in \mathbb{R}^d$ and $k \in \mathbb{N}$

$$\mathbb{E}(d_{2k+1}(z, \eta_0)) = 0 \quad (3.7)$$

and, for any $N \in \mathbb{N}$, R_{N+1} verifies: There exist $C > 0$ and $\ell_N \in \mathbb{N}$ such that for any $z \in \mathbb{R}^d$ and $\delta < \frac{1}{\alpha}$,

$$|\mathbb{E}(R_{N+1}(z, \delta, \eta_0))| \leq C(1 + |z|^{\ell_N}).$$

Proof. To prove this Lemma, we use the same ideas as in Lemma 3.4. We first compute d_k for all k . By induction, we rewrite d_k only in terms of d_1 , d_2 and the derivatives of V . Using the independence of η_0 with x , we can show (3.7).

To prove that $\mathbb{E}(R_{N_0})$ has polynomial growth, we show that for any $n \in \mathbb{N}$, there exist $C_n > 0$ and $k_n \in \mathbb{N}$ such that for $x \in \mathbb{R}^d$, $\delta < \frac{1}{\alpha}$ and the local notation $\theta = \sqrt{\delta}$,

$$\mathbb{E}(|\partial_\theta \psi_\theta(x)|^2) \leq C_n(1 + |x|^{k_n}).$$

◆

The proof of Proposition 3.2 in the case of the implicit Euler scheme (2.10) is similar to the case of the implicit split-step scheme (2.9), but we must use an asymptotic expansion of $D^k \phi$ to a larger order ($2N + 1 - k$ instead of $N - \lfloor (k + 1)/2 \rfloor$).

4 Modified generator

4.1 Formal series analysis

Let us now consider $\delta < \frac{1}{\alpha}$ as fixed. We want to construct a formal series

$$\mathcal{L}(\delta, x) = L(x) + \delta L_1(x) + \dots + \delta^n L_n(x) + \dots \quad (4.1)$$

where the coefficients of the operator L_n are in $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, and such that formally the solution v at time $t = \delta$ of the equation

$$\partial_t v(t, x) = \mathcal{L}(\delta, x)v(t, x), t > 0, x \in \mathbb{R}^d \quad v(0, x) = \phi(x), x \in \mathbb{R}^d$$

coincides in the sense of asymptotic expansion with the approximation of the transition semigroup $\mathbb{E}\phi(X_1)$ studied in the previous section. In other words, we want to obtain the following equality in the sense of asymptotic expansion in powers of δ

$$\exp(\delta \mathcal{L}(\delta, x))\phi = \phi + \sum_{n \geq 1} \delta^n A_n(x)\phi,$$

where the operators A_n are defined in Proposition 3.2.

Formally, this equation can be written as

$$\exp(\delta \mathcal{L}(\delta, x)) - I_d = \delta \tilde{A}(\delta, x), \quad (4.2)$$

where $\tilde{A}(\delta, x) = \sum_{n \geq 1} \delta^{n-1} A_n(x)$.

We have

$$\exp(\delta \mathcal{L}(\delta, x \partial_x)) - I_d = \delta \mathcal{L}(\delta, x) \left(\sum_{n \geq 0} \frac{\delta^n}{(n+1)!} \mathcal{L}(\delta, x)^n \right).$$

Note that the (formal) inverse of the series is given by

$$\left(\sum_{n \geq 0} \frac{\delta^n}{(n+1)!} \mathcal{L}(\delta, x)^n \right)^{-1} = \sum_{n \geq 0} \frac{B_n}{n!} \delta^n \mathcal{L}(\delta, x)^n,$$

where the B_n are the Bernoulli numbers (see [29, 37]). Hence, equations (4.1) and (4.2) are equivalent in the sense of formal series to

$$\begin{aligned} \mathcal{L}(\delta, x) &= \sum_{\ell \geq 0} \frac{B_\ell}{\ell!} \delta^\ell \mathcal{L}(\delta, x)^\ell \tilde{A}(\delta, x) \\ &= \sum_{n \geq 0} \delta^n \left(A_{n+1}(x) + \sum_{\ell=1}^n \frac{B_\ell}{\ell!} \sum_{n_1+\dots+n_{\ell+1}=n-\ell} L_{n_1}(x) \dots L_{n_\ell}(x) A_{n_{\ell+1}+1}(x) \right). \end{aligned} \quad (4.3)$$

Identifying the right hand sides of (4.1) and (4.3), we get the following induction formula

$$L_n(\delta, x) = A_{n+1}(x) + \sum_{\ell=1}^n \frac{B_\ell}{\ell!} \sum_{n_1+\dots+n_{\ell+1}=n-\ell} L_{n_1}(x) \dots L_{n_\ell}(x) A_{n_{\ell+1}+1}(x). \quad (4.4)$$

Each of the terms of the above sum is an operator of order $2n+2$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and therefore L_n is also an operator of order $2n+2$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$.

Note that (4.2) gives immediately the inverse relation of this formal series equation:

$$A_n(x) = \sum_{\ell=1}^n \frac{1}{\ell!} \sum_{n_1+\dots+n_\ell=n-\ell} L_{n_1}(x) \dots L_{n_\ell}(x). \quad (4.5)$$

Moreover, clearly it holds

$$L_n(x)1 = 0.$$

4.2 Approximate solution of the modified flow

In the previous section, for a given N , we have formally constructed the modified operator

$$\mathcal{L}^{(N)}(\delta, x) = L(x) + \sum_{n=1}^N \delta^n L_n(x). \quad (4.6)$$

Let the step δ be fixed. In order to perform weak backward error analysis and estimate recursively the modified invariant law of the numerical process, we should be able to define a solution v^N of the modified flow

$$\partial_t v^N(t, x) = \mathcal{L}^{(N)}(\delta, x) v^N(t, x), t > 0, x \in \mathbb{R}^d \quad v^N(0, x) = \phi(x), x \in \mathbb{R}^d. \quad (4.7)$$

However, in our situation we do not know whether this equation has a solution.

The goal of the following theorem is to give a proper definition of the modified flow associated to (4.6).

Theorem 4.1 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ such that $\int \phi d\rho = 0$. For any $N \in \mathbb{N}$, there exists an integer ℓ_N such that $\phi \in \mathcal{C}_{\ell_N}^N(\mathbb{R}^d)$. For all $n \in \mathbb{N}$, there exist functions $v_n(t, \cdot) \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ defined for all times $t \geq 0$ such that for all $t > 0$, $x \in \mathbb{R}^d$ and $n \in \mathbb{N}$,*

$$\partial_t v_n(t, x) - L(x) v_n(t, x) = \sum_{\ell=1}^n L_\ell(x) v_{n-\ell}(t, x), \quad (4.8)$$

with initial condition $v_0(0, x) = \phi(x)$ for all $x \in \mathbb{R}^d$ and $v_n(0, x) = 0$ for $n \geq 1$ and $x \in \mathbb{R}^d$. For all $N \geq 0$, $x \in \mathbb{R}^d$ and $t \geq 0$, setting

$$v^{(N)}(t, x) = \sum_{k=0}^N \delta^k v_k(t, x),$$

the following holds:

- a.** For $\delta_0 = \frac{1}{\alpha}$, there exist $C_N > 0$, $k_N \in \mathbb{N}$ and $r_N \in \mathbb{N}$ such that for all $t \geq 0$, $x \in \mathbb{R}^d$ and $\delta < \delta_0$,

$$|\mathbb{E}v^{(N)}(t, X_1) - v^{(N)}(t + \delta, x)| \leq \delta^{N+1} C_N (1 + |x|^{r_N}) \sup_{\substack{s \in]0, \delta[, \\ n=0, \dots, N}} |v_n(t + s, \cdot)|_{2N+2, k_N},$$

where $X_0 = x$.

- b.** For $\delta_0 = \frac{1}{\alpha}$, there exist $C_N > 0$ and $r_N \in \mathbb{N}$ such that for all $\delta < \delta_0$ and $x \in \mathbb{R}^d$,

$$|\mathbb{E}\phi(X_1) - v^{(N)}(\delta, x)| \leq \delta^{N+1} C_N (1 + |x|^{r_N}) \|\phi\|_{6N+2, \ell_{6N+2}},$$

where $X_0 = x$.

Note that in the previous theorem, we have constructed a function $v^{(N)}$ which is an approximate solution of (4.7). More precisely, we can easily show that we have for all time $t \geq 0$ and $x \in \mathbb{R}^d$

$$\begin{aligned} \partial_t v^{(N)}(t, x) &= L^{(N)} v^{(N)}(t, x) + R^{(N)}(t, x), \\ v^{(N)}(0, x) &= \phi(x) \end{aligned}$$

where

$$R^{(N)}(t, x) = - \sum_{\ell_1, \ell_2=0, \dots, N} \delta^{\ell_1 + \ell_2} L_{\ell_1} v_{\ell_2}(t, x)$$

is of order $\mathcal{O}(\delta^{N+1})$.

Proof. For $n = 0$, equation (4.8) reduces to $v_0 = u$, the solution of (2.17). By Proposition 2.8, we deduce that u and all its derivatives have polynomial growth in space and exponential decrease in time. Let $n \in \mathbb{N}^*$ and assume that v_j are constructed for $j = 1, \dots, n-1$. Let for $x \in \mathbb{R}^d$ and $t \geq 0$

$$F_n(t, x) = \sum_{\ell=1}^n L_\ell(x) v_{n-\ell}(t, x), \quad (4.9)$$

the right-hand side in (4.8). Then v_n is uniquely defined and given by the formula

$$v_n(t, \cdot) = \int_0^t P_{t-s} F_n(s, \cdot) ds, \quad t \geq 0. \quad (4.10)$$

Using an induction argument and Proposition 2.8, we know that v_n and all its derivatives have polynomial growth. Moreover, we have for all $i \in \mathbb{N}^*$ and $n \in \mathbb{N}^*$ that there exist integer $k_{n,i}$ and $j_{k,n}$ such that for all $t \geq 0$,

$$\|v_n(t)\|_{i, k_{n,i}} \leq P(t) \|\phi\|_{k+4n, j_{k,n}}, \quad (4.11)$$

where P is a polynomial in t which also depends on k , n and V . This proves the first part of the Theorem.

To prove **a.**, we consider a fixed time t , and define the functions $w_n(s, x) := v_n(t + s, x)$ for $s \geq 0$, $x \in \mathbb{R}^d$ and $n \in \mathbb{N}$. By definition, these functions satisfy the relations

$$\partial_s w_n(s, x) = \sum_{\ell=0}^n L_\ell(x) w_{n-\ell}(s, x), \quad s > 0, x \in \mathbb{R}^d \quad w_n(0, x) = v_n(t, x), x \in \mathbb{R}^d.$$

Let us consider the successive time derivatives of the functions w_n . We have, using the definition of w_n , for all $s > 0$ and $x \in \mathbb{R}^d$

$$\partial_s^2 w_n(s, x) = \sum_{\ell=0}^n L_\ell(x) \partial_s w_{n-\ell}(s, x) = \sum_{k=0}^n \sum_{\ell_1+\ell_2=k} L_{\ell_1}(x) L_{\ell_2}(x) w_{n-k}(s, x),$$

and we see by induction that for all $m \geq 1$, $x \in \mathbb{R}^d$ and $s > 0$

$$\partial_s^m w_n(s, x) = \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1}(x) \dots L_{\ell_m}(x) w_{\ell_{m+1}}(s, x).$$

Using the fact that the operators L_ℓ are of order $2\ell + 2$ with no terms of order zero and the coefficients of L_ℓ have polynomial growth, we see that there exist a constant C depending on n and m and a constant r_n , such that for all $s > 0$, $x \in \mathbb{R}^d$ and $m \geq 1$

$$|\partial_s^m w_n(s, x)| \leq C(1 + |x|^{r_n}) \sup_{\substack{k=0, \dots, n \\ 1 \leq j \leq 2(n-k)+2m}} |\partial_j w_k(s, x)|.$$

Now let us consider the Taylor expansion of $w_n(\delta, \cdot)$, for $\delta < \delta_0$. We have for $\delta < \delta_0$, $x \in \mathbb{R}^d$ and $n = 0, \dots, N$,

$$\begin{aligned} w_n(\delta, x) &= \sum_{m=0}^{N-n} \frac{\delta^m}{m!} \partial_s^m w_n(0, x) + \int_0^\delta \frac{\sigma^{N-n}}{(N-n)!} \partial_s^{N-n+1} w_n(\sigma, x) d\sigma \\ &= \sum_{m=0}^{N-n} \frac{\delta^m}{m!} \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1}(x) \dots L_{\ell_m}(x) w_{\ell_{m+1}}(0, x) + R_{N,n}(\delta, x). \end{aligned}$$

Using the bounds on the time derivatives of w_n , we obtain the existence of a constant ℓ_N such that for all $0 < \delta < \delta_0$, $x \in \mathbb{R}^d$ and all $n = 0, \dots, N$,

$$|R_{N,n}(\delta, x)| \leq C\delta^{N-n+1}(1 + |x|^{r_N}) \sup_{\substack{s \in]0, \delta[, \\ i=0, \dots, N \\ 1 \leq j \leq 2N+2}} |\partial_j w_i(s, x)|$$

for some constants depending on N, n . After summation in n , and using the expression (4.5) of the operators A_n and the definition of w_n , we get for all $x \in \mathbb{R}^d$, $t \geq 0$ and $0 < \delta < \delta_0$

$$v^{(N)}(t + \delta, x) = \sum_{n=0}^N \delta^n \sum_{m=0}^n A_m(x) v_{n-m}(t, x) + R_N(t, \delta, x)$$

where for all $t \geq 0$ and $0 < \delta < \delta_0$,

$$|R_N(t, \delta, x)| \leq C_N \delta^{N+1} (1 + |x|^{r_N}) \sup_{\substack{s \in]0, \delta[, \\ n=0, \dots, N \\ 1 \leq j \leq 2N+2}} |\partial_j v_n(t + s, x)|.$$

To conclude, we apply (3.1) to $\phi = v^{(N)}(t)$ and use the fact that $\delta < \delta_0$. The second estimate **b.** is then a consequence of **a.** with $t = 0$ and (4.11). ◆

5 Asymptotic expansion of the invariant measure and long time behavior

We now analyze the long time behavior of the solution of the modified flow associated to (4.7). We recall that for a given operator B , we denote by B^* its formal adjoint with respect to the $L^2(\rho)$ product. We start by an asymptotic expansion of a formal invariant measure for the numerical schemes.

Proposition 5.1 *Let $\delta_0 < \frac{1}{\alpha}$. Let $(L_n)_{n \geq 0}$ be the collection of operators defined recursively by (4.4). There exists a collection of functions $(\mu_n)_{n \geq 0}$ such that $\mu_0 = 1$, $\int_{\mathbb{R}^d} \mu_n(x) \rho(x) dx = 0$ for $n \geq 1$, and for all $n \geq 1$, $\mu_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and*

$$L\mu_n = - \sum_{\ell=1}^n (L_\ell)^* \mu_{n-\ell}. \quad (5.1)$$

Let $N \geq 0$ be fixed and the function $\mu^{(N)}$ be defined for $x \in \mathbb{R}^d$ and $0 < \delta < \delta_0$ by

$$\mu^{(N)}(\delta, x) = 1 + \sum_{n=1}^N \delta^n \mu_n(x).$$

Then for all $0 < \delta < \delta_0$, $\mu^{(N)}(\delta, \cdot) \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and $\mu^{(N)}$ satisfies for $0 < \delta < \delta_0$

$$\int_{\mathbb{R}^d} \mu^{(N)}(\delta, x) \rho(x) dx = 1.$$

Remark 5.2 *We consider equation (5.1) because $L^* = L$.*

Proof. Let $n \geq 1$. Assume that $\mu_0 = 1$ and μ_j are known, for $j = 1, \dots, n-1$. Let us consider equation (5.1) given by

$$L\mu_n = - \sum_{\ell=1}^n (L_\ell)^* \mu_{n-\ell} =: G_n$$

Note that $G_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and satisfies

$$\begin{aligned} \int_{\mathbb{R}^d} G_n(x) \rho(x) dx &= - \sum_{\ell=1}^n \int_{\mathbb{R}^d} (L_\ell)^*(x) \mu_{n-\ell}(x) \rho(x) dx \\ &= - \sum_{\ell=1}^n \int_{\mathbb{R}^d} \mu_{n-\ell}(x) L_\ell(x) 1 \rho(x) dx = 0. \end{aligned}$$

Using the Lemma 2.7, we easily obtain the existence of a function $\mu_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ satisfying (5.1) and $\int_{\mathbb{R}^d} \mu_n(x) \rho(x) dx = 0$. This completes the proof. \blacklozenge

Proposition 5.3 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$. For all n and k there exist a positive polynomial function $P_{k,n}$ and integers $\ell_{n,k}$ and $m_{n,k} \geq \ell_{n,k}$ such that $\phi \in \mathcal{C}_{\ell_{k,n}}^{k+4n}(\mathbb{R}^d)$ and for all $t \geq 0$*

$$\| v_n(t) - \int_{\mathbb{R}^d} \phi(y) \mu_n(y) \rho(y) dy \|_{k, m_{n,k}} \leq P_{k,n}(t) e^{-\lambda t} \| \phi - \langle \phi \rangle \|_{k+4n, \ell_{n,k}}, \quad (5.2)$$

where $\langle \phi \rangle = \int_{\mathbb{R}^d} \phi(x) \rho(x) dx$.

Proof. Using the fact that $\mu_0 = 1$ and $v_0 = u$, we see that estimate (5.2) is satisfied for $n = 0$ (Proposition 2.8). Let $n \geq 1$ and assume that v_j , $j = 0, \dots, n-1$ satisfy for $k \in \mathbb{N}^*$, $i \in \mathbb{N}^*$ and $t \geq 0$:

$$\|v_j(t) - \int_{\mathbb{R}^d} \phi(y) \mu_j(y) \rho(y) dy\|_{k, m_j, k} \leq P_{k, j}(t) e^{-\lambda t} \|\phi - \langle \phi \rangle\|_{k+4j, \ell_j, k},$$

where ℓ_j, k is such that $\phi \in C_{\ell_j, k}^{k+4j}(\mathbb{R}^d)$. Let us set for $t \geq 0$

$$c_n(t) = \sum_{m=0}^n \int_{\mathbb{R}^d} v_{n-m}(t, x) \mu_m(x) \rho(x) dx.$$

We claim that c_n does not depend on time. Indeed, for all $t \geq 0$,

$$\begin{aligned} \sum_{m=0}^n \partial_t \int_{\mathbb{R}^d} v_{n-m}(t, x) \mu_m(x) \rho(x) dx &= \sum_{m=0}^n \partial_t \int_{\mathbb{R}^d} v_m(t, x) \mu_{n-m}(x) \rho(x) dx \\ &= \sum_{m=0}^n \sum_{\ell=0}^m \int_{\mathbb{R}^d} L_{m-\ell}(x) v_\ell(t, x) \mu_{n-m}(x) \rho(x) dx \\ &= \sum_{\ell=0}^{n-1} \int_{\mathbb{R}^d} v_\ell(t, x) \sum_{m=1}^{n-\ell} L_m^*(x) \mu_{n-\ell-m}(x) \rho(x) dx \\ &\quad + \sum_{\ell=0}^{n-1} \int_{\mathbb{R}^d} v_\ell(t, x) L(x) \mu_{n-\ell}(x) \rho(x) dx \\ &\quad + \int_{\mathbb{R}^d} v_n(t, x) L(x) 1 d\rho \\ &= 0, \end{aligned}$$

by definition of the coefficients μ_n (see (5.1)) and by (2.15). Note that the computation above is justified because $\forall n$, v_n and μ_n are in $C_{pol}^\infty(\mathbb{R}^d)$. We deduce for all $t \geq 0$

$$\int_{\mathbb{R}^d} \partial_t v_n(t, x) \rho(x) dx = - \sum_{m=1}^n \int_{\mathbb{R}^d} \partial_t v_{n-m}(t, x) \mu_m(x) \rho(x) dx. \quad (5.3)$$

Now, we compute the average of F_n defined by (4.9). By (4.8) and (5.3), we have for all $t \geq 0$

$$\begin{aligned} \langle F_n(t) \rangle &= \int_{\mathbb{R}^d} F_n(t, x) \rho(x) dx = \int_{\mathbb{R}^d} \partial_t v_n(t, x) \rho(x) dx - \int_{\mathbb{R}^d} L(x) v_n(t, x) \rho(x) dx \\ &= \int_{\mathbb{R}^d} \partial_t v_n(t, x) \rho(x) dx \\ &= - \sum_{m=1}^n \int_{\mathbb{R}^d} \partial_t v_{n-m}(t, x) \mu_m(x) dx. \end{aligned}$$

We rewrite (4.10) as follows: for all $t \geq 0$ and $x \in \mathbb{R}^d$

$$v_n(t, x) = \int_0^t \langle F_n(s) \rangle ds + \int_0^t P_{t-s}(F_n(s, x) - \langle F_n(s) \rangle) ds.$$

Using the previous expression obtained for $\langle F_n(s) \rangle$ and recalling the initial data for v_n , we deduce that for all $x \in \mathbb{R}^d$ and $t \geq 0$

$$\begin{aligned} v_n(t, x) &= - \sum_{m=1}^n \int_{\mathbb{R}^d} v_{n-m}(t, y) \mu_m(y) \rho(y) dy + \int_{\mathbb{R}^d} \phi(y) \mu_n(y) \rho(y) dy \\ &\quad + \int_0^t P_{t-s}(F_n(s, x) - \langle F_n(s) \rangle) ds. \end{aligned}$$

Then, using $\int_{\mathbb{R}^d} \mu_m(x) \rho(x) dx = 0$, for $m \in \mathbb{N}^*$ (Proposition 5.1), we get for $x \in \mathbb{R}^d$ and $t \geq 0$

$$\begin{aligned} v_n(t, x) &- \int_{\mathbb{R}^d} \phi(y) \mu_n(y) \rho(y) dy \\ &= - \sum_{m=1}^n \int_{\mathbb{R}^d} \left(v_{n-m}(t, y) - \int_{\mathbb{R}^d} \phi(z) \mu_{n-m}(z) \rho(z) dz \right) \mu_m(y) \rho(y) dy \\ &\quad + \int_0^t P_{t-s}(F_n(s, x) - \langle F_n(s) \rangle) ds. \end{aligned}$$

Note that, since L_ℓ , $\ell \in \mathbb{N}$ is a differential operator of order $2\ell + 2$ whose coefficients belong to $\mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and contain no zero order terms, there exists an integer $\beta_{n,k}$ such that for $s \geq 0$

$$\begin{aligned} \| F_n(s) - \langle F_n(s) \rangle \|_{k, \beta_{n,k}} &\leq \sum_{\ell=0}^{n-1} c_{k,\ell} |v_\ell(s)|_{2(n-\ell)+2+k, m_{\ell, k+2(n-\ell)+2}} \\ &\leq \sum_{\ell=0}^{n-1} c_{k,\ell} \| v_\ell(s) - \int_{\mathbb{R}^d} \phi(y) \mu_\ell(y) \rho(y) dy \|_{2(n-\ell)+2+k, m_{\ell, k+2(n-\ell)+2}}. \end{aligned}$$

We have used

$$|v_\ell(s)|_{2(n-\ell)+2+k, m_{\ell, k+2(n-\ell)+2}} = |v_\ell(s) - \int_{\mathbb{R}^d} \phi(y) \mu_\ell(y) \rho(y) dy|_{2(n-\ell)+2+k, m_{\ell, k+2(n-\ell)+2}}.$$

Let s be fixed. As $\int_{\mathbb{R}^d} (F_n(s, x) - \langle F_n(s) \rangle) \rho(x) dx = 0$ and $v_s(t, x) := P_t(F_n(s, x) - \langle F_n(s) \rangle)$ is the unique solution of

$$\frac{d}{dt} v_s(t, x) = L(x) v_s(t, x), \quad x \in \mathbb{R}^d, \quad t > 0, \quad v_s(0, x) = (F_n(s, x) - \langle F_n(s) \rangle), \quad x \in \mathbb{R}^d,$$

we can use Proposition 2.8 to bound $|P_{t-s}(F_n(s, x) - \langle F_n(s) \rangle)|$.

Then, for $t \geq 0$, $i \in \mathbb{N}^*$, $x \in \mathbb{R}^d$ and $\mathbf{k} \in \mathbb{N}^d$, there exists an integer $\alpha_{n,\mathbf{k}}$ such that

$$\begin{aligned} |\partial_{\mathbf{k}}(v_n(t, x) - \int_{\mathbb{R}^d} \phi(y) \mu_n(y) \rho(y) dy)| &\leq \\ &\sum_{m=1}^n \left(\int_{\mathbb{R}^d} |v_{n-m}(t, y) - \int_{\mathbb{R}^d} \phi(z) \mu_{n-m}(z) \rho(z) dz|^2 \rho(y) dy \right)^{1/2} \left(\int_{\mathbb{R}^d} |\mu_m(y)|^2 \rho(y) dy \right)^{1/2} \\ &\quad + \int_0^t C_{\mathbf{k},n} e^{-\lambda(t-s)} \| F_n(s) - \langle F_n(s) \rangle \|_{|\mathbf{k}|, \beta_{n,|\mathbf{k}|}} ds (1 + |x|^{\alpha_{n,\mathbf{k}}}). \end{aligned}$$

Using the induction assumption, we have for $t \geq 0$, $i \in \mathbb{N}^*$ and $\mathbf{k} \in \mathbb{N}^d$

$$\begin{aligned} |\partial_{\mathbf{k}}(v_n(t, x) - \int_{\mathbb{R}^d} \phi(y) \mu_n(y) \rho(y) dy)| &\leq \sum_{m=1}^n c_m P_{0,n-m}(t) e^{-\lambda t} \| \phi - \langle \phi \rangle \|_{4n, \ell_{n,0}} \\ &\quad + \sum_{\ell=0}^{n-1} \int_0^t C_{\mathbf{k},n} P_{\mathbf{k},\ell}(s) e^{-\lambda(t-s)} e^{-\lambda s} ds \| \phi - \langle \phi \rangle \|_{|\mathbf{k}|+4n, \ell_{n,|\mathbf{k}|}} (1 + |x|^{\alpha_{n,\mathbf{k}}}). \end{aligned}$$

The conclusion follows. \blacklozenge

The following Proposition completes the proof of our main result Theorem 2.10.

Proposition 5.4 *Let N and ℓ_N be fixed. Let $\delta_0 = \frac{1}{\alpha}$. Let X_p be the discrete process defined by the implicit Euler scheme (2.10) or the implicit split-step scheme (2.9). Let $0 \leq \delta < \delta_0$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d) \cap \mathcal{C}_{\ell_N}^{6N+8}(\mathbb{R}^d)$. Then there exist $C_N > 0$ and $p_N \in \mathbb{N}$ such that for all $p \in \mathbb{N}$ and $x \in \mathbb{R}^d$,*

$$|\mathbb{E}\phi(X_p) - v^{(N)}(t_p, x)| \leq C_N(1 + |x|^{p_N}) \|\phi - \langle \phi \rangle\|_{6N+8, \ell_N} \delta^{N+1}, \quad (5.4)$$

where $t_p = p\delta$ and $X_0 = x$.

Moreover, for $0 \leq \delta < \delta_0$ and for all function $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d) \cap \mathcal{C}_{\ell_N}^{6N+8}(\mathbb{R}^d)$, there exist $C_N > 0$ and $p_N \in \mathbb{N}$ and a positive polynomial function P_N satisfying the following: For all $p \in \mathbb{N}$ and $x \in \mathbb{R}^d$,

$$|\mathbb{E}\phi(X_p) - \int_{\mathbb{R}^d} \phi(y) \mu^N(y) \rho(y) dy| \leq \|\phi - \langle \phi \rangle\|_{6N+8, \ell_N} \left(e^{-\lambda t_p} P_N(t_p) + C_N \delta^{N+1} \right) (1 + |x|^{p_N}),$$

where $t_p = p\delta$ and $X_0 = x$.

Proof. Let N and ℓ_N be fixed. Let $\delta_0 = \frac{1}{\alpha}$. Let X_p be the discrete process defined by the implicit Euler scheme (2.10) or the implicit split-step scheme (2.9). Let $0 \leq \delta < \delta_0$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d) \cap \mathcal{C}_{\ell_N}^{6N+8}(\mathbb{R}^d)$. For all p , where $t_j = j\delta$ for $j \leq p$, we have for $x \in \mathbb{R}^d$ such that $X_0 = x$

$$\begin{aligned} \mathbb{E}\phi(X_p) - v^{(N+1)}(t_p, x) &= \mathbb{E}v^{(N+1)}(0, X_p) - v^{(N+1)}(t_p, x) \\ &= \mathbb{E} \sum_{j=0}^{p-1} \mathbb{E}^{X_{p-j-1}} \left(v^{(N+1)}(t_j, X_{p-j}) - v^{(N+1)}(t_{j+1}, X_{p-j-1}) \right). \end{aligned}$$

Here we have used the notation $\mathbb{E}^{X_{p-j-1}}$ for the conditional expectation with respect to the filtration generated by X_{p-j-1} . We obtain:

$$\begin{aligned} \mathbb{E}^{X_{p-j-1}} \left(v^{(N+1)}(t_j, X_{p-j}) - v^{(N+1)}(t_{j+1}, X_{p-j-1}) \right) \\ = \mathbb{E}^{X_{p-j-1}} \left(v^{(N+1)}(t_j, X_1(X_{p-j-1})) - v^{(N+1)}(t_{j+1}, X_{p-j-1}) \right), \end{aligned}$$

where $X_1(x)$ is the first step of the scheme (2.10) or (2.9) when the initial condition is x . Using Theorem 4.1 with $t = t_j$, Proposition 2.6 and (5.2), we deduce that there exist integers p_N and k_N such that

$$\begin{aligned} |\mathbb{E}\phi(X_p) - v^{(N+1)}(t_p, x)| &\leq \delta^{N+2} C_N \sum_{j=0}^{p-1} \sup_{\substack{s \in]0, \delta[\\ n=0, \dots, N+1}} |v_n(t_{j+1}, \cdot)|_{2N+4, k_N} (1 + |x|^{p_N}) \\ &\leq \delta^{N+2} C_N \sum_{j=0}^{p-1} e^{-\lambda t_j} P_N(t_j) \|\phi - \langle \phi \rangle\|_{6N+8, \ell_N} (1 + |x|^{p_N}) \\ &\leq \delta^{N+2} C_N \|\phi - \langle \phi \rangle\|_{6N+8, \ell_N} \sum_{j=0}^{p-1} e^{-\lambda t_j} (1 + |x|^{p_N}), \end{aligned}$$

for some constant C_N . We have used:

$$|v_n(t_{j+1}, \cdot)|_{2N+4, k_N} = |v_n(t_{j+1}, \cdot) - \int_{\mathbb{R}^d} \phi(x) \mu_n(x) \rho(x) dx|_{2N+4, k_N}.$$

We conclude by using the fact that for a fixed constant $\hat{\gamma} > 0$, it holds true

$$\sum_{j=0}^{p-1} e^{-\hat{\gamma}j\delta} \leq \frac{1}{1 - e^{-\hat{\gamma}\delta}} \leq \frac{C}{\delta},$$

where the constant C depends on $\tilde{\gamma}$ and δ_0 . This implies

$$|\mathbb{E}\phi(X_p) - v^{(N+1)}(t_p, x)| \leq C_N \|\phi - \langle \phi \rangle\|_{6N+8, \ell_N} \delta^{N+1} (1 + |x|^{pN}).$$

To prove (5.4), we note that

$$v^{(N+1)}(t_p, x) = v^{(N)}(t_p, x) + \delta^{N+1} v_{N+1}(t_p, x)$$

and, for all $p \in \mathbb{N}$,

$$\begin{aligned} |v_{N+1}(t_p, x)| &\leq |v_{N+1}(t_p, x) - \int_{\mathbb{R}^d} \phi(x) \mu_{N+1}(x) \rho(x) dx| + \left| \int_{\mathbb{R}^d} (\phi - \langle \phi \rangle) \mu_{N+1}(x) \rho(x) dx \right| \\ &\leq C_N \|\phi - \langle \phi \rangle\|_{4(N+1), \ell_{4(N+1), 0}} (1 + |x|^{m_{N+1, 0}}), \end{aligned}$$

using (5.2) and its notations. The second estimate is a consequence of (5.2). \blacklozenge

6 Appendix : Proof of Proposition 2.8

The aim of this appendix is to prove Proposition 2.8. We will proceed as follow

1. First, we show that $u \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and that Proposition 2.8 holds true for all $t \leq 1$.
2. We show a point-wise estimate for u .
3. Then, using the Bismuth-Elworthy formulas, we show Proposition 2.8 for $t = 1$.
4. Finally, using the last two items, we show Proposition 2.8 for $t \geq 1$.

In the following, the constants may vary from line to line and we usually do not mention dependence on the parameters in order to use lighter notation. We use the generic notation C for such constants.

6.1 The polynomial growth of u and its derivatives

Lemma 6.1 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$. The function u , defined by (2.16), and all its derivatives have polynomial growth: For all p , there exist some constants $s_p, \ell_p \in \mathbb{N}$, γ_p and C such that $\phi \in \mathcal{C}_{2\ell_p}^p(\mathbb{R}^d)$ and for all $x \in \mathbb{R}^d$, $\mathbf{k} \in \mathbb{N}^d$ such that $|\mathbf{k}| = p$ and $t > 0$,*

$$|\partial_{\mathbf{k}} u(t, x)| \leq C \exp(\gamma_p t) (1 + |x|^{2s_p}) \|\phi\|_{p, 2\ell_p}. \quad (6.1)$$

Proof. Let us show the result (6.1) for $p = 0$. Let us assume that $\phi \in \mathcal{C}_{2\ell_0}^0(\mathbb{R}^d)$. Using Proposition 2.2, we have for all $x \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} u(t, x) &= \mathbb{E}(\phi(X_x(t))) \\ |u(t, x)| &\leq \|\phi\|_{0, 2\ell_0} (\mathbb{E}|X_x(t)|^{2\ell_0} + 1) \\ &\leq C \|\phi\|_{0, 2\ell_0} (|x|^{2\ell_0} + 1). \end{aligned}$$

Let us now show the result (6.1) for $p = 1$. It holds that for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$Du(t, x) \cdot h = \mathbb{E}(D\phi(X_x(t)) \cdot \eta_x^h(t)), \quad (6.2)$$

where $\eta_x^h(t) \in \mathbb{R}^d$ is a process defined for $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$ by

$$\eta_x^h(t) = DX_x(t) \cdot h \quad \text{for } t > 0$$

and $\eta_x^h(0) = h$. Moreover, we have for all $t > 0$, $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$

$$\frac{d}{dt}\eta_x^h(t) = -D^2V(X_x(t)) \cdot \eta_x^h(t).$$

By definition of ϕ , we have that there exists $\ell_1 \in \mathbb{N}$ such that $\phi \in \mathcal{C}_{\ell_1}^1(\mathbb{R}^d)$. Then, using Proposition 2.2 and (6.2), we have for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} |Du(t, x) \cdot h| &\leq \|\phi\|_{1, \ell_1} \left(\mathbb{E}(|X_x(t)|^{\ell_1} |\eta_x^h(t)|) + \mathbb{E}(|\eta_x^h(t)|) \right) \\ &\leq \|\phi\|_{1, \ell_1} \left((\mathbb{E}|X_x(t)|^{2\ell_1} \mathbb{E}|\eta_x^h(t)|^2)^{1/2} + (\mathbb{E}|\eta_x^h(t)|^2)^{1/2} \right) \\ &\leq C \|\phi\|_{1, \ell_1} (|x|^{\ell_1} + 1) (\mathbb{E}|\eta_x^h(t)|^2)^{1/2}. \end{aligned}$$

Moreover, by semi-convexity assumption B-2, we get for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\frac{d}{dt}|\eta_x^h(t)|^2 = -2D^2V(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) \leq 2\alpha|\eta_x^h(t)|^2,$$

where α is the constant of semi-convexity of V . Using Gronwall's lemma, we obtain for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$|\eta_x^h(t)|^2 \leq e^{2\alpha t} |h|^2 \quad (6.3)$$

and

$$|Du(t, x) \cdot h| \leq C \|\phi\|_{1, \ell_1} \exp(2\alpha t) (|x|^{\ell_1} + 1) |h|.$$

Then, we have for all $x \in \mathbb{R}^d$, $t > 0$ and $i \in \{1, \dots, d\}$

$$|\partial_i u(t, x)| \leq C \|\phi\|_{1, \ell_1} \exp(2\alpha t) (|x|^{\ell_1} + 1).$$

Let us show Lemma 6.1 for $p = 2$. We have for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$D^2u(t, x) \cdot (h, h) = \mathbb{E}\left(D^2\phi(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) + D\phi(X_x(t)) \cdot \xi_x^h(t)\right),$$

where $\xi_x^h(t) \in \mathbb{R}^d$ is a process defined for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ by

$$\xi_x^h(t) = D^2X_x(t) \cdot (h, h) \quad \text{for } t > 0,$$

and $\xi_x^h(0) = 0$. Moreover, we have for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\frac{d}{dt}\xi_x^h(t) = -D^3V(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) - D^2V(X_x(t)) \cdot \xi_x^h(t).$$

Using assumption B-1 on the polynomial growth of V , we have the existence of $p_1 \in \mathbb{N}$ such that $V \in \mathcal{C}_{2p_1}^3(\mathbb{R}^d)$. Using semi-convexity assumption B-2, we have for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} \frac{d}{dt}|\xi_x^h(t)|^2 &= -2(D^3V(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t), \xi_x^h(t)) - D^2V(X_x(t)) \cdot (\xi_x^h(t), \xi_x^h(t))) \\ &\leq 2\|V\|_{3, 2p_1} (|X_x(t)|^{2p_1} + 1) |\eta_x^h(t)|^2 |\xi_x^h(t)| + 2\alpha |\xi_x^h(t)|^2 \\ &\leq C_1 \left[(|X_x(t)|^{2p_1} + 1)^2 |\eta_x^h(t)|^4 + |\xi_x^h(t)|^2 \right]. \end{aligned}$$

Using Gronwall's lemma and Proposition 2.2, we obtain that the existence of $\tilde{\gamma} > 0$ depending of C_1 and of the constant of semi-convexity α such that for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} \mathbb{E}|\xi_x^h(t)|^2 &\leq C \exp(4\alpha t)|h|^4(|x|^{4p_1} + 1) + (|x|^{4p_1} + 1)|h|^4 \int_0^t C \exp(4\alpha s) \exp((2\alpha + C_1)s) ds \\ &\leq C \exp(\tilde{\gamma}t)(|x|^{4p_1} + 1)|h|^4. \end{aligned}$$

Moreover, we have that there exists $\ell_2 \in \mathbb{N}$ such that $\phi \in \mathcal{C}_{\ell_2}^2(\mathbb{R}^d)$. Finally, we have that there exist some constants k_2 and γ_2 such that for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} |D^2u(t, x) \cdot (h, h)| &\leq \|\phi\|_{2, \ell_2} \mathbb{E}(|X_x(t)|^{\ell_2} + 1)|\eta_x^h(t)|^2 \\ &\quad + \|\phi\|_{2, \ell_2} \left(\mathbb{E}(|X_x(t)|^{2\ell_2} + 1) \mathbb{E}|\xi_x^h(t)|^2 \right)^{1/2} \\ &\leq C \|\phi\|_{2, \ell_2} \exp(\gamma_2 t) (1 + |x|^{2k_2}) |h|^2. \end{aligned}$$

This shows the result (6.1) for $p = 2$.

To prove the result for higher derivatives, we use an induction, the Faà di Bruno's formula and the same methods as used for the first derivatives. Moreover, we can prove that for all $k \geq 0$, there exist some constants q_k , α_k and C such that for all $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\mathbb{E}|D^{k+1}X_x(t) \cdot (h, \dots, h)|^2 \leq C \exp(\alpha_k t) (1 + |x|^{2q_k})^2 |h|^{2(k+1)}. \quad (6.4)$$

◆

Remark 6.2 Proposition 2.8 for $t \leq 1$ is a consequence of this Lemma.

6.2 Estimate of u

Proposition 6.3 Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ be fixed such that $\int_{\mathbb{R}^d} \phi(x) \rho(x) dx = 0$ and u be the solution of (2.17). Let us assume that $\phi \in \mathcal{C}_{2\ell_0}^0(\mathbb{R}^d)$. There exist real numbers $C > 0$ and $\lambda > 0$ such that for all $x \in \mathbb{R}^d$ and $t \geq 0$

$$|u(t, x)| \leq C \|\phi\|_{0, 2\ell_0} \exp(-\lambda t) (1 + |x|^{2\ell_0}).$$

A proof of this result can be found in [43]. Our equation is dissipative and has noise in all directions, hence Proposition 6.3 is a corollary of Theorem 4.4 of [43].

6.3 Estimate of the derivatives of u

We can now show an estimate of the derivatives of u at the time $t = 1$:

Lemma 6.4 Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$ and $k \in \mathbb{N}^*$ be fixed and u be the solution of (2.17). Let us assume that $\phi \in \mathcal{C}_{2\ell_0}^0(\mathbb{R}^d)$. There exist constants C and $m_k \geq 2\ell_0$ such that for all $x \in \mathbb{R}^d$ and $\mathbf{j} \in \mathbb{N}^d$ such that $|\mathbf{j}| = k$, it holds

$$|\partial_{\mathbf{j}}u(1, x)| \leq C \|\phi\|_{0, 2\ell_0} (1 + |x|^{m_k}).$$

The Lemma 6.4 is a corollary of the following lemma.

Lemma 6.5 Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d) \cap \mathcal{C}_{2\ell_0}^0(\mathbb{R}^d)$ be fixed and u be the solution of (2.17). For $k \in \mathbb{N}^*$, there exist constants C and $m_k \geq 2\ell_0$ such that for $0 < t \leq 1$, $x \in \mathbb{R}^d$ and $\mathbf{j} \in \mathbb{N}^d$ such that $|\mathbf{j}| = k$, it holds

$$|\partial_{\mathbf{j}}u(t, x)| \leq C \|\phi\|_{0, 2\ell_0} t^{-k/2} (1 + |x|^{m_k}). \quad (6.5)$$

Proof. We only prove the result for the two first derivatives, as the result for the higher order follows from analogous arguments and by induction.

Let us show the result (6.5) for $k = 1$. We have the Bismuth-Elworthy formula (see [27]): for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $0 < t \leq 1$

$$Du(t, x) \cdot h = \frac{1}{t} \mathbb{E} \left(u(0, X_x(t)) \int_0^t \langle \eta_x^h(s), dW(s) \rangle \right),$$

where $\eta_x^h(t) = DX_x(t) \cdot h \in \mathbb{R}^d$ for $t > 0$ and $\eta_x^h(0) = h$.

Using Cauchy-Schwarz inequality, Burkholder-Davis-Gundy inequality and (6.3) which bounds $\eta_x^h(t)$, we have for $t \leq 1$, $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$

$$\begin{aligned} |Du(t, x) \cdot h| &\leq t^{-1} (\mathbb{E}(|u(0, X_x(t))|^2))^{1/2} (\mathbb{E}(\int_0^t |\eta_x^h(s)|^2 ds))^{1/2} \\ &\leq t^{-1/2} (\mathbb{E}(|\phi(X_x(t))|^2))^{1/2} C|h|. \end{aligned}$$

Using $\phi \in \mathcal{C}_{2\ell_0}^0(\mathbb{R}^d)$ and Proposition 2.2 on the moment of the solution of (2.1), we get (6.5) for $k=1$.

Let us show it for $k = 2$. We have the Bismuth-Elworthy at the second order (see [27]): for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} D^2u(t, x) \cdot (h, h) &= \frac{2}{t} \left[\mathbb{E} \left(Du(t/2, X_x(t/2)) \cdot (DX_x(t/2) \cdot h) \int_0^{t/2} \langle DX_x(t/2) \cdot h, dW(s) \rangle \right) \right. \\ &\quad \left. + \mathbb{E} \left(\int_0^{t/2} Du(t-s, X_x(s)) \cdot (D^2X_x(s) \cdot (h, h)) ds \right) \right]. \end{aligned} \quad (6.6)$$

Using Cauchy-Schwarz inequality, Burkholder-Davis-Gundy inequality, (6.4) and (6.3) which bound $DX_x(t) \cdot h$ and $D^2X_x(t) \cdot (h, h)$, we get for $0 < t \leq 1$, $x \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$

$$\begin{aligned} &|D^2u(t, x) \cdot (h, h)| \\ &\leq \frac{2}{t} \left(\mathbb{E} |Du(t/2, X_x(t/2))|^4 \right)^{1/4} \left(\mathbb{E} |DX_x(t/2) \cdot h|^4 \right)^{1/4} \left(\mathbb{E} \left(\int_0^{t/2} |DX_x(t/2) \cdot h|^2 ds \right) \right)^{1/2} \\ &\quad + \frac{2}{t} \int_0^{t/2} \left(\mathbb{E} |Du(t-s, X_x(s))|^2 \right)^{1/2} \left(\mathbb{E} |D^2X_x(s) \cdot (h, h)|^2 \right)^{1/2} ds \\ &\leq \frac{C}{t} (1 + |x|^q) |h|^2 \left[t^{1/2} \left(\mathbb{E} |Du(t/2, X_x(t/2))|^4 \right)^{1/4} + \int_0^{t/2} \left(\mathbb{E} |Du(t-s, X_x(s))|^2 \right)^{1/2} ds \right]. \end{aligned}$$

To conclude, we use the result (6.5) for $k = 1$ and the Proposition 2.2 on the moment of the solution of the equation (2.1).

Using the proof of (6.6) done in [27], we show the following formula at the order 3 for $x \in \mathbb{R}^d$, $h \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} &D^3u(t, x) \cdot (h, h, h) \\ &= \frac{2}{t} \left[\mathbb{E} \left(D^2u(t/2, X_x(t/2)) \cdot (DX_x(t/2) \cdot h, DX_x(t/2) \cdot h) \int_0^{t/2} \langle DX_x(s) \cdot h, dW(s) \rangle \right) \right. \\ &\quad + \mathbb{E} \left(Du(t/2, X_x(t/2)) \cdot (D^2X_x(t/2) \cdot (h, h)) \int_0^{t/2} \langle DX_x(s) \cdot h, dW(s) \rangle \right) \\ &\quad + 2\mathbb{E} \left(\int_0^{t/2} D^2u(t-s, X_x(s)) \cdot (D^2X_x(s) \cdot (h, h), DX_x(s) \cdot h) ds \right) \\ &\quad \left. + \mathbb{E} \left(\int_0^{t/2} Du(t-s, X_x(s)) \cdot (D^3X_x(s) \cdot (h, h, h)) ds \right) \right]. \end{aligned}$$

We use the same arguments as previously to prove (6.5) for $k = 3$. The proof for higher order use the same ideas. \blacklozenge

We can now show Proposition 2.8 for $t \geq 1$.

Lemma 6.6 *Let $\phi \in C_{pol}^\infty(\mathbb{R}^d)$ be fixed such that $\phi \in C_{2\ell_0}^0(\mathbb{R}^d)$ and u be the solution of (2.17). For all $k \in \mathbb{N}^*$, there exist constant C_k and m_k such that for all $t \geq 1$, $\mathbf{j} = (j_1, \dots, j_d) \in \mathbb{N}^d$ such that $|\mathbf{j}| = k$ and $x \in \mathbb{R}^d$,*

$$|\partial_{\mathbf{j}}u(t, x)| \leq C_k \exp(-\lambda t)(1 + |x|^{m_k}) \|\phi\|_{0,2\ell_0},$$

where λ is defined in Proposition 6.3.

Remark 6.7 *The constant m_k depends of the polynomial growth of all the derivatives of ϕ of order less than k and the polynomial growth of all the derivatives of V of order less than $k + 1$.*

Proof. Let $x \in \mathbb{R}^d$ and $t \geq 1$ be fixed. Let us assume that $\phi \in C_{2\ell_0}^0(\mathbb{R}^d)$. We have for all $t \geq 1$,

$$u(t, x) = \mathbb{E}(u(t-1, X_x(1))) = \mathbb{E}(P_{t-1}(X_x(1))).$$

Let v defined for all $s > 0$ by $v(s, x) = \mathbb{E}P_{t-1}(X_x(s))$, then $u(t, x) = v(1, x)$. Using Proposition 6.3, we have for all $y \in \mathbb{R}^d$

$$|P_{t-1}(y)| \leq C(1 + |y|^{2\ell_0}) \exp(-\lambda t) \|\phi\|_{0,2\ell_0}.$$

For $k \in \mathbb{N}^*$, using Lemma 6.5 on v and $t \geq 1$, we get that there exist constants $m_k \geq 2\ell_0$ and C such that for any $\mathbf{j} \in \mathbb{N}^d$ such that $|\mathbf{j}| = k$

$$\begin{aligned} |\partial_{\mathbf{j}}u(t, x)| &\leq C \|P_{t-1}\|_{0,2\ell_0} (1 + |x|^{m_k}) \\ &\leq C(1 + |x|^{m_k}) \exp(-\lambda t) \|\phi\|_{0,2\ell_0}. \end{aligned}$$

\blacklozenge

Chapter 3

Weak backward error analysis for Langevin process

1 Introduction

In the last decades, backward error analysis has become a powerful tool to analyze the long time behavior of numerical schemes applied to evolution equations - see [37, 59, 76]. The main idea can be described as follows: Let us consider an ordinary differential equation of the form

$$\dot{y}(t) = f(y(t)),$$

where $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a smooth vector field, and denote by $\phi_t^f(p)$ the associated flow. By definition, a numerical method defines for a small time step δ an approximation Φ_δ of the exact flow ϕ_δ^f : We have for bounded $p \in \mathbb{R}^d$, $\Phi_\delta(p) = \phi_\delta^f(p) + \mathcal{O}(\delta^{r+1})$ where r is the order of the method.

The idea of backward error analysis is to show that Φ_δ can be interpreted as the exact flow $\phi_\delta^{f_\delta}$ of a modified vector field defined as a series in powers of δ

$$f_\delta = f + \delta^r f_r + \delta^{r+1} f_{r+1} + \dots,$$

where f_l , $l \geq r$ are vector fields depending on the numerical method. In general, the series defining f_δ does not converge, but it can be shown that for bounded y , we have for arbitrary N

$$\Phi_\delta(y) = \phi_\delta^{f_\delta^N}(y) + C_N \delta^{N+1},$$

where f_δ^N is the truncated series:

$$f_\delta^N = f + \delta^r f_r + \dots + \delta^N f_N.$$

Under some analytic assumptions, the constant $C_N \delta^{N+1}$ can be optimized in N , so that the error term in the previous equation can be made exponentially small with respect to δ .

Such a result is very important and has many applications in the case where f has some strong geometric properties, such as Hamiltonian - see [36, 37, 59, 71, 76]. In this situation, and under some compatibility conditions on the numerical method Φ_δ , the modified vector field f_δ inherits the structure of f .

More recently, these ideas have been extended in some situations to Hamiltonian PDEs : First in the linear case [23] and then in the semi linear case - nonlinear Schrödinger or wave equations - see [29, 30].

In [22], the authors give a weak backward error analysis for SDEs defined on the d -dimensional torus. The aim of this chapter is to extend the result of [22] to the Langevin process on \mathbb{R}^{2d} . This process is defined by the stochastic Hamiltonian equation:

$$\begin{aligned} dq(t) &= M^{-1}p(t)dt, \\ dp(t) &= -\partial_q V(q(t))dt - \gamma p(t)dt + \sigma M^{1/2}dW(t), \end{aligned} \quad (1.1)$$

where V is the potential energy function of a classical model for a molecular system, M is a mass matrix, $\gamma > 0$ is a free parameter, the friction coefficient and the term $\sigma dW(t)$ is a fluctuation term bringing energy into the system. This equation can be used to give an approximation of the following integral

$$\int_{\mathbb{R}^{2d}} \phi(q, p) Z^{-1} \exp(-\beta H(q, p)) dq dp,$$

where $\beta = \frac{1}{k_B T} = \frac{2\gamma}{\sigma^2}$, T is temperature, k_B is Boltzmann's constant, $H(q, p) = \frac{1}{2}p^t M^{-1}p + V(q)$, ϕ is a smooth function and $Z = \int_{\mathbb{R}^{2d}} \exp(-\beta H(q, p)) dq dp$ - see [9, 57, 60] for more explanations.

In this work, we investigate the weak error which concerns the law of the solution. More particularly, we study behavior for long time of weak approximations of the Langevin process.

Let us recall that given a SDE in \mathbb{R}^d of the form

$$dX = f(X)dt + g(X)dW, \quad (1.2)$$

discretized by an explicit Euler scheme $(X_n)_{n \in \mathbb{N}}$ with time step δ , then, under assumptions on f , g and $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ - see [64, 69, 83, 84] - the explicit Euler scheme $(X_n)_{n \in \mathbb{N}}$ has weak error order 1:

$$|\mathbb{E}(\phi(X_n)) - \mathbb{E}(\phi(X(n\delta)))| \leq c(\phi, T)\delta, \quad n = 0, \dots, \lfloor T/\delta \rfloor, \quad T > 0.$$

Error estimates on long times for elliptic and hypoelliptic SDEs have already been proved, especially in the case of explicit scheme - [82, 83, 85] - or on the torus - [64]. In [82, 83], it is shown that for a sufficiently small time step the explicit Euler scheme defines an ergodic process and that the invariant measure of the Euler scheme is close to the invariant measure of the SDE. In [85], under the assumption of the existence of a unique invariant measure associated to the SDE, Talay and Tubaro have shown that the weak error and the invariant measure associated to the Euler scheme can be expanded in powers of the time step δ . The assumptions on f and g used in [82, 83, 85] are restrictive. Moreover, the results described in these papers are valid only for explicit schemes.

In [64], a larger class of schemes is studied. It is shown that given an elliptic or hypoelliptic SDE, the ergodic averages provided by a class of implicit and explicit schemes are asymptotically close to the average of the invariant measure of the SDE. The authors also show an expansion in expectation of the invariant measure for any time-step. Unfortunately, they work on the d -dimensional torus.

The long time behavior of approximations of the Langevin equation has already been studied, but the authors need the time step to be small enough [43, 84] or work on the torus for the position [58]. In [43], under certain assumptions and in particular in the case of the Langevin equation, it is shown that for sufficiently small time steps, two kinds of implicit schemes are ergodic processes. They also show that the invariant measures associated with these schemes converge to the invariant measure of the Langevin equation. In [84], Talay shows the exponential convergence of the solution associated to the Kolmogorov equation

and, for a sufficiently small time step δ , an expansion with respect to δ of the invariant measure to the implicit scheme which is close to the invariant measure of the SDE. In [58], the authors study the Langevin equation and work with explicit splitting methods. They provide error estimates on the invariant distribution for small step size, and compare the sampling bias obtained for various choices of explicit splitting methods.

In this paper, we work on \mathbb{R}^{2d} and V and all its derivatives are not necessarily bounded but have at most polynomial growth at infinity. The aim of this paper is, under assumptions on V , to show a weak backward error analysis result: We show an expansion with respect to the time step δ of $\mathbb{E}\phi(q_k, p_k)$ where (q_k, p_k) is obtained by an implicit scheme. Unlike [43, 84], we do not need that the time step is small enough and our assumptions are less restrictive than in [84].

The idea to extend the backward error analysis to SDE has already been developed in [1, 22, 50, 80]. In [1], the authors use this approach to construct new methods of weak order two to approximate stochastic differential equations. In [22], the authors study a SDE defined on the d -dimensional torus and its approximation by the explicit Euler scheme. They show, without any restriction on the time step, an expansion of $\mathbb{E}\phi(X_k)$ where $X_k = (q_k, p_k)$ is obtained by the explicit Euler scheme. In [80, 89], the authors show that it is possible to build of a modified SDE associated with the Euler scheme, but only up to second order, i.e. for $N = 2$. In this case, they are able to write down a modified SDE:

$$d\tilde{X} = \tilde{f}(\tilde{X})dt + \tilde{g}(\tilde{X})dW,$$

such that

$$|\mathbb{E}(\phi(X_k)) - \mathbb{E}(\phi(\tilde{X}(k\delta)))| \leq c_1(\phi, T)\delta^2, \quad k = 0, \dots, \lfloor T/\delta \rfloor, \quad T > 0.$$

In this paper, we take the approach described in [22, 50]. We show that the generator associated with the solution of the SDE (1.1) coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. It is known - see [84] - that given $\phi : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ and denoting by $(q_{q^0}(t), p_{p^0}(t))$ the solution of (1.1) satisfying $(q(0), p(0)) = (q^0, p^0)$, the function u defined for $t \geq 0$ and $(q^0, p^0) \in \mathbb{R}^{2d}$ by $u(t, q^0, p^0) = \mathbb{E}(\phi(q_{q^0}(t), p_{p^0}(t)))$ satisfies the Kolmogorov equation

$$\begin{aligned} \partial_t u(t, q, p) &= Lu(t, q, p), \quad t > 0, \quad q \in \mathbb{R}^d, \quad p \in \mathbb{R}^d \\ u(0, q, p) &= \phi(q, p), \quad q \in \mathbb{R}^d, \quad p \in \mathbb{R}^d \end{aligned} \tag{1.3}$$

where L is the Kolmogorov operator associated with the SDE.

We show that with the numerical solution, we can associate a modified Kolmogorov operator of the form

$$\mathcal{L}(\delta, q, p, \partial_q, \partial_p) = L(q, p, \partial_q, \partial_p) + \delta L_1(q, p, \partial_q, \partial_p) + \delta^2 L_2(q, p, \partial_q, \partial_p) + \dots,$$

where L_l , $l \geq 1$ are some modified operators of order $2l + 2$. The series does not converge but we consider truncated series:

$$\begin{aligned} L^{(N)}(\delta, q, p, \partial_q, \partial_p) &= L(q, p, \partial_q, \partial_p) + \delta L_1(q, p, \partial_q, \partial_p) + \delta^2 L_2(q, p, \partial_q, \partial_p) + \dots \\ &\quad + \delta^N L_N(q, p, \partial_q, \partial_p). \end{aligned}$$

Note that this operator is no longer of order 2 and we can not define easily a solution to the modified equation

$$\partial_t v^N(t, q, p) = L^{(N)}(\delta, q, p, \partial_q, \partial_p)v^N(t, q, p).$$

However, in our case, we can build an approximated solution $v^{(N)}$ such that

$$\left| \mathbb{E}(\phi(q_k, p_k)) - v^{(N)}(k\delta, q_0, p_0) \right| \leq c_2(\phi, N, q_0, p_0) \delta^{N+1}, \quad k = 0, \dots, [T/\delta], \quad T > 0.$$

As the constant c_2 does not depend on T , we have an approximation result valid on very long times. We also show that there exists a modified invariant measure for $L^{(N)}(\delta, q, p, \partial_q, \partial_p)$.

Three tools are necessary to prove our main result (see Theorem 2.17). First, we need to find a scheme which has moments of all orders bounded uniformly in time. As we wish to investigate the asymptotic properties of our implicit schemes, we need results on the long time behavior of the law of u the solution of (1.3). More precisely, we need exponential convergence of u and all its derivatives in an appropriate sense and regularity of the solution of the Poisson equation associated with L , i.e. the equation $L(q, p, \partial_q, \partial_p)h = g$. This last tool is also used in [64]. A proof of the exponential convergence to equilibrium of u and all its derivatives can be found in [84], but we need to know more precisely the dependence on the bound. Moreover, using a result described in [43], we simplify the proof in [84] (see Appendix for more details).

In Section 2, we first introduce the SDE, the assumptions that we need and the numerical schemes that we use. Then, we give some results on the Kolmogorov operator and on the solution of the Kolmogorov equation. More precisely, we describe the behavior in long time of the solution of the Kolmogorov equation. We end this section with the statement of our main result. The other sections describe the proof of our main result. The first step is to build the operators L_i for $i \in \mathbb{N}$. The principal idea is to give an asymptotic expansion of the weak approximation (Section 3) and then use it to build the operators L_i for $i \in \mathbb{N}$ (Section 4.1) and a function $v^{(N)}$ such that the weak approximation and $v^{(N)}$ are close to an error with respect to the time step. In Section 5, we analyze the long time behavior of $v^{(N)}$ and we finish to prove our main result.

We decided to work with two implicit schemes: an implicit Euler scheme and an implicit split-step scheme. However, if we consider another scheme which has moments of all order bounded uniformly in time, it is easy to adapt our proof. The principal issue is the building of the operators L_i for $i \in \mathbb{N}$. As said previously, we build it by an asymptotic expansion of the weak approximation. If we can associate with our scheme an adapted continuous process which interpolates it, then it is easier to have an asymptotic expansion of the weak approximation than in our case. Indeed, we can use Itô formula to have it.

2 Preliminaries

2.1 Presentation of the SDE

We warn the reader that constants may vary from line to line during the proofs, and that in order to use lighter notations we usually forget to mention dependence of the parameters. We use the generic notation C for such constants.

Throughout this chapter, we use the following notation: $\mathbb{N} = \{0, 1, 2, \dots\}$ and $\mathbb{N}^* = \{1, 2, \dots\}$. We write the dot product of two vectors $q = (q_1, \dots, q_d) \in \mathbb{R}^d$ and $p = (p_1, \dots, p_d) \in \mathbb{R}^d$ as

$$\langle q, p \rangle = \sum_{i=1}^d q_i p_i.$$

For a multi-index $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d$, we set $|\mathbf{k}| = k_1 + \dots + k_d$ and for a function

$\phi \in C^\infty(\mathbb{R}^d)$

$$\partial_q^{\mathbf{k}} \phi(q) = \frac{\partial^{|\mathbf{k}|} \phi(q)}{\partial^{k_1} q_1 \dots \partial^{k_d} q_d}, \quad q = (q_1, \dots, q_d) \in \mathbb{R}^d.$$

For $p \in \mathbb{R}^d$, we set $\partial_p = (\frac{\partial}{\partial p_1}, \dots, \frac{\partial}{\partial p_d})^\top$ and for $k \in \mathbb{N}^*$, ∂_p^k is the differential of order k . We also use the following notation

$$\begin{aligned} C_{pol}^\infty(\mathbb{R}^d) &= \{f \in C^\infty(\mathbb{R}^d) \text{ such that } f \text{ and all its derivatives have polynomial growth}\} \\ &= \{f \in C^\infty(\mathbb{R}^d) \text{ such that for all } \mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d, \exists C_{\mathbf{k}} > 0, n_{\mathbf{k}} \in \mathbb{N}^* \\ &\quad \text{such that for all } q \in \mathbb{R}^d, \quad |\partial_q^{\mathbf{k}} f(q)| \leq C_{\mathbf{k}}(1 + |q|^{n_{\mathbf{k}}})\}. \end{aligned}$$

Let $(\Omega, \mathcal{F}, \mathcal{F}_t, \mathbf{P})$, $t \geq 0$, be a filtered probability space and $W(t) = (W_1(t), \dots, W_d(t))$ be a d -dimensional $\{\mathcal{F}_t\}_{t \geq 0}$ -adapted standard Wiener process. We consider a process $(q(t), p(t))_{t \in \mathbb{R}_+}$ on \mathbb{R}^{2d} which verifies the stochastic Hamiltonian differential system

$$\begin{aligned} q(t) &= q(0) + M^{-1} \int_0^t p(s) ds, \\ p(t) &= p(0) - \int_0^t \partial_q V(q(s)) ds - \gamma \int_0^t p(s) ds + \sigma M^{1/2} W(t), \quad t > 0, \end{aligned}$$

where $\gamma > 0$ is a friction coefficient, $\sigma > 0$ and M is a positive diagonal mass matrix. The function V verifies the following conditions, called Assumptions **B**:

B-1: $V \in C_{pol}^\infty(\mathbb{R}^d)$.

B-2: There exist $\kappa > 0$ and $\beta \in]0, 1[$ such that for all $q \in \mathbb{R}^d$

$$\frac{1}{2} \langle \partial_q V(q), q \rangle \geq \beta V(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)} |q|^2 - \kappa. \quad (2.1)$$

B-3: The function V is semi-convex: There exist a bounded function $V_1 \in C^\infty(\mathbb{R}^d)$ with bounded derivatives and a convex function $V_2 \in C^\infty(\mathbb{R}^d)$ such that $V = V_1 + V_2$.

B-4: There exists a constant κ_1 such that for all $q \in \mathbb{R}^d$, $V(q) \geq \kappa_1 |q|^2$.

Remark 2.1 We can replace assumption **B-4** by

$$\exists \kappa_1, \kappa_2 : \quad V(q) \geq \kappa_1 |q|^2 - \kappa_2 \quad \text{for all } q \in \mathbb{R}^d,$$

however it is more convenient to assume that $V \geq 0$.

As a consequence of the semi-convexity of V - assumption **B-3** - we obtain the existence of a positive constant θ , usually called the constant of semi-convexity, such that for all $q \in \mathbb{R}^d$ and $h \in \mathbb{R}^d$,

$$\partial_q^2 V(q)(h, h) \geq -\theta |h|^2. \quad (2.2)$$

As a consequence of the assumption **B-2** we obtain a dissipativity inequality: There exists a strictly positive real number β_1 such that

$$\langle q, \partial_q V(q) \rangle \geq \beta_1 |q|^2 - \kappa \quad \text{for all } q \in \mathbb{R}^d. \quad (2.3)$$

Moreover, a polynomial function V , growing at infinity like $|q|^{2k}$, where $k \in \mathbb{N}^*$, satisfies Assumptions **B**.

To slightly simplify the presentation that follows, we make the change of variables $q \rightarrow M^{-1/2}q$, $p \rightarrow M^{1/2}p$, with a corresponding adjustment of the potential. This is equivalent to assuming $M = I$ and the new potential the verifies same assumptions as V .

Hence, for now on, we consider the following equation:

$$\begin{aligned} q(t) &= q(0) + \int_0^t p(s)ds, \\ p(t) &= p(0) - \int_0^t \partial_q V(q(s))ds - \gamma \int_0^t p(s)ds + \sigma W(t), \quad t > 0, \end{aligned} \quad (2.4)$$

where V satisfies the conditions **B**.

Remark 2.2 *Under these assumptions, we have that $(q(t), p(t))$ is well-defined for all $t > 0$ - see Chapter III, Theorem 4.1 in [47].*

We also consider the Hamiltonian function H defined for $(q, p) \in \mathbb{R}^{2d}$ by

$$H(q, p) := \frac{1}{2}|p|^2 + V(q).$$

We define the Kolmogorov operator L associated with (2.4) for $\phi \in C^\infty(\mathbb{R}^{2d})$ and $(q, p) \in \mathbb{R}^{2d}$ by

$$L\phi(q, p) := \langle p, \partial_q \phi(q, p) \rangle - \langle \partial_q V(q) + \gamma p, \partial_p \phi(q, p) \rangle + \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \phi(q, p).$$

For the study of (2.4), it is useful to define the Lyapunov function Γ defined for all $(q, p) \in \mathbb{R}^{2d}$ by

$$\Gamma(q, p) = \frac{1}{2}|p|^2 + V(q) + \frac{\gamma}{2} \langle q, p \rangle + \frac{\gamma^2}{4}|q|^2 + 1. \quad (2.5)$$

Under assumptions **B**, the function Γ verifies the following properties:

Lemma 2.3 *We have for all $(q, p) \in \mathbb{R}^{2d}$*

$$\Gamma(q, p) \geq \frac{1}{8}|p|^2 + \frac{\gamma^2}{12}|q|^2 + 1. \quad (2.6)$$

Moreover, for every $\ell \geq 1$, there exist strictly positive real numbers a_ℓ and d_ℓ such that we have for every $(q, p) \in \mathbb{R}^{2d}$

$$L\Gamma^\ell(q, p) \leq -a_\ell \Gamma^\ell(q, p) + d_\ell. \quad (2.7)$$

Remark 2.4 *We can find a similar proof of Lemma 2.3 in [43].*

Proof. We first show (2.6). We have, for all $\varepsilon > 0$ and $(q, p) \in \mathbb{R}^{2d}$,

$$\gamma \langle p, q \rangle \geq -\frac{\varepsilon}{2}|p|^2 - \frac{\gamma^2}{2\varepsilon}|q|^2,$$

then, using the positivity of V , we get for all $(q, p) \in \mathbb{R}^{2d}$ and $\varepsilon > 0$

$$\Gamma(q, p) \geq \left(\frac{1}{2} - \frac{\varepsilon}{4}\right)|p|^2 + \gamma^2 \left(\frac{1}{4} - \frac{1}{4\varepsilon}\right)|q|^2 + 1.$$

Taking $\varepsilon = \frac{3}{2}$, we show (2.6).

We now show the other property of Γ (2.7). We first consider the case $\ell = 1$. We have for any $(q, p) \in \mathbb{R}^{2d}$ and $\varepsilon > 0$

$$\Gamma(q, p) \leq \frac{1}{2}|p|^2 + V(q) + \frac{\gamma}{2}\left(\frac{\varepsilon}{2}|p|^2 + \frac{1}{2\varepsilon}|q|^2\right) + \frac{\gamma^2}{4}|q|^2 + 1.$$

Multiplying by β , taking $\varepsilon = \frac{2(1-\beta)}{\gamma\beta}$ and using assumption **B-2** on the derivative of V , we get for all $(q, p) \in \mathbb{R}^{2d}$

$$\beta\Gamma(q, p) \leq \frac{1}{2}|p|^2 + \beta V(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)}|q|^2 + \beta \leq \frac{1}{2}|p|^2 + \frac{1}{2}\langle \partial_q V(q), q \rangle + \kappa + \beta. \quad (2.8)$$

Using this inequality, we can now show (2.7) for $\ell = 1$. Indeed, we have for all $(q, p) \in \mathbb{R}^{2d}$

$$\begin{aligned} L\Gamma(q, p) &= -\frac{\gamma}{2}|p|^2 - \frac{\gamma}{2}\langle q, \partial_q V(q) \rangle + \frac{d\sigma^2}{2} \\ &\leq \frac{d\sigma^2}{2} + (\kappa + \beta)\gamma - \beta\gamma\Gamma(q, p). \end{aligned}$$

We have shown (2.7) for $\ell = 1$ with $d_1 = \frac{d\sigma^2}{2} + \gamma(\kappa + \beta)$ and $a_1 = \beta\gamma$.

Let $\ell \geq 2$ be an integer. We now calculate $L\Gamma^\ell$. We have, for $(q, p) \in \mathbb{R}^{2d}$ and $i \in \{1, \dots, 2d\}$, with the notation $x = (q, p)$,

$$\begin{aligned} \frac{\partial}{\partial x_i}\Gamma^\ell(q, p) &= \ell\Gamma^{\ell-1}(q, p)\frac{\partial}{\partial x_i}\Gamma(q, p), \\ \frac{\partial^2}{\partial x_i\partial x_i}\Gamma^\ell(q, p) &= \ell\Gamma^{\ell-1}(q, p)\frac{\partial^2}{\partial x_i\partial x_i}\Gamma(q, p) + \ell(\ell-1)\Gamma^{\ell-2}(q, p)\left(\frac{\partial}{\partial x_i}\Gamma(q, p)\right)^2, \end{aligned}$$

then we get for all $(q, p) \in \mathbb{R}^{2d}$

$$L\Gamma^\ell(q, p) = \ell\Gamma^{\ell-1}(q, p)L\Gamma(q, p) + \frac{\ell(\ell-1)}{2}\sigma^2\Gamma^{\ell-2}(q, p)\left|p + \frac{\gamma}{2}q\right|^2.$$

Using for $(q, p) \in \mathbb{R}^{2d}$

$$\left|p + \frac{\gamma}{2}q\right|^2 \leq 2\Gamma(q, p)$$

and computations for $\ell = 1$, we get for $(q, p) \in \mathbb{R}^{2d}$

$$\begin{aligned} L\Gamma^\ell(q, p) &\leq \ell\Gamma^{\ell-1}(q, p)(d_1 - a_1\Gamma(q, p)) + \ell(\ell-1)\sigma^2\Gamma^{\ell-1}(q, p) \\ &= -a_1\ell\Gamma^\ell(q, p) + \ell(d_1 + \ell - 1)\Gamma^{\ell-1}(q, p). \end{aligned}$$

Using the fact that for any $x \in \mathbb{R}$ and $\varepsilon > 0$

$$|x|^{\ell-1} \leq \varepsilon|x|^\ell + C_\varepsilon,$$

we get

$$L\Gamma^\ell(q, p) \leq (-a_1\ell + \varepsilon\ell(d_1 + \ell - 1))\Gamma^\ell(q, p) + \ell(d_1 + \ell - 1)C_\varepsilon.$$

Choosing $\varepsilon = \frac{a_1}{\ell(d_1 + \ell - 1)}$, $a_\ell = a_1(\ell - 1)$ and d_ℓ large enough, we obtain (2.7) for ℓ . \blacklozenge

Using assumptions **B** and properties of Γ , we have the following result on the moments of the solution:

Lemma 2.5 *Let a process $(q(\cdot), p(\cdot))$ which satisfies (2.4). We have for each $\ell \geq 1$ such that $\mathbb{E}|q(0)|^{2\ell} < \infty$ and $\mathbb{E}|p(0)|^{2\ell} < \infty$ that there exist strictly positive real numbers $k_\ell \geq 2\ell$, α_ℓ and C_ℓ such that for all $t > 0$*

$$\mathbb{E}(|q(t)|^{2\ell} + |p(t)|^{2\ell}) \leq C_\ell \left(1 + (\mathbb{E}|p(0)|^{k_\ell} + \mathbb{E}|q(0)|^{k_\ell}) \exp(-\alpha_\ell t)\right).$$

Proof. Let $N \in \mathbb{N}^*$ be fixed. We consider

$$\tau_N = \inf\{t, \text{ such that } \max(|q(t)|, |p(t)|) \geq N\}.$$

Let $\ell \in \mathbb{N}^*$ be fixed. We will show the following: There exists a positive real number C such that for all $t \geq 0$

$$\mathbb{E}\left(\Gamma^\ell(q(t), p(t))\right) \leq C \left(1 + \Gamma^\ell(q(0), p(0)) \exp(-\alpha t)\right). \quad (2.9)$$

Let a_ℓ be the constant defined in (2.7). Let $\alpha < a_\ell$ be fixed. We apply the Itô formula to $\Gamma^\ell(q(t), p(t)) \exp(\alpha t)$. We obtain for all $t \geq 0$

$$\begin{aligned} & \Gamma^\ell(q(t \wedge \tau_N), p(t \wedge \tau_N)) \exp(\alpha(t \wedge \tau_N)) \\ &= \Gamma^\ell(q(0), p(0)) + \alpha \int_0^{t \wedge \tau_N} \Gamma^\ell(q(s), p(s)) \exp(\alpha s) ds \\ & \quad + \int_0^{t \wedge \tau_N} \langle p(s), \partial_q \Gamma^\ell(q(s), p(s)) \rangle \exp(\alpha s) ds \\ & \quad - \int_0^{t \wedge \tau_N} \langle \partial_q V(q(s)) + \gamma p(s), \partial_p \Gamma^\ell(q(s), p(s)) \rangle \exp(\alpha s) ds \\ & \quad + \sigma \int_0^{t \wedge \tau_N} \partial_p \exp(\alpha s) \langle \Gamma^\ell(q(s), p(s)), dW(s) \rangle \\ & \quad + \frac{\sigma^2}{2} \int_0^{t \wedge \tau_N} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \Gamma^\ell(q(s), p(s)) \exp(\alpha s) ds \\ &= \Gamma^\ell(q(0), p(0)) + \alpha \int_0^{t \wedge \tau_N} \Gamma^\ell(q(s), p(s)) \exp(\alpha s) ds \\ & \quad + \int_0^{t \wedge \tau_N} L \Gamma^\ell(q(s), p(s)) \exp(\alpha s) ds \\ & \quad + \sigma \int_0^{t \wedge \tau_N} \exp(\alpha s) \langle \partial_p \Gamma^\ell(q(s), p(s)), dW(s) \rangle. \end{aligned}$$

The stochastic integral is a square integrable martingale because $\Gamma(q(\cdot), p(\cdot))$ is bounded on $[0, t \wedge \tau_N]$. Thus its average vanishes. Using the positivity of Γ , the inequality (2.7) and $\alpha < a_\ell$, we obtain for all $t \geq 0$

$$\begin{aligned} & \mathbb{E}\left(\Gamma^\ell(q(t \wedge \tau_N), p(t \wedge \tau_N)) \exp(\alpha(t \wedge \tau_N))\right) \\ & \leq \Gamma^\ell(q(0), p(0)) + \frac{d_\ell}{\alpha} \mathbb{E}(\exp(\alpha(t \wedge \tau_N))) \\ & \quad + (\alpha - a_\ell) \mathbb{E}\left(\int_0^{t \wedge \tau_N} \Gamma^\ell(q(s), p(s)) \exp(\alpha s) ds\right) \\ & \leq \Gamma^\ell(q(0), p(0)) + \frac{d_\ell}{\alpha} \mathbb{E}(\exp(\alpha(t \wedge \tau_N))). \end{aligned}$$

Fatou's lemma on the left hand side and the Monotone convergence Theorem on the right hand side of the last inequality now leads to (2.9). To conclude, we use property (2.6) and the polynomial growth of Γ . \blacklozenge

Remark 2.6 *We can find another proof of Lemma 2.5 in [84].*

2.2 Numerical schemes

For a small time step δ and $x \in \mathbb{R}^{2d}$, the classical explicit Euler method applied to (1.2), is defined for $i = 1, \dots, 2d$, by $X_0 = x$ and the formula

$$X_{n+1}^i = X_n^i + \delta f^i(X_n) + \sum_{\ell=1}^m g_\ell^i(X_n)(W^\ell((n+1)\delta) - W^\ell(n\delta)), \quad n \geq 0. \quad (2.10)$$

The ordinary Euler scheme (2.10) may be unstable when the coefficients of the differential equation (2.4) are unbounded - see [43]. We are led to avoid explicit schemes. In fact, we study two different implicit schemes. For a small time step $\delta > 0$, we consider an implicit split-step scheme defined by $q_0 = q(0)$, $p_0 = p(0)$ and for $n \in \mathbb{N}$

$$\begin{cases} q_{n+1} &= q_n + \delta p_n^* \\ p_n^* &= p_n - \delta \gamma p_n^* - \delta \partial_q V(q_{n+1}), \\ p_{n+1} &= p_n^* + \sigma(W((n+1)\delta) - W(n\delta)) = p_n^* + \sqrt{\delta} \sigma \eta_n, \end{cases} \quad (2.11)$$

where $\eta_n = {}^t(\eta_{n,1}, \dots, \eta_{n,d})$ is a \mathbb{R}^d -valued random variable and $\{\eta_{n,i} : n \in \mathbb{N}, i \in \{1, d\}\}$ is a collection of i.i.d. real-valued random variables satisfying $\eta_{1,1} \sim \mathcal{N}(0, 1)$. We also consider the implicit Euler scheme defined by $q_0 = q(0)$, $p_0 = p(0)$ and for $n \in \mathbb{N}$

$$\begin{cases} q_{n+1} &= q_n + \delta p_{n+1} \\ p_{n+1} &= p_n - \delta \partial_q V(q_{n+1}) - \gamma \delta p_{n+1} + \sqrt{\delta} \sigma \eta_n, \end{cases} \quad (2.12)$$

where $\eta_n = {}^t(\eta_{n,1}, \dots, \eta_{n,d})$ is as above.

The following Lemma shows that for q_n and p_n fixed, q_{n+1} is well-defined for $\delta < \delta_0 := \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$ where θ is the constant of semi-convexity of V and γ is the friction coefficient. Using this result, we have that our two schemes are well-defined for $\delta < \delta_0 := \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$.

Lemma 2.7 *Let $(q, p) \in \mathbb{R}^{2d}$ and $\delta < \delta_0 := \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$. Under the assumption of semi-convexity of V - **B-3** - and the dissipativity inequality (2.3), there exists a unique $z \in \mathbb{R}^d$ such that $z = q + \frac{\delta}{1+\gamma\delta}(p - \delta \partial_q V(z))$.*

Proof. Let $(q, p) \in \mathbb{R}^{2d}$ and $\delta < \delta_0$. Let $P : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be defined for $z \in \mathbb{R}^d$ by $P(z) = -z + q + \frac{\delta}{1+\gamma\delta}(p - \delta \partial_q V(z))$. We have that $P \in C^\infty$. Using the dissipativity inequality (2.3), we obtain for all $z \in \mathbb{R}^d$

$$\begin{aligned} \langle P(z), z \rangle &= -|z|^2 + \langle q, z \rangle - \frac{\delta^2}{1+\delta\gamma} \langle \partial_q V(z), z \rangle + \frac{\delta}{1+\delta\gamma} \langle p, z \rangle \\ &\leq -|z|^2 \left(1 + \frac{\beta_1 \delta^2}{1+\delta\gamma}\right) + \frac{\delta}{1+\delta\gamma} \langle p, z \rangle + \kappa \frac{\delta^2}{1+\delta\gamma} + \langle q, z \rangle. \end{aligned}$$

Thus, for $|z|^2$ large enough we have $\langle P(z), z \rangle < 0$. Then, using a Corollary of Brouwer fixed-point theorem - see for instance [62] - we conclude that there exists $z \in \mathbb{R}^d$ such that $P(z) = 0$. Therefore, we have shown the existence of $z \in \mathbb{R}^d$ such that $z = q + \frac{\delta}{1+\gamma\delta}(p - \delta \partial_q V(z))$. Let us show the uniqueness.

Let $z_1 \in \mathbb{R}^d$ and $z_2 \in \mathbb{R}^d$ such that $P(z_1) = P(z_2) = 0$ and $z_1 \neq z_2$. We have

$$z_1 - z_2 = -\frac{\delta^2}{1+\delta\gamma} (\partial_q V(z_1) - \partial_q V(z_2)).$$

Due to the assumption of semi-convexity - $\mathbf{B-3}$ - we get

$$|z_1 - z_2|^2 = -\frac{\delta^2}{1 + \delta\gamma} \int_0^1 \partial_q^2 V(z_1 + t(z_2 - z_1))(z_1 - z_2, z_1 - z_2) dt \leq \frac{\delta^2 \theta}{1 + \delta\gamma} |z_1 - z_2|^2.$$

Since $\delta < \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$, we have $\frac{\delta^2 \theta}{1 + \delta\gamma} < 1$ and $z_1 = z_2$. \blacklozenge

Remark 2.8 *The condition $\delta < \delta_0 := \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$ is necessary only in the uniqueness part of the proof. We have the existence for all δ . Moreover, in the case where V is convex, the inequality on the second derivative holds true for all $\theta \geq 0$ and therefore we can show uniqueness for all $\delta > 0$.*

Another proof of the fact that the implicit split-step scheme is well defined can be found in [43].

Moreover for δ small enough, we have that these two schemes have moments of all order. More exactly, we have:

Proposition 2.9 *Let $k \in \mathbb{N}^*$ and $\delta < \delta_0 := \frac{\gamma\beta}{4\theta}$ be fixed. Assume that $q_0 = q(0)$ and $p_0 = p(0)$. Under assumptions \mathbf{B} , the implicit split-step scheme (2.11) and the implicit Euler scheme (2.12) satisfy: There exist positive numbers C_k and ℓ_k such that for all $n \in \mathbb{N}$*

$$\mathbb{E}(|q_n|^{2k} + |p_n|^{2k}) < C_k(1 + |q(0)|^{\ell_k} + |p(0)|^{\ell_k}). \quad (2.13)$$

Remark 2.10 *Since $\frac{\gamma\beta}{4\theta} < \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$, the schemes considered are well defined. If we assume that $\delta_0 < 1$ then we can choose C_k independent of δ_0 .*

We will prove this result only for the implicit Euler scheme. The proof for the implicit split-step scheme is similar. A proof for the moment of order 2 of the implicit split-step scheme can be found in [43]. The two proofs use the same ideas.

To prove Proposition 2.9 for the implicit Euler scheme (2.12), we need the following three Lemmas:

Lemma 2.11 *Let $V \in C^\infty(\mathbb{R}^d)$. Let us assume that V is semi-convex, then V verifies for any $q \in \mathbb{R}^d$ and $p \in \mathbb{R}^d$*

$$V(q) - V(p) \leq \langle \partial_q V(q), q - p \rangle + \frac{\theta}{2} |q - p|^2, \quad (2.14)$$

where θ is the constant of semi-convexity of V .

Proof. Let $q \in \mathbb{R}^d$ and $p \in \mathbb{R}^d$. Using the Taylor expansion on V and the semi-convexity assumption $\mathbf{B-3}$ on V , we have

$$\begin{aligned} V(p) - V(q) &= \langle \partial_q V(q), p - q \rangle + \int_0^1 (1 - s) \partial_q^2 V(q + s(p - q))(p - q, p - q) ds \\ &\geq \langle \partial_q V(q), p - q \rangle - \frac{\theta}{2} |q - p|^2. \end{aligned}$$

Finally, we get

$$V(q) - V(p) \leq \langle \partial_q V(q), q - p \rangle + \frac{\theta}{2} |q - p|^2. \quad \blacklozenge$$

Lemma 2.12 Let $0 < \delta < \frac{\gamma\beta}{4\theta}$ and $\Gamma_\delta \in C^\infty(\mathbb{R}^{2d})$ be defined for any $(q, p) \in \mathbb{R}^{2d}$ by

$$\begin{aligned}\Gamma_\delta(q, p) &= \Gamma(q, p) + \frac{\gamma\delta}{4}|p|^2 \\ &= \frac{1}{2}|p|^2 + V(q) + \frac{\gamma}{2}\langle q, p \rangle + \frac{\gamma^2}{4}|q|^2 + 1 + \frac{\gamma\delta}{4}|p|^2,\end{aligned}\quad (2.15)$$

then Γ_δ verifies the following properties: for any $(q, p) \in \mathbb{R}^{2d}$

$$\Gamma_\delta(q, p) \geq \frac{1}{8}|p|^2 \quad (2.16)$$

and for any $n \in \mathbb{N}$

$$(1 + \gamma(1 - \varepsilon)\delta\beta)\Gamma_\delta(q_{n+1}, p_{n+1}) \leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) + \gamma\delta(\kappa + \beta), \quad (2.17)$$

where (q_n, p_n) is the implicit Euler scheme defined by (2.12) and $0 < \varepsilon < 1$ is such that $\delta < \frac{\varepsilon\gamma\beta}{4\theta}$.

Proof. Inequality (2.16) is a consequence of property (2.6) on Γ .

By the definition of the implicit Euler scheme (2.12), we have

$$\begin{aligned}\Gamma_\delta(q_{n+1}, p_{n+1}) &= \frac{1}{2}|p_{n+1}|^2 + V(q_n + \delta p_{n+1}) + \frac{\gamma}{2}\langle q_n, p_{n+1} \rangle + \frac{\gamma\delta}{2}|p_{n+1}|^2 \\ &\quad + \frac{\gamma^2}{4}\left(|q_n|^2 + 2\delta\langle q_n, p_{n+1} \rangle + \delta^2|p_{n+1}|^2\right) + 1 + \frac{\gamma\delta}{4}|p_{n+1}|^2.\end{aligned}$$

Using inequality (2.14) on V , we get

$$\begin{aligned}\Gamma_\delta(q_{n+1}, p_{n+1}) &\leq \Gamma_\delta(q_n, p_{n+1}) + \delta\langle \partial_q V(q_{n+1}), p_{n+1} \rangle + \left(\frac{\delta\gamma}{2} + \frac{\theta\delta^2}{2} + \frac{\gamma^2\delta^2}{4}\right)|p_{n+1}|^2 \\ &\quad + \frac{\gamma^2\delta}{2}\langle q_n, p_{n+1} \rangle.\end{aligned}$$

Since $q_n = q_{n+1} - \delta p_{n+1}$ and, for any $(q, p) \in \mathbb{R}^{2d}$,

$$|p|^2 - |q|^2 = \langle p - q, p + q \rangle = 2\langle p - q, p \rangle - |p - q|^2 \leq 2\langle p - q, p \rangle,$$

we get

$$\begin{aligned}\Gamma_\delta(q_n, p_{n+1}) &= \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) \\ &\quad + \frac{1}{2}\left(|p_{n+1}|^2 - |(1 + \delta\gamma)p_{n+1} + \delta\partial_q V(q_{n+1})|^2\right) \\ &\quad - \frac{\gamma\delta}{2}\langle q_{n+1}, \partial_q V(q_{n+1}) \rangle - \frac{\gamma^2\delta}{2}\langle q_{n+1}, p_{n+1} \rangle \\ &\quad + \frac{\gamma\delta^2}{2}\langle p_{n+1}, \partial_q V(q_{n+1}) + \gamma p_{n+1} \rangle \\ &\quad + \frac{\gamma\delta}{4}\left(|p_{n+1}|^2 - |(1 + \delta\gamma)p_{n+1} + \delta\partial_q V(q_{n+1})|^2\right) \\ &\leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) - \gamma\delta|p_{n+1}|^2 - \delta\langle \partial_q V(q_{n+1}), p_{n+1} \rangle \\ &\quad - \frac{\gamma\delta}{2}\langle q_{n+1}, \partial_q V(q_{n+1}) \rangle - \frac{\gamma^2\delta}{2}\langle q_{n+1}, p_{n+1} \rangle.\end{aligned}$$

Then, we get

$$\begin{aligned}\Gamma_\delta(q_{n+1}, p_{n+1}) &\leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) + \left(\frac{\theta\delta^2}{2} - \frac{\gamma^2\delta^2}{4}\right)|p_{n+1}|^2 \\ &\quad - \frac{\delta\gamma}{2}\left(\langle q_{n+1}, \partial_q V(q_{n+1}) \rangle + |p_{n+1}|^2\right).\end{aligned}$$

Using (2.8) and $\beta < 1$, we have

$$\begin{aligned}\Gamma_\delta(q_n, p_{n+1}) &\leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) - \gamma\delta\beta\Gamma_\delta(q_{n+1}, p_{n+1}) \\ &\quad + \left(\frac{\theta\delta^2}{2} + \frac{\gamma^2\delta^2}{4}(\beta - 1)\right)|p_{n+1}|^2 + (\kappa + \beta)\gamma\delta \\ &\leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) - \gamma\delta\beta\Gamma_\delta(q_{n+1}, p_{n+1}) \\ &\quad + \frac{\theta\delta^2}{2}|p_{n+1}|^2 + (\kappa + \beta)\gamma\delta.\end{aligned}$$

Using property (2.16), we get

$$\begin{aligned}\Gamma_\delta(q_{n+1}, p_{n+1}) &\leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) + \left(\frac{\theta\delta^2}{2} - \beta\frac{\gamma\delta\varepsilon}{8}\right)|p_{n+1}|^2 \\ &\quad + (\kappa + \beta)\gamma\delta - \gamma\delta\beta(1 - \varepsilon)\Gamma_\delta(q_{n+1}, p_{n+1}).\end{aligned}$$

Since $\delta \leq \frac{\varepsilon\gamma\beta}{4\theta}$ it follows that

$$(1 + \gamma(1 - \varepsilon)\delta\beta)\Gamma_\delta(q_{n+1}, p_{n+1}) \leq \Gamma_\delta(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) + \gamma\delta(\kappa + \beta).$$

◆

Lemma 2.13 *Let $\delta < \delta_0 := \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$ be fixed. Let the processes $P_n(\cdot)$ be defined for $t \in [n\delta, (n+1)\delta]$ and $n \in \mathbb{N}^*$ by*

$$P_n(t) = p_n + \sigma(W(t) - W(n\delta)).$$

Then, there exists $C(\delta_0) > 0$ such that for all $n \in \mathbb{N}$ and $t \in [n\delta, (n+1)\delta]$

$$\mathbb{E}(\Gamma_\delta^\ell(q_n, P_n(t))) \leq \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + C(\delta_0) \sum_{i=0}^{\ell-1} (t - n\delta)^{\ell-i} \mathbb{E}(\Gamma_\delta^i(q_n, p_n)). \quad (2.18)$$

Proof. We will show (2.18) by induction on ℓ . Let $n \in \mathbb{N}^*$ be fixed. Using the definition of Γ_δ , independence of q_n with $W(t) - W(n\delta)$ for $t \geq n\delta$ and properties of W , we easily have

$$E(\Gamma_\delta(q_n, p_n + \sigma(W(t) - W(n\delta)))) \leq \mathbb{E}(\Gamma_\delta(q_n, p_n)) + (t - n\delta) \frac{\sigma^2}{2} \left(1 + \frac{\delta_0\gamma}{2}\right).$$

Let $\ell \in \mathbb{N}^*$. Let us assume that (2.18) is true for all $j \leq \ell - 1$ and let us show it for ℓ . Let $n \in \mathbb{N}^*$ be fixed. Using the Itô formula on $\Gamma_\delta(q_n, P_n(t))$, we get for $t \in [n\delta, (n+1)\delta]$

$$\begin{aligned}\Gamma_\delta^\ell(q_n, P_n(t)) &= \Gamma_\delta^\ell(q_n, p_n) + \sigma\ell \int_{n\delta}^t \Gamma_\delta^{\ell-1}(q_n, P_n(s)) \left\langle \left(1 + \frac{\gamma\delta}{2}\right)P_n(s) + \frac{\gamma}{2}q_n, dW(s) \right\rangle \\ &\quad + \frac{1}{2}\ell\left(1 + \frac{\delta\gamma}{2}\right) \int_{n\delta}^t \Gamma_\delta^{\ell-1}(q_n, P_n(s)) ds \\ &\quad + \frac{\ell(\ell-1)}{2} \int_{n\delta}^t \left| \left(1 + \frac{\gamma\delta}{2}\right)P_n(s) + \frac{\gamma}{2}q_n \right|^2 \Gamma_\delta^{\ell-2}(q_n, P_n(s)) ds.\end{aligned}$$

We take the expectation. The second term in the right hand side vanishes because it is a square integrable martingale. Using for $(q, p) \in \mathbb{R}^{2d}$

$$\left| \left(1 + \frac{\gamma\delta}{2}\right)p + \frac{\gamma}{2}q \right|^2 \leq 16\left(1 + \frac{\gamma\delta_0}{2}\right)^2 \Gamma_\delta(q, p),$$

we get, for $t \in [n\delta, (n+1)\delta]$,

$$\mathbb{E}(\Gamma_\delta^\ell(q_n, P_n(t))) \leq \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + C_\ell(\delta_0) \int_{n\delta}^t \mathbb{E}(\Gamma_\delta^{\ell-1}(q_n, P_n(s))) ds.$$

Then, by induction we get (2.18) for ℓ . ◆

Proof of Proposition 2.9 in the case of the implicit Euler scheme (2.12). First, we rewrite the implicit Euler scheme (2.12) as

$$\begin{aligned} q_n &= q_{n+1} - \delta p_{n+1} \\ p_n + \sqrt{\delta} \sigma \eta_n &= p_{n+1} + \delta \partial_q V(q_{n+1}) + \gamma \delta p_{n+1}. \end{aligned} \quad (2.19)$$

Let $\ell \in \mathbb{N}^*$. Using (2.18) for $t = (n+1)\delta$, we see that

$$\begin{aligned} \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n + \sigma\sqrt{\delta}\eta_n)) &\leq \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + C \sum_{i=0}^{\ell-1} \delta^{\ell-i} \mathbb{E}(\Gamma_\delta^i(q_n, p_n)) \\ &\leq \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + C\delta \sum_{i=0}^{\ell-1} \mathbb{E}(\Gamma_\delta^i(q_n, p_n)), \end{aligned}$$

where we can choose C independent of δ . Using the fact that for any $x \in \mathbb{R}$, $i \in \mathbb{N}^*$ such that $i < \ell$ and $\varepsilon_1 > 0$

$$|x|^i \leq \varepsilon_1 |x|^\ell + C_{\varepsilon_1}, \quad (2.20)$$

we get

$$\mathbb{E}(\Gamma_\delta^\ell(q_n, p_n + \sigma\sqrt{\delta}\eta_n)) \leq (1 + \varepsilon_1 \delta C) \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + C C_{\varepsilon_1} \delta \quad (2.21)$$

Moreover, using (2.20) and (2.17), we get that for $\varepsilon_2 > 0$

$$(1 + \gamma(1 - \varepsilon)\delta\beta)^\ell \Gamma_\delta^\ell(q_{n+1}, p_{n+1}) \leq (1 + \delta\varepsilon_2) \Gamma_\delta^\ell(q_n, p_{n+1} + \delta\gamma p_{n+1} + \delta\partial_q V(q_{n+1})) + \delta C_{\varepsilon_2}, \quad (2.22)$$

where $0 < \varepsilon < 1$ is defined in (2.17). Then, using (2.21), (2.19) and (2.22), we get

$$(1 + \gamma(1 - \varepsilon)\delta\beta)^\ell \mathbb{E}(\Gamma_\delta^\ell(q_{n+1}, p_{n+1})) \leq (1 + \delta\varepsilon_2)(1 + \varepsilon_1 \delta C) \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) + \delta C_{\varepsilon_1, \varepsilon_2}.$$

Choosing $\varepsilon_1 = \frac{\gamma(1-\varepsilon)\beta}{2C}$ and $\varepsilon_2 = \lambda\gamma(1-\varepsilon)\beta$ such that $\lambda \leq \frac{1}{2(1+1/2(1-\varepsilon)\gamma\beta\delta_0)}$, we get, $(1 + \varepsilon_1 C)(1 + \varepsilon_2) \leq 1 + \gamma(1 - \varepsilon)\beta$. Then, by induction on n , we get

$$\begin{aligned} \mathbb{E}(\Gamma_\delta^\ell(q_n, p_n)) &\leq \Gamma_\delta^\ell(q, p) + C\delta \sum_{i=1}^n \frac{1}{(1 + \gamma(1 - \varepsilon)\delta\beta)^{(\ell-1)i}} \\ &\leq \Gamma_\delta^\ell(q, p) + C. \end{aligned}$$

To conclude, we use the fact the Γ_δ has polynomial growth and for any $(q, p) \in \mathbb{R}^{2d}$

$$\frac{1}{8}|p|^2 + \frac{\gamma^2}{12}|q|^2 \leq c\Gamma_\delta(q, p).$$

◆

2.3 Preliminary results

Before giving the main result, we will introduce some notations and give results on the Kolmogorov generator L . In particular, we will describe the two important properties that we need to prove our main result.

For $(x, y) \in \mathbb{R}^{2d}$, we denote by $(q_x(t), p_y(t))_{t \geq 0}$ the process that satisfies (2.4) and has for initial data $q_x(0) = x$ and $p_y(0) = y$. From now on, $(P_t)_{t \geq 0}$ is the transition semigroup associated with the Markov process $(q_x(t), p_y(t))_{t \geq 0}$.

In all this chapter, we consider the following spaces: for $k \in \mathbb{N}$ and $\ell \in \mathbb{N}$

$$\mathcal{C}_k^\ell(\mathbb{R}^{2d}) := \left\{ f \in C^\ell(\mathbb{R}^{2d}) \text{ such that for all } \mathbf{j} = (j_1, \dots, j_{2d}) \in \mathbb{N}^d, |\mathbf{j}| \leq \ell, \right. \\ \left. \sup_{x \in \mathbb{R}^{2d}} |\partial^{\mathbf{j}} f(x)| \Gamma^{-k}(x) < \infty \right\}.$$

Let ℓ and k be two integers. For a function $f \in \mathcal{C}_k^\ell(\mathbb{R}^{2d})$, we define the following norm

$$\|f\|_{\ell,k} := \sup_{\substack{\mathbf{j}=(j_1, \dots, j_{2d}) \\ |\mathbf{j}| \leq \ell}} \sup_{x \in \mathbb{R}^{2d}} \left| \frac{\partial^{\mathbf{j}} f(x)}{\Gamma^k(x)} \right|.$$

We also define the semi-norm

$$|f|_{\ell,k} := \sup_{\substack{\mathbf{j}=(j_1, \dots, j_{2d}) \\ 1 \leq |\mathbf{j}| \leq \ell}} \sup_{x \in \mathbb{R}^{2d}} \left| \frac{\partial^{\mathbf{j}} f(x)}{\Gamma^k(x)} \right|.$$

We recall that we denote by L the Kolmogorov generator associated with the stochastic differential equation (2.4): It is defined for all $\phi \in C^\infty(\mathbb{R}^{2d})$ and $(q, p) \in \mathbb{R}^{2d}$ by

$$L\phi(q, p) := \langle p, \partial_q \phi(q, p) \rangle - \langle \partial_q V(q) + \gamma p, \partial_p \phi(q, p) \rangle + \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \phi(q, p). \quad (2.23)$$

Moreover its formal adjoint L^\top in $L^2(\mathbb{R}^{2d})$ is defined for all $\phi \in C^\infty(\mathbb{R}^{2d})$ and $(q, p) \in \mathbb{R}^{2d}$ by

$$L^\top \phi(q, p) = -\langle p, \partial_q \phi(q, p) \rangle + \langle \partial_q V(q), \partial_p \phi(q, p) \rangle + \gamma \langle p, \partial_p \phi(q, p) \rangle \\ + \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \phi(q, p) + d\gamma \phi(q, p). \quad (2.24)$$

The following equality will be useful: For any functions $\phi \in C^\infty(\mathbb{R}^{2d})$ and $\psi \in C^\infty(\mathbb{R}^{2d})$, we have

$$L(\phi\psi) = \psi L\phi + \phi L\psi + \sigma^2 \langle \partial_p \phi, \partial_p \psi \rangle. \quad (2.25)$$

We define the measure $d\rho := \rho(q, p) dq dp$ where for all $(q, p) \in \mathbb{R}^{2d}$,

$$\rho(q, p) = \frac{1}{Z} \exp\left(-\frac{2\gamma}{\sigma^2} H(q, p)\right)$$

and $Z = \int_{\mathbb{R}^{2d}} \exp\left(-\frac{2\gamma}{\sigma^2} H(q, p)\right) dq dp$. A consequence of assumption **B-4** is that for all $k \in \mathbb{N}$ and $j \in \mathbb{N}$

$$\int_{\mathbb{R}^{2d}} |q|^{2k} |p|^{2j} e^{-\frac{2\gamma}{\sigma^2} H(q,p)} dq dp < \infty.$$

It is easy to verify that the measure $d\rho$ is invariant by P_t : $L^\top \rho = 0$.

We also define the following space:

$$L^2(\rho) = \left\{ f : \mathbb{R}^{2d} \rightarrow \mathbb{R}; \int |f|^2 d\rho < \infty \right\}.$$

We will now give some results on the law of the solution of (2.4). We consider a function $\phi \in C_{pol}^\infty(\mathbb{R}^{2d})$ and we set for all $q \in \mathbb{R}^d$, $p \in \mathbb{R}^d$ and $t \geq 0$:

$$u(t, q, p) = \mathbb{E}(\phi(q_q(t), p_p(t))). \quad (2.26)$$

It is a classical result that u is a C^∞ function on $\mathbb{R}^+ \times \mathbb{R}^{2d}$. Moreover, one can show the following result on the regularity of u - see [84]:

Lemma 2.14 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. Let u be defined by (2.26). For any integer m , there exists an integer s such that for all $T \geq 0$ there exists a strictly positive real number $C_m(T)$ such that for $t \in [0, T]$, $q \in \mathbb{R}^d$ and $p \in \mathbb{R}^d$*

$$|D^m u(t, q, p)| \leq C_m(T)(1 + |q|^s + |p|^s),$$

where $D^m u(t)$ denotes the vector of all the spatial derivatives of $u(t)$ of order m .

By Itô formula, it is possible to show that u verifies the Kolmogorov equation

$$\frac{du}{dt}(t, q, p) = Lu(q, p), \quad q \in \mathbb{R}^d, \quad p \in \mathbb{R}^d, \quad t > 0, \quad u(0, q, p) = \phi(q, p), \quad q \in \mathbb{R}^d, \quad p \in \mathbb{R}^d. \quad (2.27)$$

In the following, we write: $u(t) = P_t \phi$. Note that we use the standard identification $u(t) = u(t, \cdot)$.

As we wish to investigate the asymptotic properties of the implicit Euler scheme and the implicit split-step scheme, we need results on the long time behavior of the solution of (2.27). More precisely, we need exponential convergence of u and all its derivatives in an appropriate sense:

Proposition 2.15 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int \phi d\rho = 0$. Let u be the unique solution of (2.27). There exists a strictly positive real number λ_0 such that, for any $m \in \mathbb{N}$ and $0 < \lambda < \lambda_0$, there exist a positive real number C and integers r_{m+d+1} and $\ell_m \geq 2r_{m+d+1}$ such that if $\phi \in \mathcal{C}_{r_{m+d+1}}^{m+d+1}(\mathbb{R}^{2d})$ then for all $t \geq 0$*

$$\|u(t)\|_{m, \ell_m} \leq C \exp(-\lambda t) \|\phi\|_{d+1+m, r_{m+d+1}}.$$

We also need the existence of a solution to the Poisson equation associated with the operator L :

Lemma 2.16 *We denote by L^* the formal adjoint of L in $L^2(\rho)$. Let $g \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int g d\rho = 0$. Then there exists a unique function $h \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that*

$$L^* h = g \quad \text{and} \quad \int h d\rho = 0.$$

The proof of these two results can be found in the appendix.

2.4 Main result

Our main result can be stated as follows:

Theorem 2.17 *Let N be fixed. Let $\delta_0 := \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$. Let (q_k, p_k) be the discrete process defined by the implicit Euler scheme (2.12) or by the implicit split-step scheme (2.11). Then for all $\delta < \delta_0$, there exists a modified function $\mu^{(N)}$ defined for all $(q, p) \in \mathbb{R}^{2d}$ by*

$$\mu^{(N)}(q, p) = 1 + \sum_{n=1}^N \delta^n \mu_n(q, p)$$

such that $\mu^{(N)} \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and

$$\int_{\mathbb{R}^{2d}} \mu^{(N)}(q, p) \rho(q, p) dq dp = 1.$$

For all functions $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d}) \cap \mathcal{C}_{\ell_N}^{\alpha_N}(\mathbb{R}^{2d})$ where $\alpha_N = 6N + 8 + (d + 1)(N + 2)$ and $0 < \lambda < \lambda_0$, where λ_0 is defined in Proposition 2.15, there exist a positive real number C_N and an integer $k_N \geq \ell_N$ satisfying the following : For all $k \in \mathbb{N}$,

$$\left| \mathbb{E}\phi(q_k, p_k) - \int \phi \mu^{(N)} d\rho \right| \leq C_N \left(e^{-\lambda t_k} + \delta^{N+1} \right) (1 + |q_0|^{k_N} + |p_0|^{k_N}) \|\phi - \langle \phi \rangle\|_{\alpha_N, \ell_N},$$

where $t_k = k\delta$ and $\langle \phi \rangle = \int \phi d\rho$.

This result can be viewed as a discrete version of Proposition 2.15 in the case of $m = 0$. We have, for (q_k, p_k) , the discrete process defined by the implicit Euler scheme (2.12) or the implicit split-step scheme (2.11), that $\mathbb{E}\phi(q_k, p_k)$, which is an approximation of u , has the same property as u : $\mathbb{E}\phi(q_k, p_k)$ converges exponentially fast to a constant in $\mathcal{C}_{k_N}^0(\mathbb{R}^{2d})$ up to an error $\delta^N C_N$. At a fixed k , we can optimize this error with a good choice of N .

Our result can be compared with [22, 50, 64, 82, 83]. As in [22, 50, 64], the only assumption made on δ is that $\delta < \delta_0 := \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$. We also recover an expansion of the invariant measure as in [85].

Our result is similar to the result in the case of SDE on the torus described in [22] and to the result for the overdamped Langevin equation described in [50].

The constant C_N appearing in the above estimate depends on N , the constant of semi-convexity θ , the parameters of the equation γ and σ and the polynomial growth of V and all its derivatives.

To prove Theorem 2.17, we will proceed in several steps and will use the same strategy as [22]. In Section 3, we give an asymptotic expansion of the weak error for the first step. Then, we use this expansion to build a modified operator $\mathcal{L}^{(N)}$ and a function $v^{(N)}$ such that the weak error at the first step and $v^{(N)}$ are close to an error δ^{N+1} (Section 4). In Section 5, using Lemma 2.15, we build the modified function μ^N and, using Proposition 2.16, we show the exponential convergence of $v^{(N)}$ to a constant depending of μ^N . Finally, by the Markov property and Proposition 2.9, we complete the proof of Theorem 2.17.

3 Asymptotic expansion of the weak error

We now examine in detail the first time step and its asymptotic properties in terms of the law. By the Markov property, it is sufficient to obtain information for all steps. It is easy to have an expansion of u . Indeed, by Taylor expansion in time, we have the formal expansion for small t and $(q, p) \in \mathbb{R}^{2d}$:

$$u(t, q, p) = \phi(q, p) + tL\phi(q, p) + \frac{t^2}{2}L^2\phi(q, p) + \dots + \frac{t^n}{n!}L^n\phi(q, p) + \dots$$

Since the solution $u(t)$ of the Kolmogorov equation is in $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$, the above formal expansion can be justified in $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. Indeed, we have the following easy result whose proof is left to the reader.

Proposition 3.1 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and $\delta_1 > 0$ be fixed. Then, for all N , there exist constants $C(N)$ and ℓ such that for all $\delta < \delta_1$,*

$$|u(\delta, q, p) - \sum_{n=0}^N \frac{\delta^n}{n!} L^n(q, p)\phi(q, p)| \leq C(N)\delta^{N+1}(1 + |q|^\ell + |p|^\ell) \|\phi\|_{2N+2, r_{2N+2}},$$

where r_{2N+2} is defined such that $\phi \in \mathcal{C}_{r_{2N+2}}^{2N+2}(\mathbb{R}^{2d})$.

We would like to have an expansion similar to the last Proposition in the case of processes defined by the implicit Euler scheme (2.12) or the implicit split-step scheme (2.11).

Proposition 3.2 *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$. Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. For any $N \in \mathbb{N}$, there exists an integer r_N such that $\phi \in \mathcal{C}_{r_N}^N(\mathbb{R}^{2d})$. For all $n \geq 1$, there exist operators A_n of order $2n$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ which depend on the scheme chosen - (2.11) or (2.12) -, such that for all integer $N \geq 1$ there exist a constant C_N and an integer ℓ_N such that for $0 < \delta < \delta_0$ and $(q, p) := (q_0, p_0)$,*

$$|\mathbb{E}\phi(q_1, p_1) - \sum_{n=0}^N \delta^n A_n(q, p)\phi(q, p)| \leq C_N \delta^{N+1} (1 + |q|^{\ell_N} + |p|^{\ell_N}) |\phi|_{2N+2, r_{2N+2}}. \quad (3.1)$$

Moreover, we have $A_0 = I$ and $A_1 = L$.

Remark 3.3 *This result is similar of the asymptotic expansion of the weak error described in [22], but the proof is different. Indeed, we can not use Itô's lemma because the schemes considered here are implicit.*

We consider the implicit split-step scheme (2.11). Let $0 < \delta < \delta_0$. Let us recall that we have

$$\begin{aligned} q_1 &= q_0 + \delta p_0^* \\ p_0^* &= p_0 - \delta \gamma p_0^* - \delta \partial_q V(q_1) \\ p_1 &= p_0^* + \sqrt{\delta} \sigma \eta_0. \end{aligned}$$

To prove Proposition 3.2, we first need an asymptotic expansion for q_1 , p_1 and p_0^* . We define the function Ψ_δ which associates to (q, p) the solution z of $(1 + \gamma\delta)z = (1 + \gamma\delta)q + \delta p - \delta^2 \partial_q V(z)$. The function Ψ_δ is well defined - see Lemma 2.7 - and we have $q_1 = \Psi_\delta(q_0, p_0)$. Moreover, we have that $(\delta, q, p) \mapsto \Psi_\delta(q, p)$ is C^∞ on $]0, \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}[\times \mathbb{R}^{2d}$. Let $\Omega_1 =]0, \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}[\times \mathbb{R}^{3d}$ and the function $f \in C^\infty$ defined on Ω_1 by

$$f(\delta, q, p, z) = -(1 + \delta\gamma)z + (1 + \delta\gamma)q + \delta p - \delta^2 \partial_q V(z).$$

Using the semi-convexity of V , we have that, for all $(\delta, q, p, z) \in \Omega_1$, $\partial_z f(\delta, q, p, z)$ is invertible. By implicit function Theorem, we obtain that the function defined by $(\delta, q, p) \mapsto \Psi_\delta(q, p) = z$ is C^∞ on a neighborhood of each point of $]0, \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}[\times \mathbb{R}^{2d}$.

We have the following asymptotic expansion:

Lemma 3.4 *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$ and $(q, p) \in \mathbb{R}^{2d}$ such that $q_0 = q$ and $p_0 = p$ be fixed. We have for $0 < \delta < \delta_0$ and $N \in \mathbb{N}$,*

$$q_1 = \Psi_\delta(q, p) = q + \sum_{k=1}^N \delta^k d_k(q, p) + \delta^{N+1} R_{N+1}(q, p, \delta), \quad (3.2)$$

where, for all $k \geq 0$, $d_k \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ is defined for all $(x, y) \in \mathbb{R}^{2d}$ by

$d_1(x, y) = y$, and for $k \geq 2$

$$\begin{aligned} d_k(x, y) &= (-1)^{k-1} \gamma^{k-2} (\gamma y + \partial_q V(x)) \\ &+ \sum_{j=2}^{k-1} (-1)^{j-1} \gamma^{j-2} \sum_{n=1}^{k-j} \frac{1}{n!} \sum_{\substack{k_1 + \dots + k_n = k-j-n, \\ 0 \leq k_i \leq N}} \partial_q^{n+1} V(x)(d_{k_1+1}(x, y), \dots, d_{k_n+1}(x, y)). \end{aligned}$$

and R_{N+1} verifies: There exist $C > 0$ and $\ell_N \in \mathbb{N}$ such that for any $(x, y) \in \mathbb{R}^{2d}$ and $\delta < \delta_0$

$$|R_{N+1}(x, y, \delta)| \leq C(1 + |x|^{\ell_N} + |y|^{\ell_N}). \quad (3.3)$$

Proof. Let $0 < \delta < \delta_0$. We have previously shown that $(\delta, q, p) \mapsto \Psi_\delta(q, p)$ is C^∞ on $]0, \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}[\times \mathbb{R}^{2d}$. Then, for $(q, p) \in \mathbb{R}^{2d}$ fixed, we have that $d_k(q, p)$ is the k^{th} term of the Taylor expansion of $\delta \mapsto \Psi_\delta(q, p)$ and we can write (3.2). We now search an expression for d_k .

Let $(q, p) \in \mathbb{R}^{2d}$ such that $q_0 = q$ and $p_0 = p$. Let $\ell \in \mathbb{N}$. We use the temporary notation, for all $0 \leq k \leq \ell - 1$, $g_{k,\ell} = d_{k+1}$ and $g_{\ell,\ell} = R_{\ell+1}$. Hence, we have

$$\begin{aligned} q_1 &= q + \sum_{k=1}^{\ell} \delta^k d_k(q, p) + \delta^{\ell+1} R_{\ell+1}(q, p, \delta) \\ &= q + \delta z_{1,\ell}, \end{aligned}$$

where $z_{1,\ell} = \sum_{k=0}^{\ell} g_{k,\ell}(q, p)$. Using Taylor expansion, we obtain

$$\begin{aligned} \partial_q V(q_1) &= \partial_q V(q + \delta z_{1,\ell}) = \partial_q V(q) + \sum_{n=1}^{\ell} \frac{1}{n!} \partial_q^{n+1} V(q)(\delta z_{1,\ell}, \dots, \delta z_{1,\ell}) + \delta^{\ell+1} \theta_\ell(q, p) \\ &= \partial_q V(q) + \sum_{n=1}^{\ell} \frac{1}{n!} \delta^n \partial_q^{n+1} V(q) \left(\sum_{k=0}^{\ell} \delta^k g_{k,\ell}(q, p), \dots, \sum_{k=0}^{\ell} \delta^k g_{k,\ell}(q, p) \right) + \delta^{\ell+1} \theta_\ell(q, p) \\ &= \partial_q V(q) + \sum_{n=1}^{\ell} \delta^n \frac{1}{n!} \sum_{m=0}^{n\ell} \delta^m \sum_{\substack{k_1 + \dots + k_n = m, \\ 0 \leq k_i \leq \ell}} \partial_q^{n+1} V(q)(g_{k_1,\ell}(q, p), \dots, g_{k_n,\ell}(q, p)) \\ &\quad + \delta^{\ell+1} \theta_\ell(q, p) \\ &= \partial_q V(q) + I_{1,\ell}(q, p) + \delta^{\ell+1} I_{2,\ell}(q, p) + \delta^{\ell+1} \theta_\ell(q, p), \end{aligned}$$

where

$$\begin{aligned} \theta_\ell(q, p) &= \int_0^1 \frac{(1-t)^\ell}{\ell!} \partial_q^{\ell+2} V(q + t\delta z_1)(z_1, \dots, z_1) dt, \\ I_{1,\ell}(q, p) &= \sum_{n=1}^{\ell} \frac{1}{n!} \delta^n \sum_{m=0}^{j-n} \delta^m \sum_{\substack{k_1 + \dots + k_n = m, \\ 0 \leq k_i \leq \ell}} \partial_q^{n+1} V(q)(g_{k_1,\ell}(q, p), \dots, g_{k_n,\ell}(q, p)), \\ &= \sum_{j=1}^{\ell} \delta^j \sum_{n=1}^j \frac{1}{n!} \sum_{\substack{k_1 + \dots + k_n = \ell - n, \\ 0 \leq k_i \leq \ell - 1}} \partial_q^{n+1} V(q)(d_{k_1+1}(q, p), \dots, d_{k_n+1}(q, p)), \\ I_{2,\ell}(q, p) &= \sum_{n=1}^{\ell} \frac{1}{n!} \delta^n \sum_{m=\ell-n+1}^{n\ell} \delta^{m-\ell-1} \sum_{\substack{k_1 + \dots + k_n = m, \\ 0 \leq k_i \leq \ell}} \partial_q^{n+1} V(q)(g_{k_1,\ell}(q, p), \dots, g_{k_n,\ell}(q, p)). \end{aligned}$$

Let N be fixed, using the above computations, we have

$$\begin{aligned}
 q_1 &= q + (1 + \gamma\delta)^{-1}(\delta p - \delta^2 \partial_q V(q_1)) \\
 &= q + \sum_{k=0}^{N-1} (-\gamma)^k \delta^{k+1} p + \delta^{N+1} g(q, p) \\
 &\quad + \sum_{k=0}^{N-2} (-\gamma)^k \delta^{k+2} \left(\partial_q V(q) - \delta^2 I_{1, N-k-2}(q, p) - \delta^{N-k-1} (I_{2, N-k-2}(q, p) + \theta_{N-k-2}(q, p)) \right) \\
 &= q + \delta p + \sum_{k=2}^N (-1)^{k-1} \gamma^{k-2} \delta^k (\gamma p + \partial_q V(q)) + J(q, p) + \delta^{N+1} G(q, p), \tag{3.4}
 \end{aligned}$$

where

$$\begin{aligned}
 J(q, p) &= - \sum_{k=0}^{N-2} (-\gamma)^k I_{1, N-k-2}(q, p) \delta^{k+2} \\
 &= \sum_{k=2}^N (-1)^{k-1} \gamma^{k-2} \sum_{j=1}^{N-k} \delta^{j+k} \sum_{n=1}^j \frac{1}{n!} \sum_{\substack{k_1+\dots+k_n=j-n, \\ 0 \leq k_i \leq N}} \partial_q^{n+1} V(q)(d_{k_1+1}(q, p), \dots, d_{k_n+1}(q, p)) \\
 &= \sum_{k=3}^N \delta^k \sum_{j=2}^{k-1} (-1)^{j-1} \gamma^{j-2} \sum_{n=1}^{k-j} \frac{1}{n!} \sum_{\substack{k_1+\dots+k_n=k-j-n, \\ 0 \leq k_i \leq N}} \partial_q^{n+1} V(q)(d_{k_1+1}(q, p), \dots, d_{k_n+1}(q, p)), \\
 G(q, p) &= g(q, p) - \sum_{k=0}^{N-1} (-\gamma)^k I_{2, N-k-2}(q, p), \\
 g(q, p) &= - \frac{(-\gamma)^{N-1}}{1 + \delta\gamma} (\gamma p + \partial_q V(q_1)).
 \end{aligned}$$

Identifying the terms in the two expansions (3.4) and (3.2), we get

$$q_1 = q + \sum_{k=1}^N \delta^k d_k(q, p) + \delta^{N+1} R_{N+1}(\delta, q, p),$$

where, for all $k \geq 0$, d_k is defined for all $(q, p) \in \mathbb{R}^{2d}$ by

$$\begin{aligned}
 d_1(q, p) &= p, \text{ and for } k \geq 2, \\
 d_k(q, p) &= (-1)^{k-1} \gamma^{k-2} (\gamma p + \partial_q V(q)) \\
 &\quad + \sum_{j=2}^{k-1} (-1)^{j-1} \gamma^{j-2} \sum_{n=1}^{k-j} \frac{1}{n!} \sum_{\substack{k_1+\dots+k_n=k-j-n, \\ 0 \leq k_i}} \partial_q^{n+1} V(q)(d_{k_1+1}(q, p), \dots, d_{k_n+1}(q, p)),
 \end{aligned}$$

moreover, by induction, we have, for all $k \in \mathbb{N}$, $d_k \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$.

The above identification does not give an easy expression of R_N , then we have not immediately (3.3). To show this result, we will use that, for $N, q \in \mathbb{R}^d$ and $p \in \mathbb{R}^d$ fixed, $R_N(q, p, \cdot)$ is the remainder of order N of $\delta \mapsto \Psi_\delta(q, p)$. Therefore, if we show that, for any $n \in \mathbb{N}$, there exist $C > 0$ and $\ell_n \in \mathbb{N}$ such that for any $0 < \delta < \delta_0$ and $(q, p) \in \mathbb{R}^{2d}$,

$$|\partial_\delta^n \Psi_\delta(q, p)|^2 \leq C(1 + |q|^{\ell_n} + |p|^{\ell_n}), \tag{3.5}$$

then we show (3.3) and Lemma 3.4 is shown.

Let us show the result (3.5) by induction on n . Let $0 < \delta < \delta_0$ and $(q, p) \in \mathbb{R}^{2d}$ be fixed. We have, by definition of Ψ_δ ,

$$\Psi_\delta(q, p)(1 + \delta\gamma) + \delta^2 \partial_q V(\Psi_\delta(q, p)) = \delta p + (1 + \delta\gamma)q. \quad (3.6)$$

We multiply this equation by $\Psi_\delta(q, p)$ and use dissipativity inequality (2.3). We get

$$\begin{aligned} \langle p, \Psi_\delta(q, p) \rangle \delta + \langle q, \Psi_\delta(q, p) \rangle (1 + \delta\gamma) &= (1 + \delta\gamma) |\Psi_\delta(q, p)|^2 + \delta^2 \langle \partial_q V(\Psi_\delta(q, p)), \Psi_\delta(q, p) \rangle \\ &\geq (1 + \delta\gamma + \beta_1 \delta^2) |\Psi_\delta(q, p)|^2 - \kappa \delta^2. \end{aligned}$$

Since

$$2\langle a, b \rangle \leq \varepsilon |a|^2 + \frac{1}{\varepsilon} |b|^2 \quad \text{for all } \varepsilon > 0, a \in \mathbb{R}^d \text{ and } b \in \mathbb{R}^d, \quad (3.7)$$

we get, for any positive constants ε_1 and ε_2 :

$$\begin{aligned} |\Psi_\delta(q, p)|^2 &\left[1 + \delta\gamma + \beta_1 \delta^2 - \frac{\varepsilon_1}{2} - \frac{\varepsilon_2}{2} \right] \\ &\leq \kappa \delta^2 + \frac{\delta}{2\varepsilon_2} |p|^2 + \frac{1 + \delta\gamma}{2\varepsilon_1} |q|^2. \end{aligned}$$

We choose $\varepsilon_1 = \varepsilon_2 = \frac{1}{2}$, then we have that there exists a positive constant C , which is independent of δ , such that

$$|\Psi_\delta(q, p)|^2 \leq C(1 + |q|^2 + |p|^2).$$

This proves (3.5) for $n = 0$ and $\ell_0 = 2$.

Let us assume the result (3.5) is true for all $0 \leq j < n$ and let us show it for n . Let $0 < \delta < \delta_0$ and $(q, p) \in \mathbb{R}^{2d}$ be fixed. Differentiating (3.6), we have

$$\begin{aligned} (1 + \delta\gamma) \partial_\delta^n \Psi_\delta(q, p) &= -n\gamma \partial_\delta^{n-1} \Psi_\delta(q, p) + (\gamma q + p) \mathbf{1}_{\{n=1\}} \\ &\quad - 2n \partial_\delta^{n-1} \left(\partial_q V(\Psi_\delta(q, p)) \right) - \delta^2 \partial_\delta^n \left(\partial_q V(\Psi_\delta(q, p)) \right) \\ &\quad - 2 \binom{n}{2} \delta \partial_\delta^{n-2} \left(\partial_q V(\Psi_\delta(q, p)) \right) \\ &=: B_1(\delta, q, p) - 2n B_2(\delta, q, p) - \delta^2 B_3(\delta, q, p) - \delta B_4(\delta, q, p). \end{aligned}$$

By induction hypothesis, we have that B_1 has polynomial growth in (q, p) . Moreover, using Faà di Bruno's formula, we get

$$\begin{aligned} B_2(\delta, q, p) &= \sum \frac{(n-1)!}{m_1! m_2! (2!)^{m_2} \dots m_{n-1}! ((n-1)!)^{m_{n-1}}} \partial_q^{m_1 + \dots + m_{n-1} + 1} V(\Psi_\delta(q, p)) \\ &\quad \times \prod_{j=1}^{n-1} (\partial_\delta^j \Psi_\delta(q, p))^{m_j}, \end{aligned}$$

where $m_1 + 2m_2 + \dots + (n-1)m_{n-1} = n-1$. Using the polynomial growth of V and its derivatives (B-1) and induction hypothesis, we have that B_2 has polynomial growth in (q, p) . Using the same method, we have that B_4 has polynomial growth in (q, p) . Using Faà di Bruno's formula, we also have

$$\begin{aligned} B_3(\delta, q, p) &= \sum \frac{n!}{m_1! m_2! (2!)^{m_2} \dots m_n! (n!)^{m_n}} \partial_q^{m_1 + \dots + m_n + 1} V(\Psi_\delta(q, p)) \\ &\quad \times \prod_{j=1}^n (\partial_\delta^j \Psi_\delta(q, p))^{m_j} \\ &= \delta \partial_q^2 V(q + \delta \Psi_\delta(q, p)) \partial_\delta^n \Psi_\delta(q, p) + B_5(\delta, q, p), \end{aligned}$$

where $m_1 + 2m_2 + \dots + nm_n = n$ and

$$B_5(\delta, q, p) = \sum \frac{n!}{k_1!k_2!(2!)^{k_2}\dots k_{n-1}!(n-1)!^{k_{n-1}}} \partial_q^{k_1+\dots+k_{n-1}+1} V(\Psi_\delta(q, p)) \\ \times \prod_{j=1}^{n-1} (\partial_\delta^j \Psi_\delta(q, p))^{k_j}, \\ k_1 + 2k_2 + \dots + (n-1)k_{n-1} = n.$$

Then we have that B_1, B_2, B_4 and B_5 have polynomial growth in (q, p) and we get

$$((1 + \delta\gamma)I + \delta^2 \partial_q^2 V(q + \delta \Psi_\delta(q, p))) \partial_\delta^n \Psi_\delta(q, p) = B_6(\delta, q, p)$$

where $B_6 := -n\gamma B_1 - 2nB_2 - \delta B_4 - \delta^2 B_5$ has polynomial growth in (q, p) .

Multiplying by $\delta_\delta^n \Psi_\delta(q, p)$, and using (3.7) on $|\langle B_6(\delta, q, p), \partial_\delta^n \Psi_\delta(q, p) \rangle|$ and semi-convexity assumption **B-3**, we get

$$|\partial_\delta^n \Psi_\delta(q, p)|^2 (1 + \gamma\delta - \theta\delta^2 - \frac{1}{2}) \leq \frac{1}{2} B_6^2(\delta, q, p),$$

where θ is the constant of semi-convexity and B_6 has polynomial growth in (q, p) . Since $\delta < \frac{\gamma}{\theta}$, we have that there exist constants C and $\ell_n \in \mathbb{N}$ such that

$$|\partial_\delta^n \Psi_\delta(q, p)|^2 \leq C(1 + |q|^{\ell_n} + |p|^{\ell_n}),$$

which proves (3.5). \blacklozenge

Corollary 3.5 *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$ and $(q^0, p^0) \in \mathbb{R}^{2d}$ such that $q_0 = q^0$ and $p_0 = p^0$ be fixed. We have for $0 < \delta < \delta_0$ and $N \in \mathbb{N}$,*

$$q_1 = q^0 + \sum_{k=1}^N \delta^k d_k(q^0, p^0) + \delta^{N+1} R_{N+1}(q^0, p^0, \delta), \\ p_1 = \sum_{k=0}^N \delta^k d_{k+1}(q^0, p^0) + \delta^{N+1} R_{N+2}(q^0, p^0, \delta) + \sqrt{\delta} \sigma \eta_0$$

where, for all $k \geq 0$, $d_k \in C_{pol}^\infty(\mathbb{R}^{2d})$ is defined for all $(x, y) \in \mathbb{R}^{2d}$ by

$$d_1(x, y) = y, \text{ and for } k \geq 2$$

$$d_k(x, y) = (-1)^{k-1} \gamma^{k-2} (\gamma y + \partial_q V(x)) \\ + \sum_{j=2}^{k-1} (-1)^{j-1} \gamma^{j-2} \sum_{n=1}^{k-j} \frac{1}{n!} \sum_{\substack{k_1+\dots+k_n=k-j-n, \\ 0 \leq k_i}} \partial_q^{n+1} V(x)(d_{k_1+1}(x, y), \dots, d_{k_n+1}(x, y)).$$

and R_{N+1} verifies: There exist $C > 0$ and $\ell_N \in \mathbb{N}$ such that for any $(x, y) \in \mathbb{R}^{2d}$ and $\delta < \delta_0$

$$|R_{N+1}(x, y, \delta)| \leq C(1 + |x|^{\ell_N} + |y|^{\ell_N}).$$

Proof of Proposition 3.2 in the case of the implicit split-step scheme (2.11). Let N fixed. We have, with the notation of Corollary 3.5, for all $N_0 \in \mathbb{N}$

$$q_1 = q + \sum_{k=1}^{N_0} \delta^k d_k(q, p) + \delta^{N_0+1} R_{N_0+1}(q, p, \delta) = q + \delta R_1(q, p, \delta), \\ p_1 = \sum_{k=0}^{N_0} \delta^k d_{k+1}(q, p) + \delta^{N_0+1} R_{N_0+2}(q, p, \delta) + \sqrt{\delta} \sigma \eta_0 \\ = p + \sqrt{\delta} \sigma \eta_0 + \delta R_2(q, p, \delta) = z + \sqrt{\delta} \sigma \eta_0.$$

Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$, for any $n \in \mathbb{N}$, there exists an integer r_n such that $\phi \in \mathcal{C}_{r_n}^n(\mathbb{R}^{2d})$. Using Taylor expansion, we get

$$\begin{aligned}\phi(q_1, p_1) &= \phi(q_1, z + \sqrt{\delta}\sigma\eta_0) \\ &= \phi(q_1, z) + \sum_{k=1}^{2N+1} \frac{1}{k!} \delta^{k/2} \sigma^k \partial_p^k \phi(q_1, z)(\eta_0, \dots, \eta_0) \\ &\quad + \int_0^1 \frac{(1-t)^{2N+1}}{(2N+1)!} \delta^{N+1} \sigma^{2N+2} \partial_p^{2N+2} \phi(q_1, z + t\sqrt{\delta}\sigma\eta_0)(\eta_0, \dots, \eta_0) dt.\end{aligned}$$

Let $\lfloor \cdot \rfloor$ denotes the integer part. Using Taylor expansion on $\partial_p^k \phi(q_1, z)$ and computations done in the proof of Lemma 3.4, we obtain

$$\phi(q_1, p_1) = I_1(x, \eta_0) + I_2(x, \eta_0) + I_3(x, \eta_0) + I_4(x, \eta_0),$$

where $x = (q, p)$ and

$$\begin{aligned}I_1(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \sigma^k \left(\delta^{k/2} \partial_p^k \phi(x)(\eta_0, \dots, \eta_0) + \sum_{n=1}^{\ell_k} \frac{1}{n!} \sum_{\ell=0}^n \binom{n}{\ell} \sum_{m=n}^{\ell_k} \delta^{m+k/2} \right. \\ &\quad \times \left. \sum_{\substack{k_1+\dots+k_\ell \\ +\tilde{k}_1+\dots+\tilde{k}_{n-\ell}=m \\ 0 < k_i \leq \ell_k \\ 0 < \tilde{k}_i \leq \ell_k}} \partial_q^\ell \partial_p^{n-\ell+k} \phi(x)(d_{k_1}(x), \dots, d_{k_\ell}(x), d_{\tilde{k}_1+1}(x), \dots, d_{\tilde{k}_{n-\ell}+1}(x), \eta_0, \dots, \eta_0) \right), \\ I_2(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \sigma^k \sum_{n=0}^{\ell_k} \frac{1}{n!} \sum_{\ell=0}^n \binom{n}{\ell} \sum_{m=\ell_k+1}^{n(\ell_k+1)} \delta^{m+k/2} B_{m,n,\ell,k}(x_1, \eta_0), \\ I_3(x, \eta_0) &= \sum_{k=0}^{2N+1} \frac{1}{k!} \sigma^k \delta^{k/2} \delta^{\ell_k+1} \int_0^1 \frac{(1-t)^{\ell_k}}{(\ell_k)!} \sum_{\ell=0}^{\ell_k+1} \binom{\ell_k+1}{\ell} \\ &\quad \times \partial_q^\ell \partial_p^{\ell_k+1-\ell+k} \phi(q + t\delta R_1(x, \delta), p + t\delta R_2(x, \delta)) \\ &\quad \times (R_1(x, \delta), \dots, R_1(x, \delta), R_2(x, \delta), \dots, R_2(x, \delta), \eta_0, \dots, \eta_0) dt, \\ I_4(x, \eta_0) &= \delta^{N+1} \sigma^{2N+2} \int_0^1 \frac{(1-t)^{2N+1}}{(2N+1)!} \partial_p^{2N+2} \phi(q + \delta R_1(x, \delta), z + t\sqrt{\delta}\eta_0)(\eta_0, \dots, \eta_0) dt, \\ \ell_k &= N - \left\lfloor \frac{k+1}{2} \right\rfloor\end{aligned}$$

and, with the temporary notation: for all $0 \leq k \leq 2N+1$ and $1 \leq i \leq \ell_k$, $\tilde{g}_{k,i} = d_{i+1}$, $g_{k,i} = d_i$, $\tilde{g}_{k,\ell_k+1} = R_{\ell_k+2}$ and $g_{k,\ell_k+1} = R_{\ell_k+1}$,

$$B_{m,n,\ell,k}(x, \eta_0) = \sum_{\substack{k_1+\dots+k_\ell \\ +\tilde{k}_1+\dots+\tilde{k}_{n-\ell}=m \\ 0 < k_i \leq \ell_k+1 \\ 0 < \tilde{k}_i \leq \ell_k+1}} \partial_q^\ell \partial_p^{n-\ell+k} \phi(x)(g_{k_1}(x), \dots, g_{k_\ell}(x), \tilde{g}_{\tilde{k}_1}(x), \dots, \tilde{g}_{\tilde{k}_{n-\ell}}(x), \eta_0, \dots, \eta_0).$$

We have, for all $\ell \in \mathbb{N}$, $\mathbb{E}(\eta_{0,i}^{2\ell+1}) = 0$ and $\eta_{0,i}$ are independent of q, p and $\eta_{0,j}$ for $j \neq i$,

then the expectation of all the odd term in k in I_1 , I_2 and I_3 vanish. Hence we have

$$\begin{aligned}\mathbb{E}(I_2(x, \eta_0)) &= \sum_{k=0}^N \frac{1}{(2k)!} \sigma^{2k} \sum_{n=0}^{N-k} \frac{1}{n!} \sum_{\ell=0}^n \binom{n}{\ell} \sum_{m=N-k+1}^{n(N-k+1)} \delta^{m+k} \mathbb{E}(B_{m,n,\ell,2k}(x, \eta_0)), \\ \mathbb{E}(I_3(x, \eta_0)) &= \sum_{k=0}^N \frac{1}{(2k)!} \delta^{N+1} \sigma^{2k} \int_0^1 \frac{(1-t)^{N-k}}{(N-k)!} \sum_{\ell=0}^{N-k+1} \binom{N-k+1}{\ell} \\ &\quad \times \mathbb{E} \left(\partial_q^\ell \partial_p^{N-k+1-\ell+k} \phi(q + t\delta R_1(x, \delta), p + t\delta R_2(x, \delta)) \right. \\ &\quad \left. \times (R_1(x, \delta), \dots, R_1(x, \delta), R_2(x, \delta), \dots, R_2(x, \delta), \eta_0, \dots, \eta_0) \right) dt.\end{aligned}$$

In $\mathbb{E}(I_2(x, \eta_0))$, we have $m+k \geq N+1$, then we can factor δ^{N+1} . Moreover, if $n = \ell = 0$ then $B_{m,n,\ell,2k} = 0$, hence, in each term of $\mathbb{E}(I_2(x, \eta_0))$, we have at least one derivative of ϕ . Using $\phi \in \mathcal{C}_{r_{2N+2}}^{2N+2}(\mathbb{R}^{2d})$ and the polynomial growth of d_j , \tilde{R}_{N_0+1} and R_{N_0+1} for $j \in \mathbb{N}^*$ and $N_0 \in \mathbb{N}$, we get that there exist integers n_1 , n_2 and n_3 such that

$$\begin{aligned}|\mathbb{E}(I_2(q, p, \eta_0))| &\leq C_N \delta^{N+1} (1 + |p|^{n_1} + |q|^{n_1}) |\phi|_{2N, r_{2N}}, \\ |\mathbb{E}(I_4(q, p, \eta_0))| &\leq C_N \delta^{N+1} (1 + |p|^{n_2} + |q|^{n_2}) \|D^{2N+2}\phi\|_{0, r_{2N+2}} \\ |\mathbb{E}(I_3(q, p, \eta_0))| &\leq C_N \delta^{N+1} (1 + |p|^{n_3} + |q|^{n_3}) \|D^N\phi\|_{N+1, r_{2N+1}}.\end{aligned}$$

Hence, we have that there exists $k_1 \in \mathbb{N}^*$ such that

$$|\mathbb{E}\phi(q_1, p_1) - \mathbb{E}(I_1)| \leq C_N \delta^{N+1} (1 + |p|^{k_1} + |q|^{k_1}) |\phi|_{2N+2, r_{2N+2}},$$

where

$$\begin{aligned}\mathbb{E}(I_1) &= \sum_{j=0}^N \frac{1}{(2j)!} \sigma^{2j} \delta^j \mathbb{E} \left(\partial_p^{2j} \phi(q, p)(\eta_0, \dots, \eta_0) \right) \\ &\quad + \sum_{j=0}^N \frac{1}{(2j)!} \sigma^{2j} \sum_{n=1}^{N-j} \frac{1}{n!} \sum_{\ell=0}^n \binom{n}{\ell} \sum_{m=n}^{N-j} \delta^{m+j} \sum_{\substack{k_1+\dots+k_\ell \\ +\tilde{k}_1+\dots+\tilde{k}_{n-\ell}=m \\ \tilde{k}_i, k_i \geq 1}} \mathbb{E} \left(\partial_q^\ell \partial_p^{n-\ell+2j} \phi(q, p) \right. \\ &\quad \left. \times (d_{k_1}(q, p), \dots, d_{k_\ell}(q, p), d_{\tilde{k}_1+1}(q, p), \dots, d_{\tilde{k}_{n-\ell}+1}(q, p), \eta_0, \dots, \eta_0) \right), \\ &= \sum_{k=0}^N \delta^k A_k(q, p) \phi(q, p),\end{aligned}$$

and

$$\begin{aligned}A_k(q, p) \phi(q, p) &= \frac{\sigma^{2k}}{(2k)!} \mathbb{E}(\partial_p^{2k} \phi(q, p)(\eta_0, \dots, \eta_0)) + \sum_{j=0}^{k-1} \frac{1}{(2j)!} \sigma^{2j} \sum_{n=1}^{k-j} \frac{1}{n!} \sum_{\ell=0}^n \binom{n}{\ell} \\ &\times \sum_{\substack{k_1+\dots+k_\ell \\ +\tilde{k}_1+\dots+\tilde{k}_{n-\ell}=k-j \\ 0 < k_i, \tilde{k}_i}} \mathbb{E} \left(\partial_q^\ell \partial_p^{n-\ell+2j} \phi(q, p)(d_{k_1}(q, p), \dots, d_{k_\ell}(q, p), d_{\tilde{k}_1+1}(q, p), \dots, d_{\tilde{k}_{n-\ell}+1}(q, p), \eta_0, \dots, \eta_0) \right)\end{aligned}$$

Using property of η_0 , we get that $A_0 = I$,

$$A_1 \phi(q, p) = \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \phi(q, p) + \langle \partial_p \phi, d_2(q, p) \rangle + \langle \partial_q \phi(q, p), d_1(q, p) \rangle = L$$

and A_k is an operator of order $2k$. ◆

The proof for the scheme (2.12) uses the same arguments.

We need asymptotic expansions for $q_1 = q + \delta p_1$ and $p_1 = p - \delta \gamma p_1 - \partial_q V(q_1) \delta + \sqrt{\delta} \sigma \eta_0$. We use the local notation $\alpha = \sqrt{\delta}$. We define the function ψ_α which associates to (q, p) the solution z of $(1 + \gamma \alpha^2)z = (1 + \gamma \alpha^2)q + \alpha^2 p - \alpha^4 \partial_q V(z) + \alpha \sigma \eta_0$. This function is well defined (see Lemma 2.7). Moreover, using same arguments as for the scheme (2.11), we can show that $(\alpha, q, p) \mapsto \psi_\alpha(q, p)$ is C^∞ on $]0, \sqrt{\delta_1}[\times \mathbb{R}^{2d}$, where $\delta_1 = \frac{\gamma + \sqrt{\gamma^2 + 4\theta}}{2\theta}$.

We have the following lemma:

Lemma 3.6 *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$ and $(q^0, p^0) \in \mathbb{R}^{2d}$ such that $q_0 = q^0$ and $p_0 = p^0$ be fixed. For $0 < \delta < \delta_0$ and the local notation $\alpha = \sqrt{\delta}$, we have*

$$\begin{aligned} \forall N_0 \in \mathbb{N}, \quad q_1 &= \psi_\alpha(q, p) = q + \sum_{k=2}^{2N_0+1} \delta^{\frac{k}{2}} d_k(q, p, \eta_0) + \delta^{N_0+1} R_{N_0+1}(q, p, \delta, \eta_0), \\ p_1 &= \sum_{k=0}^{2N_0+1} \delta^{\frac{k}{2}} d_{k+2}(q, p, \eta_0) + \delta^{N_0+1} R_{N_0+2}(q, p, \delta, \eta_0), \end{aligned}$$

where, $\forall k \geq 2$, d_k is defined for all $(q, p) \in \mathbb{R}^{2d}$ by

$$d_2(q, p, \eta_0) = p, d_3(q, p, \eta_0) = \sigma \eta_0$$

and $\forall k \geq 2$

$$\begin{aligned} d_{2k}(q, p, \eta_0) &= (-1)^{k-1} \gamma^{k-2} (\gamma p + \partial_q V(q)) \\ &+ \sum_{i=2}^{k-1} (-1)^{i+1} \gamma^i \sum_{n=1}^{k-i} \frac{1}{n!} \sum_{\substack{k_1 + \dots + k_n = 2(k-i) \\ k_s \geq 2}} \partial_q^n V(q)(d_{k_1}(q, p, \eta_0), \dots, d_{k_i}(q, p, \eta_0)), \\ d_{2k+1}(q, p, \eta_0) &= (-1)^{k-1} \gamma^{k-1} \sigma \eta_0 \\ &+ \sum_{i=2}^k (-1)^{i+1} \gamma^i \sum_{n=1}^{k-i} \frac{1}{n!} \sum_{\substack{k_1 + \dots + k_n = 2(k-i)+1 \\ k_s \geq 2}} \partial_q^n V(q)(d_{k_1}(q, p, \eta_0), \dots, d_{k_i}(q, p, \eta_0)). \end{aligned}$$

Moreover, we have that for any $k \geq 2$, $\mathbb{E}(d_k) \in C_{pol}^\infty(\mathbb{R}^{2d})$,

$$\mathbb{E}(d_{2k+1}(q, p, \eta_0)) = 0 \tag{3.8}$$

and, for any $N \in \mathbb{N}$, R_N verifies: There exist $C > 0$ and $\ell_N \in \mathbb{N}$ such that for any $(x, y) \in \mathbb{R}^{2d}$ and $\delta < \delta_0$

$$|\mathbb{E}(R_N(q, p, \delta, \eta_0))| \leq C(1 + |q|^{\ell_N} + |p|^{\ell_N}).$$

Proof. To prove this Lemma, we use the same ideas as in Lemma 3.4. We first compute d_k for all k . By induction, we rewrite d_k only in terms of d_1 , d_2 and the derivatives of V evaluate in q . Using the independence of η_0 with (q, p) , we can show (3.8).

To prove that $\mathbb{E}(R_N)$ has polynomial growth, we show that, for $n \in \mathbb{N}$, there exist $C_n > 0$ and $k_n \in \mathbb{N}$ such that, for $(q, p) \in \mathbb{R}^{2d}$, $\delta < \delta_0$ and the local notation $\alpha = \sqrt{\delta}$, we have

$$\mathbb{E}(|\partial_\alpha^n \psi_\alpha(q, p)|^2) \leq C_n(1 + |q|^{k_n} + |p|^{k_n}).$$

◆

The proof of Proposition 3.2 in the case of the scheme (2.12) is similar to the case of the scheme (2.11), but we must use an asymptotic expansion of $\partial_p^k \phi$ to a larger order $-2N + 1 - k$ instead of $N - \lfloor (k+1)/2 \rfloor$.

4 Modified generator

4.1 Formal series analysis

Let us now consider δ as fixed. We want to construct a formal series

$$\mathcal{L} = L + \delta L_1 + \dots + \delta^n L_n + \dots \quad (4.1)$$

where the coefficients of the operator L_n are in $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and such that formally the solution v at time $t = \delta$ of the equation

$$\partial_t v(t, q) = \mathcal{L}(q, p)v(t, q, p), t > 0, (q, p) \in \mathbb{R}^{2d} \quad v(0, q, p) = \phi(q, p), (q, p) \in \mathbb{R}^{2d}$$

coincides in the sense of asymptotic expansion with the approximation of the transition semigroup $\mathbb{E}\phi(q_1, p_1)$ studied in the previous section. In other words, we want to have the following equality in the sense of asymptotic expansion in powers of δ

$$\exp(\delta \mathcal{L})\phi = \phi + \sum_{n \geq 1} \delta^n A_n \phi,$$

where the operators A_n are defined in Proposition 3.2.

Formally, this equation can be written as

$$\exp(\delta \mathcal{L}) - I_d = \delta \tilde{A}(\delta), \quad (4.2)$$

where $\tilde{A}(\delta) = \sum_{n \geq 1} \delta^{n-1} A_n$.

We have

$$\exp(\delta \mathcal{L}) - I_d = \delta \mathcal{L} \left(\sum_{n \geq 0} \frac{\delta^n}{(n+1)!} \mathcal{L}^n \right).$$

Note that the - formal - inverse of the series is given by

$$\left(\sum_{n \geq 0} \frac{\delta^n}{(n+1)!} \mathcal{L}^n \right)^{-1} = \sum_{n \geq 0} \frac{B_n}{n!} \delta^n \mathcal{L}^n,$$

where the B_n are the Bernoulli numbers - see [29, 37]. Hence, equations (4.1) and (4.2) are equivalent in the sense of formal series to

$$\mathcal{L} = \sum_{\ell \geq 0} \frac{B_\ell}{\ell!} \delta^\ell \mathcal{L}^\ell \tilde{A}(\delta) = \sum_{n \geq 0} \delta^n \left(A_{n+1} + \sum_{\ell=1}^n \frac{B_\ell}{\ell!} \sum_{n_1 + \dots + n_{\ell+1} = n - \ell} L_{n_1} \dots L_{n_\ell} A_{n_{\ell+1} + 1} \right). \quad (4.3)$$

Identifying the right hand sides of (4.1) and (4.3), we get the following induction formula

$$L_n = A_{n+1} + \sum_{\ell=1}^n \frac{B_\ell}{\ell!} \sum_{n_1 + \dots + n_{\ell+1} = n - \ell} L_{n_1} \dots L_{n_\ell} A_{n_{\ell+1} + 1}. \quad (4.4)$$

Each of the terms of the above sum is an operator of order $2n+2$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and therefore L_n is also an operator of order $2n+2$ with coefficients $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$.

Note that (4.2) gives immediately the inverse relation of this formal series equation:

$$A_n = \sum_{\ell=1}^n \frac{1}{\ell!} \sum_{n_1 + \dots + n_\ell = n - \ell} L_{n_1} \dots L_{n_\ell}. \quad (4.5)$$

Moreover, clearly it holds

$$L_n 1 = 0.$$

4.2 Approximate solution of the modified flow

In the previous section, for a given N , we have constructed the modified operator

$$L^{(N)} = L + \sum_{n=1}^N \delta^n L_n. \quad (4.6)$$

In order to perform weak backward error analysis and recursively estimate the modified invariant law of the numerical process, we should be able to find a solution v^N of the modified flow

$$\partial_t v^N(t, q, p) = L^{(N)} v^N(t, q, p), t > 0, (q, p) \in \mathbb{R}^{2d} \quad v^N(0, q, p) = \phi(q, p), (q, p) \in \mathbb{R}^{2d}. \quad (4.7)$$

However in our situation we do not know whether this equation has a solution.

The goal of the following theorem is to give a proper definition of the modified flow associated to (4.6).

Theorem 4.1 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int \phi d\rho = 0$. For any $N \in \mathbb{N}$, there exists an integer r_N such that $\phi \in \mathcal{C}_{r_N}^N(\mathbb{R}^{2d})$. For all $n \in \mathbb{N}$, there exist functions $v_n(t, \cdot) \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ defined for all times $t \geq 0$ such that for all $t \geq 0$ and $n \in \mathbb{N}$,*

$$\partial_t v_n(t, q, p) - L v_n(t, q, p) = \sum_{\ell=1}^n L_\ell v_{n-\ell}(t, q, p), \quad (4.8)$$

with initial condition $v_0(0, \cdot) = \phi$ and $v_n(0, \cdot) = 0$ for $n \geq 1$. For all $N \geq 0$, setting

$$v^{(N)}(t, q, p) = \sum_{k=0}^N \delta^k v_k(t, q, p),$$

the following holds:

a. *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$, there exist a positive real number C_N and integers ℓ_N and k_N such that for all $t \geq 0$, $0 < \delta < \delta_0$ and $(q, p) \in \mathbb{R}^{2d}$*

$$|\mathbb{E}v^{(N)}(t, q_1, p_1) - v^{(N)}(t+\delta, q, p)| \leq \delta^{N+1} C_N (1 + |q|^{\ell_N} + |p|^{\ell_N}) \sup_{\substack{s \in]0, \delta[\\ n=0, \dots, N}} |v_n(t+s, \cdot)|_{2N+2, k_N}.$$

b. *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$, there exist a positive real number C_N and an integer ℓ_N such that for all $0 < \delta < \delta_0$ and $(q, p) \in \mathbb{R}^{2d}$*

$$|\mathbb{E}\phi(q_1, p_1) - v^{(N)}(\delta, q, p)| \leq \delta^{N+1} C_N (1 + |q|^{\ell_N} + |p|^{\ell_N}) \|\phi\|_{N(d+7)+2, r_{N(d+7)+2}}.$$

Proof. Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int \phi d\rho = 0$, for any $N \in \mathbb{N}$, there exists an integer r_N such that $\phi \in \mathcal{C}_{r_N}^N(\mathbb{R}^{2d})$. For $n = 0$, equation (4.8) reduces to $v_0 = u$, the solution of (2.27). By Proposition 2.15, we deduce that u and all its derivatives have polynomial growth. Let $n \in \mathbb{N}$ and assume that $v_j(t)$ are constructed for $j = 1, \dots, n-1$. Let for $t \geq 0$ and $(q, p) \in \mathbb{R}^{2d}$

$$F_n(t, q, p) = \sum_{l=1}^n L_l v_{n-l}(t, q, p), \quad (4.9)$$

the right-hand side in (4.8), then v_n is uniquely defined and given by the formula

$$v_n(t, \cdot) = \int_0^t P_{t-s} F_n(s, \cdot) ds, \quad t \geq 0. \quad (4.10)$$

Using an induction argument and Proposition 2.15, we know that v_n and all its derivatives have polynomial growth. Moreover, we have for all $k \in \mathbb{N}$ and $n \in \mathbb{N}^*$ that there exists an integer $\alpha_{k,n}$ such that for all $t \geq 0$

$$\|v_n(t)\|_{k, \alpha_{k,n}} \leq C(t) \|\phi\|_{k+n(d+1)+4n, r_{k+n(d+5)}}, \quad (4.11)$$

where the constant $C(t)$ depends on t , k , n and V . This proves the first part of the Theorem.

To prove **a.**, we consider a fixed time t and define the functions $w_n(s, q, p) := v_n(t + s, q, p)$ for $s \geq 0$, $(q, p) \in \mathbb{R}^{2d}$ and $n \in \mathbb{N}$. By definition, these functions satisfy the relation

$$\begin{aligned} \partial_s w_n(s, q, p) &= \sum_{\ell=0}^n L_\ell w_{n-\ell}(s, q, p), \quad s \geq 0, (q, p) \in \mathbb{R}^{2d} \\ w_n(0, q, p) &= v_n(t, q, p), \quad (q, p) \in \mathbb{R}^{2d}. \end{aligned}$$

Let us consider the successive time derivatives of the functions w_n . We have, using the definition of w_n , for all $s \geq 0$ and $(q, p) \in \mathbb{R}^{2d}$,

$$\partial_s^2 w_n(s, q, p) = \sum_{\ell=0}^n L_\ell \partial_s w_{n-\ell}(s, q, p) = \sum_{k=0}^n \sum_{\ell_1+\ell_2=k} L_{\ell_1} L_{\ell_2} w_{n-k}(s, q, p),$$

and we see by induction that for all $m \geq 1$, $(q, p) \in \mathbb{R}^{2d}$ and $s \geq 0$

$$\partial_s^m w_n(s, q, p) = \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1} \dots L_{\ell_m} w_{\ell_{m+1}}(s, q, p).$$

Using the fact that the operators L_ℓ are of order $2\ell+2$ with no terms of order zero and that their coefficients have polynomial growth, we see that there exist a constant C , depending on n and m , and an integer β_n such that

$$|\partial_s^m w_n(s, q, p)| \leq C(1 + |q|^{\beta_n} + |p|^{\beta_n}) \sup_{k=0, \dots, n} |w_k(s, \cdot)|_{2n-2k+2m, \ell_{n,k,m}},$$

where $\ell_{n,k,m} \in \mathbb{N}$ is such that $w_k(s, \cdot) \in \mathcal{C}_{\ell_{n,k,m}}^{2(n-k+m)}(\mathbb{R}^{2d})$. Now let us consider the Taylor expansion of $w_n(\delta, \cdot)$, for $\delta < \delta_0$. Let N be fixed. We have for $\delta < \delta_0$, $(q, p) \in \mathbb{R}^{2d}$ and $n = 0, \dots, N$,

$$\begin{aligned} w_n(\delta, q, p) &= \sum_{m=0}^{N-n} \frac{\delta^m}{m!} \partial_t^m w_n(0, q, p) + \int_0^\delta \frac{s^{N-n}}{(N-n)!} \partial_t^{N-n+1} w_n(s, q, p) ds \\ &= \sum_{m=0}^{N-n} \frac{\delta^m}{m!} \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1} \dots L_{\ell_m} w_{\ell_{m+1}}(0, q, p) + R_{N,n}(\delta, q, p). \end{aligned}$$

Using the bounds on the time derivatives of w_n , we obtain the existence of an integer ℓ_N such that for all $0 \leq \delta \leq \delta_0$ and all $n = 0, \dots, N$,

$$|R_{N,n}(\delta, q, p)| \leq C \delta^{N-n+1} (1 + |q|^{\ell_N} + |p|^{\ell_N}) \sup_{\substack{s \in]0, \delta[\\ n=0, \dots, N}} |w_n(s, \cdot)|_{2N+2, k_N},$$

for some constants depending on N , n and k_N such that for $n = 0, \dots, N$, $w_n \in \mathcal{C}_{k_N}^{2N+2}(\mathbb{R}^{2d})$. After summation in n and using the expression (4.5) of the operators A_n and the definition of w_n , we get for all $(q, p) \in \mathbb{R}^{2d}$, $t \geq 0$ and $0 < \delta < \delta_0$

$$v^{(N)}(t + \delta, q, p) = \sum_{n=0}^N \delta^n \sum_{m=0}^n A_m v_{n-m}(t, q, p) + R_N(t, \delta, q, p),$$

where

$$|R_N(t, \delta, q, p)| \leq C_N \delta^{N+1} (1 + |q|^{\ell_N} + |p|^{\ell_N}) \sup_{\substack{s \in]0, \delta[\\ n=0, \dots, N}} |v_n(t+s, \cdot)|_{2N+2, k_N}.$$

To conclude we apply (3.1) applied to $\phi = v^{(N)}(t, q, p)$ and use the fact that $\delta < \delta_0$. The second estimate **b.** is then a consequence of **a.** with $t = 0$ and (4.11).

Note that in the previous theorem, we have constructed a function $v^{(N)}$ which is an approximate solution of (4.7). More precisely, we can easily show that we have for all time $t \geq 0$ and $x \in \mathbb{R}^{2d}$

$$\begin{aligned} \partial_t v^{(N)}(t, x) &= L^{(N)} v^{(N)}(t, x) + R^{(N)}(t, x), \\ v^{(N)}(0, x) &= \phi(x) \end{aligned}$$

where

$$R^{(N)}(t, x) = - \sum_{\ell_1, \ell_2=0, \dots, N} \delta^{\ell_1 + \ell_2} L_{\ell_1} v_{\ell_2}(t, x)$$

is of order $\mathcal{O}(\delta^{N+1})$.

5 Asymptotic expansion of the invariant measure and long time behavior

We now analyze the long time behavior of the solution of the modified flow associated to (4.7). In the following, for a given operator B , we denote by B^* its adjoint with respect to the $L^2(\rho)$ product. We start by an asymptotic expansion of a formal invariant measure for the numerical schemes.

Proposition 5.1 *Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$. Let $(L_n)_{n \geq 0}$ be the collection of operators defined recursively by (4.4). There exists a collection of functions $(\mu_n)_{n \geq 0}$ such that $\mu_0 = 1$ and $\int \mu_n d\rho = 0$ for all $n \in \mathbb{N}^*$, and for all $n \in \mathbb{N}^*$, $\mu_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$*

$$L^* \mu_n = - \sum_{\ell=1}^n (L_\ell)^* \mu_{n-\ell}. \quad (5.1)$$

Let $N \in \mathbb{N}^*$ be fixed and the function $\mu^{(N)}$ be defined for $(q, p) \in \mathbb{R}^{2d}$ and $0 < \delta < \delta_0$ by

$$\mu^{(N)}(\delta, q, p) = 1 + \sum_{n=1}^N \delta^n \mu_n(q, p),$$

then for $0 < \delta < \delta_0$, $\mu^{(N)}(\delta, \cdot, \cdot) \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and satisfies

$$\int_{\mathbb{R}^{2d}} \mu^{(N)}(\delta, q, p) \rho(q, p) dq dp = 1.$$

Proof. Let $n \geq 1$ be fixed. Assume that $\mu_0 = 1$ and for $j = 1, \dots, n-1$, μ_j are known and $\mu_j \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. Let us consider equation (5.1) given by

$$L^* \mu_n = - \sum_{\ell=1}^n L_\ell^* \mu_{n-\ell} =: G_n$$

Note that $G_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. Indeed, μ_0, \dots, μ_{n-1} and all the coefficients of L_ℓ^* are in $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$. Moreover, G_n satisfies

$$\begin{aligned} \int_{\mathbb{R}^{2d}} G_n(q, p) \rho(q, p) dq dp &= - \sum_{\ell=1}^n \int_{\mathbb{R}^{2d}} L_\ell^* \mu_{n-\ell}(q, p) \rho(q, p) dq dp \\ &= - \sum_{\ell=1}^n \int_{\mathbb{R}^{2d}} \mu_{n-\ell}(q, p) L_\ell 1 \rho(q, p) dq dp = 0. \end{aligned}$$

Using Lemma 2.16, we easily obtain the existence of a function $\mu_n \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ satisfying (5.1) and $\int \mu_n d\rho = 0$. This completes the proof. \blacklozenge

Proposition 5.2 *Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $u(0) = \phi$, then for any $n \in \mathbb{N}$, there exists an integer r_n such that $\phi \in \mathcal{C}_{r_n}^n(\mathbb{R}^{2d})$. For all $n \in \mathbb{N}$, $k \in \mathbb{N}$ and $\lambda < \lambda_0$, there exist a positive polynomial function $P_{k,n}$ and an integer $\ell_{k,n}$ such that for all $t \geq 0$*

$$\|v_n(t) - \int \phi \mu_n d\rho\|_{k, \ell_{k,n}} \leq P_{k,n}(t) e^{-\lambda t} \|\phi - \langle \phi \rangle\|_{\beta_{k,n}, \alpha_{k,n}}, \quad (5.2)$$

where λ_0 is defined in the Proposition 2.15, $\langle \phi \rangle = \int \phi \rho dq dp$, $\beta_{k,n} = k + 4n + (n+1)(d+1)$ and $\alpha_{k,n} = r_{\beta_{k,n}}$.

Proof. Let $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $u(0) = \phi$, then for any $n \in \mathbb{N}$, there exists an integer r_n such that $\phi \in \mathcal{C}_{r_n}^n(\mathbb{R}^{2d})$. Using the fact that $\mu_0 = 1$ and $v_0 = u$, we see that the estimate (5.2) is satisfied for $n = 0$ (Proposition 2.15). Let $n \geq 1$ assume that v_j , $j = 0, \dots, n-1$ satisfy: For all $k \in \mathbb{N}$ and $\lambda < \lambda_0$, there exist a positive polynomial function $P_{k,j}$ and $\ell_{k,j}$ such that for any $t \geq 0$:

$$\|v_j(t, \cdot) - \int \phi \mu_j d\rho\|_{k, \ell_{j,k}} \leq P_{k,j}(t) e^{-\lambda t} \|\phi - \langle \phi \rangle\|_{k+4j+(j+1)(d+1), \alpha_{k,j}},$$

where $\alpha_{k,j}$ is such that $\phi \in \mathcal{C}_{\alpha_{k,j}}^{k+4j+(j+1)(d+1)}(\mathbb{R}^{2d})$. Let us set for $t \geq 0$

$$c_n(t) = \sum_{m=0}^n \int_{\mathbb{R}^{2d}} v_{n-m}(t, q, p) \mu_m(q, p) \rho(q, p) dq dp.$$

We claim that $c_n(\cdot)$ does not depend on time. Indeed, for all $t \geq 0$,

$$\begin{aligned} &\sum_{m=0}^n \partial_t \int_{\mathbb{R}^{2d}} v_{n-m}(t, q, p) \mu_m(q, p) \rho(q, p) dq dp \\ &= \sum_{m=0}^n \partial_t \int_{\mathbb{R}^{2d}} v_m(t, q, p) \mu_{n-m}(q, p) \rho(q, p) dq dp \\ &= \sum_{m=0}^n \sum_{\ell=0}^m \int_{\mathbb{R}^{2d}} L_{m-\ell} v_\ell(t, q, p) \mu_{n-m}(q, p) \rho(q, p) dq dp \\ &= \sum_{\ell=0}^n \int_{\mathbb{R}^{2d}} v_\ell(t, q, p) \sum_{m=0}^{n-\ell} L_m^* \mu_{n-\ell-m}(q, p) \rho(q, p) dq dp \\ &= 0, \end{aligned}$$

by definition of the coefficients μ_n (see (5.1)). Note that the computation above is justified because $\forall n$, v_n , μ_n and all their derivatives have polynomial growth. We deduce, for all $t \geq 0$,

$$\int_{\mathbb{R}^{2d}} \partial_t v_n(t, q, p) \rho(q, p) dq dp = - \sum_{m=1}^n \int_{\mathbb{R}^{2d}} \partial_t v_{n-m}(t, q, p) \mu_m(q, p) \rho(q, p) dq dp. \quad (5.3)$$

Now we compute the average of F_n defined by (5.3). By (4.8) and (5.3), we have for $t \geq 0$

$$\begin{aligned} \langle F_n(t) \rangle &= \int_{\mathbb{R}^{2d}} F_n(t, q, p) \rho(q, p) dq dp \\ &= \int_{\mathbb{R}^{2d}} \partial_t v_n(t, q, p) \rho(q, p) dq dp - \int_{\mathbb{R}^{2d}} L v_n(t, q, p) \rho(q, p) dq dp \\ &= \int_{\mathbb{R}^{2d}} \partial_t v_n(t, q, p) \rho(q, p) dq dp \\ &= - \sum_{m=1}^n \int_{\mathbb{R}^{2d}} \partial_t v_{n-m}(t, q, p) \mu_m(q, p) dq dp. \end{aligned}$$

We rewrite (4.10) as follows: for all $(q, p) \in \mathbb{R}^{2d}$ and $t \geq 0$,

$$v_n(t, q, p) = \int_0^t \langle F_n(s) \rangle ds + \int_0^t P_{t-s}(F_n(s, q, p) - \langle F_n(s) \rangle) ds.$$

Using the previous expression obtained for $\langle F_n(s) \rangle$ and recalling the initial data for v_n , we deduce that for all $(q, p) \in \mathbb{R}^{2d}$ and $t \geq 0$

$$\begin{aligned} v_n(t, q, p) &= - \sum_{m=1}^n \int_{\mathbb{R}^{2d}} v_{n-m}(t) \mu_m d\rho + \int \phi \mu_n d\rho \\ &\quad + \int_0^t P_{t-s}(F_n(s, q, p) - \langle F_n(s) \rangle) ds. \end{aligned}$$

Then, using $\int_{\mathbb{R}^{2d}} \mu_m(q, p) \rho(q, p) dq dp = 0$, for $m \in \mathbb{N}^*$ (Proposition 5.1), we get for all $(q, p) \in \mathbb{R}^{2d}$ and $t \geq 0$

$$\begin{aligned} v_n(t, q, p) - \int \phi \mu_n d\rho &= - \sum_{m=1}^n \int_{\mathbb{R}^{2d}} \left(v_{n-m}(t, \tilde{q}, \tilde{p}) - \int \phi \mu_{n-m} d\rho \right) \mu_m(\tilde{q}, \tilde{p}) \rho(\tilde{q}, \tilde{p}) d\tilde{q} d\tilde{p} \\ &\quad + \int_0^t P_{t-s}(F_n(s, q, p) - \langle F_n(s) \rangle) ds. \end{aligned}$$

Note that, since L_ℓ , $\ell \in \mathbb{N}$ is a differential operator of order $2\ell + 2$ whose coefficients belong to $\mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ and contain no zero order terms, we have for $k \in \mathbb{N}$ that there exist $\gamma_{k,n} \in \mathbb{N}$ and $\zeta_{k,n,l} \in \mathbb{N}$ such that for $s \geq 0$,

$$\begin{aligned} \| F_n(s) - \langle F_n(s) \rangle \|_{k, \gamma_{k,n}} &\leq \sum_{\ell=0}^{n-1} c_{k,\ell} |v_\ell(s)|_{b_{k,n,l}, \zeta_{k,n,l}} \\ &\leq \sum_{\ell=0}^{n-1} c_{k,\ell} \| v_\ell(s) - \int \phi \mu_\ell d\rho \|_{b_{k,n,l}, \zeta_{k,n,l}}, \end{aligned}$$

where $b_{k,n,l} = k + 2(n-l) + 2$ and we have used:

$$|v_n(t_{j+1}, \cdot)|_{\alpha, \beta} = |v_n(t_{j+1}, \cdot) - \int_{\mathbb{R}^{2d}} \phi(q, p) \mu_n(q, p) \rho(q, p) dq dp|_{\alpha, \beta}.$$

Then, using Proposition 2.15, we have for $k \in \mathbb{N}$ that there exists $r \in \mathbb{N}$ such that for $t \geq 0$

$$\begin{aligned} & \|v_n(t) - \int \phi \mu_n d\rho\|_{k,r} \leq \\ & \sum_{m=1}^n \left(\int_{\mathbb{R}^{2d}} |v_{n-m}(t, q, p) - \int \phi \mu_{n-m} d\rho|^2 \rho(q, p) dq dp \right)^{1/2} \left(\int_{\mathbb{R}^{2d}} |\mu_m(q, p)|^2 \rho(q, p) dq dp \right)^{1/2} \\ & \quad + \int_0^t C_{k,n,i} e^{-\lambda(t-s)} \|F_n(s) - \langle F_n(s) \rangle\|_{k+(d+1), \gamma_{k+(d+1)}} ds. \end{aligned}$$

Using the induction assumption, we have, for $k \in \mathbb{N}$ that there exists $r \in \mathbb{N}$ such that for $t \geq 0$,

$$\begin{aligned} & \|v_n(t) - \int \phi \mu_n d\rho\|_{k,r} \leq \sum_{m=1}^n \tilde{c}_m P_{0,n-m,0}(t) e^{-\lambda t} \|\phi - \langle \phi \rangle\|_{(n+1)(d+1)+4n, \alpha_{0,j}} \\ & \quad + C_{k,n} \sum_{l=0}^{n-1} c_{k,l} \int_0^t P_{k,l}(s) e^{-\lambda(t-s)} e^{-\lambda s} ds \|\phi - \langle \phi \rangle\|_{4n+k+(n+1)(d+1), \alpha_{k,j}}. \end{aligned}$$

The conclusion follows. \blacklozenge

The following Proposition finishes the proof of our main result Theorem 2.17.

Proposition 5.3 *Let N be fixed and ℓ_N be fixed. Let $\delta_0 = \min(\frac{1}{\gamma}, \frac{\gamma\beta}{4\theta})$. Let (q_k, p_k) be the discrete process defined by the implicit Euler scheme (2.12) or the implicit split-step scheme (2.11). Let $0 \leq \delta < \delta_0$, $\alpha_N = 6N + 8 + (N+2)(d+1)$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d}) \cap \mathcal{C}_{\ell_N}^{\alpha_N}(\mathbb{R}^{2d})$, then there exist strictly positive real number C_N and an integer k_N such that we have for $k \geq 0$,*

$$\|\mathbb{E}\phi(q_k, p_k) - v^{(N)}(t_k, \cdot)\|_{0, k_N} \leq \delta^{N+1} C_N \|\phi - \langle \phi \rangle\|_{\alpha_N, \ell_N}, \quad (5.4)$$

where $t_k = k\delta$.

Moreover, for $0 \leq \delta < \delta_0$, $\lambda < \lambda_0$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d}) \cap \mathcal{C}_{\ell_N}^{\alpha_N}(\mathbb{R}^{2d})$, there exist a positive real number C_N , an integer k_N and a positive polynomial function P_N satisfying the following : For all $k \in \mathbb{N}$,

$$\|\mathbb{E}\phi(q_k, p_k) - \int \phi \mu^{(N)} d\rho\|_{0, k_N} \leq C_N \left(e^{-\lambda t_k} P_N(t_k) + \delta^{N+1} \right) \|\phi - \langle \phi \rangle\|_{\alpha_N, \ell_N},$$

where $t_k = k\delta$.

Proof. Let N be fixed and ℓ_N be fixed. Let (q_k, p_k) be the discrete process defined by the implicit Euler scheme (2.12) or the implicit split-step scheme (2.11), $0 \leq \delta < \delta_0$ and $\phi \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d}) \cap \mathcal{C}_{\ell_N}^{\alpha_N}(\mathbb{R}^{2d})$ be fixed. Let $(q, p) \in \mathbb{R}^{2d}$ such that $q_0 = q$ and $p_0 = p$. For all k , with $t_k = k\delta$, we have

$$\begin{aligned} \mathbb{E}\phi(q_k, p_k) - v^{(N+1)}(t_k, q, p) &= \mathbb{E}v^{(N+1)}(0, q_k, p_k) - v^{(N+1)}(t_k, q, p) \\ &= \mathbb{E} \sum_{j=0}^{k-1} \mathbb{E}^{q_{k-j-1}, p_{k-j-1}} \left(v^{(N+1)}(t_j, q_{k-j}, p_{k-j}) - v^{(N)}(t_{j+1}, q_{k-j-1}, p_{k-j-1}) \right). \end{aligned}$$

Here we have used the notation $\mathbb{E}^{q_{k-j-1}, p_{k-j-1}}$ for the conditional expectation with respect to the filtration generated by q_{k-j-1} and p_{k-j-1} . We obtain:

$$\begin{aligned} & \mathbb{E}^{q_{k-j-1}, p_{k-j-1}} \left(v^{(N+1)}(t_j, q_{k-j}, p_{k-j}) - v^{(N+1)}(t_{j+1}, q_{k-j-1}, p_{k-j-1}) \right) \\ &= \mathbb{E}^{q_{k-j-1}, p_{k-j-1}} \left(v^{(N+1)}(t_j, q_1(q_{k-j-1}), p_1(p_{k-j-1})) - v^{(N+1)}(t_{j+1}, q_{k-j-1}, p_{k-j-1}) \right), \end{aligned}$$

where $(q_1(q), p_1(p))$ is the first step of the scheme (2.12) or of the scheme (2.11) when the initial condition is (q, p) . Using Theorem 4.1 with $t = t_j$, Proposition 2.9 and (5.2), we deduce that there exist integers r_N and k_N such that for all $k \in \mathbb{N}$

$$\begin{aligned} \|\mathbb{E}\phi(q_k, p_k) - v^{(N+1)}(t_k, \cdot)\|_{0, k_N} &\leq \delta^{N+2} C_N \sum_{j=0}^{k-1} \sup_{s \in]0, \delta[, n=0, \dots, N+1} |v_n(t_{j+1}, \cdot)|_{2N+4, r_N} \\ &\leq \delta^{N+2} C_N \|\phi - \langle \phi \rangle\|_{6N+8+(N+2)(d+1), \ell_N} \sum_{j=0}^{p-1} e^{\lambda t_j} P_N(t_j) \\ &\leq \delta^{N+2} C_N \|\phi - \langle \phi \rangle\|_{6N+8+(N+2)(d+1), \ell_N} \sum_{j=0}^{p-1} e^{-\bar{\lambda} t_j}, \end{aligned}$$

for some constant C_N . We have used:

$$|v_n(t_{j+1}, \cdot)|_{\alpha, \beta} = |v_n(t_{j+1}, \cdot) - \int_{\mathbb{R}^{2d}} \phi(q, p) \mu_n(q, p) \rho(q, p) dq dp|_{\alpha, \beta}.$$

We conclude by using the fact that for a fixed constant $\gamma_1 > 0$, it holds true

$$\sum_{j=0}^{p-1} e^{-\gamma_1 j \delta} \leq \frac{1}{1 - e^{-\gamma_1 \delta}} \leq \frac{C}{\delta},$$

where the constant C depends on γ_1 and δ_0 . This implies

$$\|\mathbb{E}\phi(q_k, p_k) - v^{(N+1)}(t_k, q, p)\|_{0, k_N} \leq C_N \delta^{N+1} \|\phi - \langle \phi \rangle\|_{6N+8+(N+2)(d+1), \ell_N}$$

To prove (5.4), we note that

$$v^{(N+1)}(t_k, q, p) = v^{(N)}(t_k, q, p) + \delta^{N+1} v_{N+1}(t_k, q, p)$$

and, for all $k \in \mathbb{N}$,

$$\begin{aligned} |v_{N+1}(t_k, q, p)| &\leq |v_{N+1}(t_k, q, p) - \int \phi \mu_{N+1} d\rho| + \left| \int (\phi - \langle \phi \rangle) \mu_{N+1} d\rho \right| \\ &\leq C_N \|\phi - \langle \phi \rangle\|_{\beta_{0, N+1}, \alpha_{0, N+1}} (1 + |q|^{\ell_{0, N+1}} + |p|^{\ell_{0, N+1}}), \end{aligned}$$

using (5.2) and its notations. The second estimate is a consequence of (5.2). \blacklozenge

6 Appendix: Estimates on u and its derivatives

6.1 Notations, assumptions and result

In all this appendix, the constant C may vary from line to line and we will use the following notations:

Let $\phi \in C_{pol}^\infty(\mathbb{R}^{2d})$, then, for all $m \in \mathbb{N}$, there exists an integer r_m such that $\phi \in C_{r_m}^m(\mathbb{R}^{2d})$. For a multi-index $\mathbf{k} = (k_1, \dots, k_{2d}) \in \mathbb{N}^d$, we set $|\mathbf{k}| = k_1 + \dots + k_{2d}$ and for a function $\phi \in C^\infty(\mathbb{R}^{2d})$, we set

$$D^{\mathbf{k}}\phi(x) = \frac{\partial^{|\mathbf{k}|}\phi(x)}{\partial_{x_1}^{k_1} \dots \partial_{x_{2d}}^{k_{2d}}}, \quad x = (x_1, \dots, x_{2d}) \in \mathbb{R}^{2d}.$$

Moreover, we will assume in all the appendix that $\int \phi d\rho = 0$. We recall that u is defined by (2.26).

The aim of this appendix is to prove the following result (Proposition 2.15):

Proposition 6.1 *There exists a strictly positive real number λ_0 such that for any $m \in \mathbb{N}$, $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$ and $0 < \lambda < \lambda_0$, there exist an integer $s > 2r_{m+1+d}$ and a strictly positive real number C such that for all $t \geq 0$ and $(q, p) \in \mathbb{R}^{2d}$*

$$|D^{\mathbf{k}}u(t, q, p)| \leq C(1 + |q|^s + |p|^s) \|\phi\|_{m+d+1, r_{m+1+d}} \exp(-\lambda t).$$

To prove this Proposition, we will use the same idea as in [84]. Unlike in [84], we need to know how the estimate depend on ϕ . Moreover, using an estimate of u described in [43], the proof is easier than in [84].

The proof proceeds as follows. We first show estimates on u and its derivatives in an appropriate space. More precisely, we will show that for any $0 < \lambda < 2\lambda_0$, $m \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, there exists a strictly positive real number C_m such that for all $t > 0$

$$\int |D^{\mathbf{k}}u(t, q, p)|^2 \pi_s(q, p) dq dp \leq C_m \exp(-\lambda t),$$

where the function π_s is defined as

$$\pi_s = \frac{1}{\Gamma_s}, \tag{6.1}$$

for some integer s .

Moreover, we have the following result on π_s : For all multi-index \mathbf{j} and integer s , there exists a function $\psi_{\mathbf{j}, s} \in C^\infty$ such that

$$\partial^{\mathbf{j}}\pi_s(q, p) = \psi_{\mathbf{j}, s}(q, p)\pi_s(q, p) \tag{6.2}$$

where

$$\psi_{\mathbf{j}, s}(q, p) \xrightarrow{|(q, p)| \rightarrow \infty} 0.$$

Then, for any $m \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, it is possible to choose an integer s_m such that we have, for all $t > 0$, $s \geq s_m$ and $0 < \zeta < 2\lambda_0$

$$\int_{\mathbb{R}^{2d}} |D^{\mathbf{k}}(u(t, q, p)\pi_s(q, p))|^2 dq dp < C_m \exp(-\zeta t).$$

We then conclude by applying Sobolev embedding Theorem (see [8]).

We will also use the following notation: for all $s \in \mathbb{N}$, $d\pi_s = \pi_s(q, p) dq dp$.

6.2 Estimates on $u(t)$ and its derivatives in $L^2(\pi_s) = \{f : \mathbb{R}^{2d} \rightarrow \mathbb{R}; \int |f|^2 d\pi_s\}$

Using expression (2.24) of L^\top and inequality (2.7) on $L\Gamma$, computations lead to

$$\begin{aligned} L^\top(\pi_s) &= s \frac{L\Gamma}{\Gamma^{s+1}} - \frac{sd\sigma^2}{\Gamma} \pi_s + \frac{s(s+1)\sigma^2}{2} \frac{|\partial_p \Gamma|^2}{\Gamma^2} \pi_s + d\gamma \pi_s \\ &\leq (-a_1 s + \gamma d) \pi_s + \Phi_s \pi_s, \end{aligned}$$

where $\Phi_s(q, p) \xrightarrow{|(q,p)| \rightarrow +\infty} 0$ and a_1 is defined by (2.7). Hence, for each $s \in \mathbb{N}^*$, there exists a real number $\nu_s > 0$ such that

$$L^\top(\pi_s) \leq \nu_s \pi_s. \quad (6.3)$$

We will now show the following proposition then we will use Sobolev inequalities to prove Proposition 6.1:

Proposition 6.2 *Let $m \in \mathbb{N}$, $0 < \zeta < 2\lambda_0$, where λ_0 is defined in the following and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$ be fixed. There exists an integer $s_m > 2r_m$ such that, for all $s \geq s_m$, there exists a strictly positive real number $C_{m,s}$ such that we have for all $T > 0$,*

$$\int |D^{\mathbf{k}}u(T)|^2 d\pi_s \leq C_{m,s} \|\phi\|_{m,r_m}^2 \exp(-\zeta T), \quad (6.4)$$

where r_m is defined at the beginning of this appendix.

Proposition 6.2 is a corollary of the following result:

Proposition 6.3 *Let λ_0 be defined in the following. For all $m \in \mathbb{N}$, $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, positive polynomial function Q and $0 < \zeta < 2\lambda_0$, there exists an integer $s_m > 2r_m$ such that for all $s \geq s_m$ there exists a strictly positive real numbers $C_{m,Q,s}$ such that we have for all $T > 0$*

$$\int_0^T \exp(\zeta t) \int Q |D^{\mathbf{k}}u(t)|^2 d\pi_s dt \leq C_{m,Q,s} \|\phi\|_{m,r_m}^2. \quad (6.5)$$

For the convenience of the reading, we will first show Propositions 6.2 and 6.3 for $m = 0$. Then, we will show Proposition 6.3 for $m = 1$ and explain how to deduce Proposition 6.2 for $m = 1$. Finally, we will show Proposition 6.3 by induction and show that Proposition 6.2 is a consequence of Proposition 6.3. The idea to prove Proposition 6.3 for $m \geq 1$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$ is the following: We first show the result for $Q|\partial_p D^{\mathbf{k}-1}|^2$ and $Q|(\alpha\partial_p - \partial_q)D^{\mathbf{k}-1}|^2$. We can then deduce the result for $Q|\partial_q D^{\mathbf{k}-1}|^2$.

To show this two Propositions for $m = 0$, we need a better point-wise estimatie of u :

Lemma 6.4 *There exists $C = C(r_0) > 0$, $\lambda_0 = \lambda_0(r_0) > 0$ such that, for all $t \geq 0$ and $(q, p) \in \mathbb{R}^{2d}$,*

$$|u(t, q, p)| \leq C\Gamma^{r_0}(q, p) \exp(-\lambda_0 t) \|\phi\|_{0,r_0}. \quad (6.6)$$

A proof of this result can be found in [43] or [38]. To show this Lemma, the two main ingredients are the property (2.6) on Γ and that for $x \in \mathbb{R}^{2d}$, $t > 0$ and open $\mathcal{O} \subset \mathbb{R}^{2d}$, the transition kernel for (2.4) satisfies $Q_t(x, \mathcal{O}) > 0$. Under Assumption **B**, the second property is true (see [43]).

We have the following Corollary:

Lemma 6.5 For $s > 2r_0$, there exists a strictly positive real number C_s such that

$$\int |u(t)|^2 d\pi_s \leq C_s \|\phi\|_{0,r_0}^2 \exp(-2\lambda_0 t) \quad \forall t \geq 0. \quad (6.7)$$

Moreover, for Q a positive polynomial function, we have, for all $s > s_Q \geq 2r_0$, that there exists a strictly positive real number $C_{Q,s}$ such that

$$\int Q|u(t)|^2 d\pi_s \leq C_{Q,s} \|\phi\|_{0,r_0}^2 \exp(-2\lambda_0 t) \quad \forall t \geq 0. \quad (6.8)$$

Then, the results (6.4) and (6.5) for $m = 0$ are a consequence of Lemma 6.5.

The following Lemma is the key of the proof of all the other Lemmas.

Lemma 6.6 Let A be a linear operator and Q a polynomial function. There exists an integer $s_{A,Q}$ such that for all $s \geq s_{A,Q}$, we have for all $\zeta > 0$ and $T > 0$

$$\begin{aligned} & \exp(\zeta T) \int Q|Au(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int Q|\partial_p(Au(t))|^2 d\pi_s dt \\ & \leq \int Q|Au(0)|^2 d\pi_s + (\zeta + \nu_s) \int_0^T \exp(\zeta t) \int Q|Au(t)|^2 d\pi_s dt \\ & + 2 \int_0^T \exp(\zeta t) \int Q\langle [A, L]u(t), Au(t) \rangle d\pi_s dt - \int_0^T \exp(\zeta t) \int |Au(t)|^2 LQ d\pi_s dt \\ & \quad - \sigma^2 \int_0^T \exp(\zeta t) \int \langle \partial_p Q, \partial_p |Au(t)|^2 \rangle d\pi_s dt, \end{aligned} \quad (6.9)$$

where, for A and B two linear operators, $[A, B] = AB - BA$.

Proof. Let s large enough such that $\int Q|Au(0)|^2 d\pi_s < \infty$. Using (2.23) and (2.25), we get

$$\begin{aligned} & \frac{d}{dt} [\exp(\zeta t) Q|Au(t)|^2] \\ & = \zeta \exp(\zeta t) Q|Au(t)|^2 + 2 \exp(\zeta t) Q\langle ALu(t), Au(t) \rangle \\ & = \zeta \exp(\zeta t) Q|Au(t)|^2 + 2 \exp(\zeta t) Q\langle LAu(t), Au(t) \rangle \\ & \quad + 2 \exp(\zeta t) Q\langle [A, L]u(t), Au(t) \rangle \\ & = \zeta \exp(\zeta t) Q|Au(t)|^2 + \exp(\zeta t) QL|Au(t)|^2 - \sigma^2 \exp(\zeta t) Q|\partial_p(Au(t))|^2 \\ & \quad + 2 \exp(\zeta t) Q\langle [A, L]u(t), Au(t) \rangle \\ & = \zeta \exp(\zeta t) Q|Au(t)|^2 + \exp(\zeta t) L(Q|Au(t)|^2) - \exp(\zeta t) |Au(t)|^2 LQ \\ & \quad - \sigma^2 \exp(\zeta t) \langle \partial_p Q, \partial_p |Au(t)|^2 \rangle - \sigma^2 \exp(\zeta t) Q|\partial_p(Au(t))|^2 \\ & \quad + 2 \exp(\zeta t) Q\langle [A, L]u(t), Au(t) \rangle. \end{aligned}$$

We integrate with respect to t ,

$$\begin{aligned} & \exp(\zeta T) Q|Au(T)|^2 \\ & = Q|Au(0)|^2 + \zeta \int_0^T \exp(\zeta t) Q|Au(t)|^2 dt + \int_0^T \exp(\zeta t) L(Q|Au(t)|^2) dt \\ & \quad - \int_0^T \exp(\zeta t) |Au(t)|^2 LQ dt - \sigma^2 \int_0^T \exp(\zeta t) \langle \partial_p Q, \partial_p |Au(t)|^2 \rangle dt \\ & \quad - \sigma^2 \int_0^T \exp(\zeta t) Q|\partial_p Au(t)|^2 dt + 2 \int_0^T \exp(\zeta t) Q\langle [A, L]u(t), Au(t) \rangle dt. \end{aligned}$$

We integrate with respect to π_s . Using the inequality (6.3) on $L^\top \pi_s$, we have (6.13). \blacklozenge

We will also need the following computations:

Lemma 6.7 *Let $k \in \mathbb{N}$, we have for any $(q, p) \in \mathbb{R}^{2d}$*

$$-LH^k(q, p) \leq 2\gamma k H^k(q, p) \quad (6.10)$$

and for all $t \geq 0$ and linear operator A ,

$$\langle \partial_p H^k, \partial_p |Au(t)|^2 \rangle \leq 2k H^k |Au(t)|^2 + 2k H^{k-1} |\partial_p Au(t)|^2. \quad (6.11)$$

Proof. For any $(q, p) \in \mathbb{R}^{2d}$ and $k \in \mathbb{N}^*$, we have

$$\partial_p H^k(q, p) = k H^{k-1}(q, p) p$$

and

$$\begin{aligned} -LH^k(q, p) &= \gamma k |p|^2 H^{k-1}(q, p) - \frac{k}{2} H^{k-1}(q, p) - \frac{k(k-1)}{2} |p|^2 H^{k-2}(q, p) \\ &\leq \gamma k |p|^2 H^{k-1}(q, p) \leq 2\gamma k H^k(q, p). \end{aligned}$$

We have used the positivity of V . Moreover, we have for any $t \geq 0$, $\ell \in \mathbb{N}$ and for each component of Au that we still write Au ,

$$\begin{aligned} \langle \partial_p H^{2\ell}, \partial_p |Au(t)|^2 \rangle &= 4\ell H^\ell Au(t) \langle p H^{\ell-1}, \partial_p Au(t) \rangle \\ &\leq 2\ell H^{2\ell} |Au(t)|^2 + 2\ell |p|^2 H^{2\ell-2} |\partial_p Au(t)|^2 \\ &\leq 2\ell H^{2\ell} |Au(t)|^2 + 4\ell H^{2\ell-1} |\partial_p Au(t)|^2 \end{aligned}$$

and

$$\begin{aligned} \langle \partial_p H^{2\ell+1}, \partial_p |Au(t)|^2 \rangle &= 2(2\ell+1) \langle H^\ell u(t) p, H^\ell \partial_p Au(t) \rangle \\ &\leq (2\ell+1) H^{2\ell} |p|^2 |u(t)|^2 + (2\ell+1) H^{2\ell} |\partial_p Au(t)|^2 \\ &\leq 2(2\ell+1) H^{2\ell+1} |u(t)|^2 + (2\ell+1) H^{2\ell} |\partial_p Au(t)|^2. \end{aligned}$$

◆

We now show the results (6.4) and (6.5) for $m = 1$. First, we show the two following preliminary Lemmas.

Lemma 6.8 *Let Q be a positive polynomial function. Let $s > 2r_0$ large enough and $0 < \zeta < 2\lambda_0$. There exists a strictly positive real number $C_{Q,s}$ such that for all $T > 0$*

$$\int_0^T \exp(\zeta t) \int Q |\partial_p u(t)|^2 d\pi_s dt \leq C_{Q,s} \|\phi\|_{0,r_0}^2. \quad (6.12)$$

Proof. Let $\zeta > 0$. We have $[Id, L] = 0$, then, using Lemma 6.6 with $A = Id$ and $Q = 1$, we get for $T > 0$

$$\begin{aligned} \exp(\zeta T) \int |u(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int |\partial_p u(t)|^2 d\pi_s dt \\ \leq \int |u(0)|^2 d\pi_s + (\zeta + \nu_s) \int_0^T \exp(\zeta t) \int |u(t)|^2 d\pi_s dt. \end{aligned}$$

We choose $0 < \zeta < 2\lambda_0$ and, using (6.7), we bound the last term. Then, we have (6.12) for $Q = 1$.

Let Q a positive polynomial function. Using Lemma 6.6 for $A = I_d$, we get for s large enough, $\zeta > 0$ and $T > 0$

$$\begin{aligned} & \exp(\zeta T) \int Q|u(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int Q|\partial_p(u(t))|^2 d\pi_s dt \\ & \leq \int Q|u(0)|^2 d\pi_s + (\zeta + \nu_s) \int_0^T \exp(\zeta t) \int Q|u(t)|^2 d\pi_s dt \\ & \quad - \int_0^T \exp(\zeta t) \int |u(t)|^2 LQ d\pi_s dt - \sigma^2 \int_0^T \exp(\zeta t) \int \langle \partial_p Q, \partial_p |u(t)|^2 \rangle d\pi_s dt, \end{aligned} \quad (6.13)$$

As $V \in \mathcal{C}_{pol}^\infty(\mathbb{R}^d)$, there exists a positive polynomial function Q_1 such that $|LQ| \leq Q_1$, then we have for any $T > 0$ and s large enough

$$\begin{aligned} & - \int_0^T \exp(\zeta t) \int |u(t)|^2 LQ d\pi_s dt - \sigma^2 \int_0^T \exp(\zeta t) \int \langle \partial_p Q, \partial_p |u(t)|^2 \rangle d\pi_s dt \\ & \leq \int_0^T \exp(\zeta t) (2Q_1 + \sigma^2 |\partial_p Q|^2) |u(t)|^2 d\pi_s dt + \sigma^2 \int_0^T \exp(\zeta t) \int |\partial_p u(t)|^2 d\pi_s dt. \end{aligned}$$

We choose $0 < \zeta < 2\lambda_0$ and use (6.8) and (6.12) with $Q = 1$ to have the result (6.12) for any positive polynomial function Q . \blacklozenge

Lemma 6.9 *Let $s > 2r_1$ large enough and $0 < \zeta < 2\lambda_0$. There exists a strictly positive real number α_s such that for $\alpha > \alpha_s$, there exists a positive real number C_s such that, for all $T > 0$,*

$$\begin{aligned} & \int_0^T \exp(\zeta t) \int |\alpha \partial_p u(t) - \partial_q u(t)|^2 d\pi_s dt + \int_0^T \exp(\zeta t) \int |\partial_p(\alpha \partial_p u(t) - \partial_q u(t))|^2 d\pi_s dt \\ & \leq C_s \|\phi\|_{1,r_1}^2. \end{aligned} \quad (6.14)$$

Let $k > 0$ an integer. For any $0 < \zeta < 2\lambda_0$ and $s > 2r_1$ large enough, there exists a strictly positive real number α_k such that $\forall \alpha \geq \alpha_k$ there exists a strictly positive real number $C_{k,s}$ such that, for all $T > 0$,

$$\begin{aligned} & \exp(\zeta T) \int H^k |\alpha \partial_p u(T) - \partial_q u(T)|^2 d\pi_s + \int_0^T \exp(\zeta t) \int H^k |\partial_p(\alpha \partial_p u(t) - \partial_q u(t))|^2 d\pi_s dt \\ & \leq C_{k,s} \|\phi\|_{1,r_1}^2. \end{aligned} \quad (6.15)$$

Proof. Let $\alpha > 0$ and $i \in \{1, \dots, d\}$. We use the following notation: $A_1 = \alpha \partial_{p_i} - \partial_{q_i}$. We have for any function $\psi \in C^\infty(\mathbb{R}^{2d})$

$$[A_1, L]\psi = -\alpha A_1 \psi + \alpha(\alpha - \gamma) \partial_{p_i} \psi + \langle \partial_{q_i} \partial_q V, \partial_p \psi \rangle.$$

Using the polynomial growth of $\partial_{q_i} \partial_q V$, we have that there exist a positive polynomial function Q_1 , $\varepsilon_1 > 0$ and $\varepsilon_2 > 0$ such that for any function $\psi \in C^\infty(\mathbb{R}^{2d})$

$$\begin{aligned} 2\langle [A_1, L]\psi, A_1 \psi \rangle & = -2\alpha |A_1 \psi|^2 + 2A_1 \psi \langle \partial_{q_i} \partial_q V, \partial_p \psi \rangle + 2\alpha(\alpha - \gamma) \partial_{p_i} \psi A_1 \psi \\ & \leq (\varepsilon_1 + \varepsilon_2 - 2\alpha) |A_1 \psi|^2 + \frac{Q_1}{\varepsilon_1} |\partial_p \psi|^2 + \frac{\alpha(\alpha - \gamma)^2}{\varepsilon_2} |\partial_{p_i} \psi|^2. \end{aligned} \quad (6.16)$$

Then, choosing s large enough and using Lemma 6.6 with $Q = 1$, we get for all $T > 0$, $\varepsilon_1, \varepsilon_2$ and $\zeta > 0$

$$\begin{aligned} & \exp(\zeta T) \int |A_1 u(T)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int |\partial_p(A_1 u(t))|^2 d\pi_s dt \\ & \leq \int |A_1 u(0)|^2 d\pi_s + \frac{1}{\varepsilon_1} \int_0^T \exp(\zeta t) \int Q_1 |\partial_p u(t)|^2 d\pi_s dt \\ & \quad + \frac{(\alpha(\alpha - \gamma))^2}{\varepsilon_2} \int_0^T \exp(\zeta t) \int |\partial_{p_i} u(t)|^2 d\pi_s dt \\ & \quad + (\nu_s + \zeta + \varepsilon_1 + \varepsilon_2 - 2\alpha) \int_0^T \exp(\zeta t) \int |A_1 u(t)|^2 d\pi_s dt. \end{aligned}$$

We choose $0 < \zeta < 2\lambda_0$ and α, ε_1 and ε_2 such that $\nu_s + \zeta + \varepsilon_1 + \varepsilon_2 - 2\alpha < 0$. We then use (6.12) to prove (6.14).

We now prove (6.15) by recursion on k . We have proved the case $k = 0$. Let us assume (6.15) is true for $k - 1$. We want to obtain it for k .

Using computations for $k = 0$, (6.16), (6.10), (6.11) and Lemma 6.6, we get for s large enough, $\varepsilon_1 > 0$, $\varepsilon_2 > 0$, $\zeta > 0$ and $T > 0$

$$\begin{aligned} & \exp(\zeta T) \int H^k |\alpha \partial_p u(t) - \partial_q u(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int H^k |\partial_p(\alpha \partial_p u(t) - \partial_q u(t))|^2 d\pi_s dt \\ & \leq \int H^k |\alpha \partial_p u(0) - \partial_q u(0)|^2 d\pi_s \\ & \quad + (\zeta + \varepsilon_2 + \varepsilon_1 - 2\alpha + 2k\sigma^2 + 2k\gamma + \nu_s) \int_0^T \exp(\zeta t) \int H^k |\alpha \partial_p u(t) - \partial_q u(t)|^2 d\pi_s dt \\ & \quad + 2k\sigma^2 \int_0^T \exp(\zeta t) \int H^{k-1} |\partial_p(\partial_p u(t) - \partial_q u(t))|^2 d\pi_s dt \\ & \quad \quad + \left(\frac{Q_1}{\varepsilon_1} + \frac{\alpha^2(\alpha + \gamma)^2}{\varepsilon_2} \right) \int_0^T \exp(\zeta t) \int H^k |\partial_p u(t)|^2 d\pi_s dt, \end{aligned}$$

where Q_1 is a positive polynomial function. We take $\zeta < 2\lambda$ and choose α, ε_2 and ε_1 such that $\varepsilon_2 + \varepsilon_1 - 2\alpha + 2k\sigma^2 + 2k\gamma + \zeta + \nu_s \leq 0$. Then, using the induction hypothesis on k , the polynomial growth of H and (6.12), we obtain (6.15) for k . \blacklozenge

Remark 6.10 Using the fact that $q^2 \leq CH(q, p)$ and $p^2 \leq 2H(q, p)$, (6.14) and (6.15), we have for $0 < \zeta < 2\lambda_0$, s large enough and Q a positive polynomial function that there exist real positive numbers α_s and $C_{Q,s}$ depending also of α_s , such that, for $T > 0$,

$$\int_0^T \exp(\zeta t) \int Q |\alpha \partial_p u(t) - \partial_q u(t)|^2 d\pi_s dt \leq C_{Q,s} \|\phi\|_{1,r_1}^2. \quad (6.17)$$

Using above Remark, we can show the following Lemma:

Lemma 6.11 Let Q be a positive polynomial function. Let $s > 2r_1$ large enough. For all $0 < \zeta < 2\lambda_0$, there exists a strictly positive real number $C_{Q,s}$ such that for all $T > 0$

$$\int_0^T \exp(\zeta t) \int Q |\partial_q u(t)|^2 d\pi_s dt \leq C_{Q,s} \|\phi\|_{1,r_1}^2. \quad (6.18)$$

Proof. Let $0 < \zeta < 2\lambda_0$. We have the following inequality: for any function $\psi \in C^\infty(\mathbb{R}^{2d})$ and $\alpha > 0$

$$|\partial_q \psi|^2 \leq |(\partial_q - \alpha \partial_p) \psi|^2 + \alpha^2 |\partial_p \psi|^2.$$

Then, using (6.17) and (6.12), we have (6.18). \blacklozenge

Using (6.12) and (6.18), we obtain (6.5) for $m = 1$. We will now show (6.4) for $m = 1$.

Lemma 6.12 *For $s > 2r_1$ large enough and $0 < \zeta < 2\lambda_0$, there exists a strictly positive real number C_s such that for $T > 0$,*

$$\int |\partial_p u(T)|^2 d\pi_s \leq C_s \|\phi\|_{1,r_1}^2 \exp(-\zeta T).$$

Proof. We have for $t \geq 0$

$$2\langle [\partial_{p_i}, L]u(t), \partial_{p_i} u(t) \rangle = 2\partial_{q_i} u(t) \partial_{p_i} u(t) - 2\gamma |\partial_{p_i} u(t)|^2 \leq |\partial_{q_i} u(t)|^2 + (1 - 2\gamma) |\partial_{p_i} u(t)|^2.$$

Then, using Lemma 6.6, we get for $T > 0$ and $\zeta > 0$

$$\begin{aligned} \exp(\zeta t) \int |\partial_p u(t)|^2 d\pi_s &\leq \int |\partial_p u(0)|^2 d\pi_s + (\zeta + \nu_s + 1 - 2\gamma) \int_0^t \exp(\zeta s) \int |\partial_p u(s)|^2 d\pi_s ds \\ &\quad + \int_0^t \exp(\zeta s) \int |\partial_{q_i} u(s)|^2 d\pi_s ds. \end{aligned} \quad (6.19)$$

We choose $0 < \zeta < 2\lambda_0$ and use (6.12) and (6.18) to conclude. \blacklozenge

Lemma 6.13 *For $s > 2r_1$ large enough and $0 < \zeta < 2\lambda_0$, there exists a strictly positive real number C_s such that for all $T > 0$,*

$$\int |\partial_q u(T)|^2 d\pi_s \leq C_s \|\phi\|_{1,r_1}^2 \exp(-\zeta T).$$

Proof. We have for $t \geq 0$

$$2\langle [\partial_{q_i}, L]u(t), \partial_{q_i} u(t) \rangle = 2\langle \partial_{q_i} DV, \partial_p u(t) \rangle \partial_{q_i} u(t) \leq Q |\partial_p u(t)|^2 + |\partial_{q_i} u(t)|^2,$$

where Q is a positive polynomial function such that $|\partial_{q_i} DV|^2 < Q$. Then, we use Lemma 6.6, $0 < \zeta < 2\lambda_0$, (6.12) and (6.18) to conclude. \blacklozenge

We have shown the result (6.4) for $m = 1$.

We will now show equation (6.5) by induction on m . We already proved the case $m = 1$. We suppose that (6.5) holds up to m and we want to obtain it for $m + 1$. First, we show a result on $\partial_p D^{\mathbf{k}} u(t)$ where $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$.

Lemma 6.14 *Let us assume that induction hypothesis (6.5) holds up to m . For $s > 2r_m$ large enough, $0 < \zeta < 2\lambda_0$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, there exists a strictly positive real number $C_{m,s}$ such that for all $T > 0$,*

$$\int_0^T \exp(\zeta t) \int |\partial_p D^{\mathbf{k}} u(t)|^2 d\pi_s dt \leq C_{m,s} \|\phi\|_{m,r_m}^2. \quad (6.20)$$

Proof. By induction, we can show for any function ψ

$$[D^{\mathbf{k}}, L]\psi \leq \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} P_{\mathbf{i}} |D^{\mathbf{i}}\psi|,$$

where $P_{\mathbf{i}}$ is a positive polynomial function which depends on the polynomial growth of V and its derivatives. Then, we get for $t > 0$

$$2\langle [D^{\mathbf{k}}, L]u(t), D^{\mathbf{k}}u(t) \rangle \leq \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} P_{\mathbf{i}}^2 |D^{\mathbf{i}}u(t)|^2 + C |D^{\mathbf{k}}u(t)|^2, \quad (6.21)$$

where C is a positive real number. Using Lemma 6.6, we get for $T > 0$ and $\zeta > 0$

$$\begin{aligned} & \exp(\zeta T) \int |D^{\mathbf{k}}u(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int |\partial_p(D^{\mathbf{k}}u(t))|^2 d\pi_s dt \\ & \leq \int |D^{\mathbf{k}}u(0)|^2 d\pi_s + (\zeta + \nu_s + C) \int_0^T \exp(\zeta t) \int |D^{\mathbf{k}}u(t)|^2 d\pi_s dt \\ & \quad + \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} \int_0^T \exp(\zeta t) \int P_{\mathbf{i}}^2 |D^{\mathbf{i}}u(t)| d\pi_s dt, \end{aligned}$$

We choose $0 < \zeta < 2\lambda_0$ and use induction hypothesis (6.5) to conclude. \blacklozenge

Lemma 6.15 *Let us assume that induction hypothesis (6.5) holds. For $0 < \zeta < 2\lambda_0$, $s > 2r_m$ large enough, $\ell \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, there exists a strictly positive real number $C_{m,\ell,s}$ such that*

$$\int_0^T \exp(\zeta t) \int H^\ell |\partial_p D^{\mathbf{k}}u(t)|^2 d\pi_s dt \leq C_{m,\ell,s} \|\phi\|_{m,r_m}^2, \quad (6.22)$$

for all $T > 0$.

Proof. We proceed by induction on ℓ .

We also have the result for $\ell = 0$ (see (6.20)). Suppose that the induction hypothesis (6.22) holds for $\ell - 1$. Using computations for $\ell = 0$ (6.21), (6.10), (6.11) and Lemma 6.6, we get for s large enough, $\varepsilon_1 > 0$, $\varepsilon_2 > 0$, $\zeta > 0$ and $T > 0$

$$\begin{aligned} & \exp(\zeta T) \int H^\ell |D^{\mathbf{k}}u(t)|^2 d\pi_s + \sigma^2 \int_0^T \exp(\zeta t) \int H^\ell |\partial_p D^{\mathbf{k}}u(t)|^2 d\pi_s dt \\ & \leq \int H^\ell |D^{\mathbf{k}}u(0)|^2 d\pi_s \\ & \quad + (\zeta + C + 2\ell\sigma^2 + 2\ell\gamma + \nu_s) \int_0^T \exp(\zeta t) \int H^\ell |D^{\mathbf{k}}u(t)|^2 d\pi_s dt \\ & \quad + 2\ell\sigma^2 \int_0^T \exp(\zeta t) \int H^{\ell-1} |\partial_p D^{\mathbf{k}}u(t)|^2 d\pi_s dt \\ & \quad + \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} \int_0^T \exp(\zeta t) \int H^\ell P_{\mathbf{i}}^2 |D^{\mathbf{i}}u(t)| d\pi_s dt, \end{aligned}$$

where C and $P_{\mathbf{i}}$ are defined in (6.21). We take $0 < \zeta < 2\lambda_0$. Then, using the induction hypothesis on ℓ , the polynomial growth of H and induction hypothesis on m , we obtain (6.15) for ℓ . \blacklozenge

Remark 6.16 *Using the same ideas as in Remark 6.10, we prove the following result. Let Q a positive polynomial function. For $s > 2r_m$ large enough, $0 < \zeta < 2\lambda_0$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, there exists a strictly positive real number $C_{m,Q,s}$ such that for all $T > 0$*

$$\exp(\zeta T) \int Q |D^{\mathbf{k}}u(T)|^2 d\pi_s + \int_0^T \exp(\zeta t) \int Q |\partial_p D^{\mathbf{k}}u(t)|^2 d\pi_s dt \leq C_{m,Q,s} \|\phi\|_{m,r_m}^2. \quad (6.23)$$

Lemma 6.17 *Let us assume that induction hypothesis (6.5) holds. Let $D_q^m u(t)$ denoted an arbitrary partial derivative of $u(t)$ of the type $\partial_{q_{i_1}} \dots \partial_{q_{i_m}}$. For $s > 2r_{m+1}$ large enough and $0 < \zeta < 2\lambda_0$, there exists a strictly positive real number $\tilde{\alpha}_0$ such that for all $\alpha \geq \tilde{\alpha}_0$, there exists a strictly positive real number C depending of m , s and α such that for all $T > 0$,*

$$\int_0^T \exp(\zeta t) \int |\alpha \partial_p (D_q^m u(t)) - \partial_q (D_q^m u(t))|^2 d\pi_s dt \leq C \|\phi\|_{m+1,r_{m+1}}^2. \quad (6.24)$$

Proof. Let $\alpha > 0$, $i \in \{1, \dots, d\}$ and $A_1 = \alpha \partial_p - \partial_q$. For any function $\psi \in C^\infty(\mathbb{R}^{2d})$, we have

$$[A_1 D_q^m, L]\psi = A_1 [D_q^m, L]\psi + [A_1, L](D_q^m \psi).$$

Moreover, by induction an m , we can show for any function $\psi \in C^\infty(\mathbb{R}^{2d})$

$$A_1 [D_q^m, L]\psi \leq \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} P_{\mathbf{i}} |\partial_p D^{\mathbf{i}} \psi|,$$

where $P_{\mathbf{i}}$ is a positive polynomial function which depends on the polynomial growth of V and its derivatives. Then, we get for $t > 0$

$$2\langle A_1 [D_q^m, L]u(t), A_1 D_q^m u(t) \rangle \leq \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} P_{\mathbf{i}}^2 |\partial_p D^{\mathbf{i}} u(t)|^2 + C |A_1 D_q^m u(t)|^2, \quad (6.25)$$

where C is a positive real number. Using (6.25) and (6.16), we have that there exist a positive polynomial function Q_1 , $\varepsilon_1 > 0$ and $\varepsilon_2 > 0$ such that

$$\begin{aligned} \langle [A_1 D_q^m, L]u(t), A_1 D_q^m u(t) \rangle &\leq \sum_{\mathbf{i} \in \mathbb{N}^{2d}, |\mathbf{i}| \leq m} P_{\mathbf{i}}^2 |\partial_p D^{\mathbf{i}} u(t)|^2 + (\varepsilon_1 + \varepsilon_2 - 2\alpha + C) |A_1 D_q^m u(t)|^2 \\ &\quad + \frac{Q_1}{\varepsilon_1} |\partial_p D_q^m u(t)|^2 + \frac{\alpha(\alpha - \gamma)^2}{\varepsilon_2} |\partial_{p_i} D_q^m u(t)|^2. \end{aligned}$$

To conclude, we proceed as Lemma 6.9: We choose s large enough and use Lemma 6.6. We the choose $\zeta < 2\lambda$ and α , ε_1 and ε_2 such that $\nu_s + \zeta + \varepsilon_1 + \varepsilon_2 - 2\alpha + C < 0$ and use (6.23). \blacklozenge

Lemma 6.18 *Let us assume that induction hypothesis (6.5) holds. Let Q a positive polynomial function. For $s > 2r_{m+1}$ large enough and $0 < \zeta < 2\lambda_0$, there exists a strictly positive real number $\tilde{\alpha}_s$ such that for all $\alpha \geq \tilde{\alpha}_s$, there exists a strictly positive real number $C_{m,s}$ which also depends on α and ζ such that for all $T > 0$,*

$$\int_0^T \exp(\zeta t) \int Q |\alpha \partial_p (D_q^m u(t)) - \partial_q (D_q^m u(t))|^2 d\pi_s dt \leq C_{m,s} \|\phi\|_{m+1,r_{m+1}}^2. \quad (6.26)$$

Proof. First, we prove this result by induction on k for H^k . We use same arguments and computations used to prove (6.15) and (6.22), then we have the result for Q (see Remark 6.10). \blacklozenge

Remark 6.19 Using (6.23) and (6.26), we prove that inequality (6.5) holds up to $m + 1$. Indeed, if there is a derivative in a direction p_1, \dots, p_d , then we use the result (6.23). In the other case, we use (6.26), (6.23) and $\partial_q D_q^m = -(\alpha \partial_{p_i} D_q^m - \partial_{q_i} D_q^m) + \alpha \partial_{p_i} D_q^m$, for $i \in \{1, \dots, d\}$.

We have shown that (6.5) is true for all m , then we have shown Proposition 6.3. We now prove that (6.4) is true for the derivatives of order m , where $m \in \mathbb{N}^*$.

Lemma 6.20 Let $m \in \mathbb{N}^*$ be fixed. For $s > 2r_m$ large enough, $0 < \zeta < 2\lambda_0$ and $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, there exists a strictly positive real number $C_{m,s}$ such that for all $T > 0$,

$$\int |D^{\mathbf{k}}u(T)|^2 d\pi_s \leq C_{m,s} \|\phi\|_{m,r_m}^2 \exp(-\zeta T).$$

Proof. We proceed as to prove Lemma 6.11 and Lemma 6.12 and we use Lemma 6.6, (6.21) and Proposition 6.3. \blacklozenge

We have shown the result (6.4).

6.3 Point-wise estimates of u and its derivatives

Proof of Proposition 6.1 Using (6.4) and (6.2), we get : For all $m \in \mathbb{N}$, $n \in \mathbb{N}$, $\mathbf{k} \in \mathbb{N}^{2d}$ such that $|\mathbf{k}| = m$, $\mathbf{l} \in \mathbb{N}^{2d}$ such that $|\mathbf{l}| = n$, $0 < \zeta < 2\lambda_0$ and s large enough, there exists a strictly positive real number $C_{m,n,s}$ such that for all $t > 0$

$$\int \left| D^{\mathbf{l}}(D^{\mathbf{k}}u(t, q, p)\pi_s(q, p)) \right|^2 dqdp \leq C_{m,n,s} \|\phi\|_{m+n, r_{m+n}}^2 \exp(-\zeta t).$$

Then, using Sobolev embedding theorem [8], we get, for $n = d + 1$

$$|D^{\mathbf{k}}u(t, q, p)|^2 \pi_s^2(q, p) \leq C_{m,d+1,s} \|\phi\|_{m+d+1, r_{m+d+1}}^2 \exp(-\zeta t),$$

for all $t > 0$ and $(q, p) \in \mathbb{R}^{2d}$. The conclusion follows. \blacklozenge

6.4 Proof of the Lemma 2.16

The two following results are consequences of Proposition 6.1:

Corollary 6.21 Let $g \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int_{\mathbb{R}^{2d}} g(q, p)\rho(q, p)dqdp = 0$, then there exists a unique function $h \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that

$$Lh = g \quad \text{and} \quad \int_{\mathbb{R}^{2d}} h(q, p)\rho(q, p)dqdp = 0.$$

Proof. It is know that the unique solution h of $Lh = g$ which verifies

$$\int_{\mathbb{R}^{2d}} h(q, p)\rho(q, p)dqdp = 0$$

is defined by

$$h(q, p) = \int_0^{+\infty} \mathbb{E}(g(q_q(t), p_p(t)))dt.$$

Then the regularity of h is a consequence of Proposition 6.1.

Remark 6.22 L and its formal adjoint in $L^2(\rho)$ have the same behavior. Indeed, we have for any function $\phi \in C^\infty(\mathbb{R}^{2d})$ and $(q, p) \in \mathbb{R}^{2d}$

$$\begin{aligned} L^*(q, p; \partial_p, \partial_q)\phi(q, p) &= -\langle p, \partial_q \phi(q, p) \rangle + \langle \partial_q V, \partial_p \phi(q, p) \rangle - \gamma \langle p, \partial_p \phi(q, p) \rangle \\ &\quad + \frac{\sigma^2}{2} \sum_{i=1}^d \frac{\partial^2}{\partial p_i \partial p_i} \phi(q, p) \\ &= L(q, -p; \partial_p, \partial_q)\phi(q, -p). \end{aligned}$$

Then we have the Lemma 2.16:

Let $g \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that $\int_{\mathbb{R}^{2d}} g(q, p)\rho(q, p)dqdp = 0$. Then there exists a unique function $h \in \mathcal{C}_{pol}^\infty(\mathbb{R}^{2d})$ such that

$$L^*h = g \quad \text{and} \quad \int_{\mathbb{R}^{2d}} h(q, p)\rho(q, p)dqdp = 0,$$

where L^* is the adjoint of L with respect to the $L^2(\rho)$ product.

Chapter 4

Approximation of the invariant law of SPDE_s: error analysis using a Poisson equation for a full-discretization scheme

1 Introduction

In this chapter, we want to analyze in a quantitative way the effect of time and space discretization schemes on the knowledge of the unique invariant law of a semi-linear Stochastic PDE of parabolic type, written in the abstract form of [16]

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t), \quad 0 < t \leq T, \\ X(0, x) &= x. \end{aligned} \tag{1.1}$$

This process takes value in an infinite-dimensional Hilbert space H - typically $H = L^2(0, 1)$; A is a negative, self-adjoint, unbounded linear operator on H , with a compact inverse - for instance, $A = \frac{\partial^2}{\partial \xi^2}$, given on the domain $H^2(0, 1) \cap H_0^1(0, 1)$ when homogeneous Dirichlet boundary conditions are applied. The coefficient F is an operator on H , on which regularity conditions are assumed and given below.

Finally, $(W(t))_{t \in [0, T]}$ is a cylindrical Wiener process on H , so that we have a space-time white noise in (1.1).

More precise assumptions are given below. In a more general setting, one could for instance intend to remove boundedness of F , or include spatially correlated noise processes. However, we already consider the main technical and conceptual difficulties in this paper.

In our setting, it is known that the SPDE (1.1) admits a unique invariant probability measure μ , and that convergence is exponentially fast. This result comes from the spatial non-degeneracy of the noise and from a dissipation relation satisfied by the drift part. Nevertheless, in general, no expression of μ is available for practical use; moreover, the support of this measure is an infinite-dimensional space.

The approximation of quantities like $\int_H \phi d\mu$ for bounded test functions ϕ is therefore complicated. The exponential convergence ensures that $\mathbb{E}\phi(X(t))$ tends to $\int_H \phi d\mu$ when t tends to infinity, exponentially fast. However, using a Monte-Carlo method to compute $\mathbb{E}\phi(X(t))$ would require the ability to simulate the H -valued random variable $X(t)$, for a large value of t . Since it is not possible to have an exact simulation, we introduce two approximations:

- a discretization in time, in order to get an approximation of the law of the random variables $X(t)$ for different, fixed values of t , using a finite number of calculations; this is done here with a semi-implicit Euler scheme;
- a discretization in space, in order to replace the H -valued random variables with finite-dimensional ones. Here, this is performed with a finite element method.

The second approximation is specific to the case of SPDEs, while the first one has already been studied a lot in the case of SDEs.

Different techniques to control the error are available in the litterature. A first one is found in [82], where an estimate of the weak error introduced by the numerical scheme is proved, holding for any value of the finite time T . The idea there is to expand the error thanks to the solution of the Kolmogorov equation associated with the diffusion, and to prove bounds on the spatial derivatives of this solution, with an exponential decrease with respect to the time variable.

This strategy has been generalized to SPDEs like (1.1) in [5], when a semi-implicit Euler scheme is used. The main additional difficulty, when compared with the SDE case, is the need for tools introduced in [20], for the estimate of the weak error at a fixed time T .

Using these tools aims at proving that on a finite time interval the weak order of convergence is twice the strong one: in other words, laws at fixed times are approximated more accurately than the trajectories. These tools have also been used in [87] to treat the time-discretization in a slightly more-general setting, and in [3] where discretization in space with a finite element method is studied. Basically, the two ingredients are the following:

- improved estimates on the derivatives of the solution of the Kolmogorov equations, with spatial regularization;
- an integration by parts formula issued from Malliavin calculus, in order to transform some stochastic expressions with insufficient spatial regularity into more suitable ones.

These tools are fundamental to treat equations with nonlinear terms; they are used again in the present work. Notice that for linear equations a specific idea simplifies the proof - so that the second tool is not used - but cannot be adapted to nonlinear parabolic equations like (1.1): see [25], and [19] where a stochastic Schrödinger equation is discretized.

Here, we are interested in another method for the approximation of the invariant measure: we want to follow the approach of [64]. There, the authors study the distance between time-averages along the realization of the numerical scheme of a test function ϕ , and its expected value with respect to the invariant law μ . They introduce the solution Ψ of the Poisson equation $\mathcal{L}\Psi = \phi - \int \phi d\mu$, where \mathcal{L} is the infinitesimal generator of the SDE - the solvability of this elliptic or hypoelliptic PDE is ensured by ergodic properties. Then they show how to expand the error for various numerical methods, in a stochastic Taylor expansion fashion.

The use of a Poisson equation to prove convergence results of Law of Large Numbers type is classical, as explained in [64]. In the context of SPDEs, it has been used in [4] and [11] for the study of the averaging principle for systems evolving with two separate time-scales.

Such a technique gives an approximation result for μ , even if the numerical method is not ergodic, having possibly several invariant laws. In the SDE case, the study of ergodicity for time-discretized processes has been the subject of [43]; there the author use general results on Markov chains, like the Harris Theorem. Up to our knowledge, no such study has been completed for SPDEs so far.

Our main result is the adaptation of the approach of [64] for SPDEs, with time and space approximation procedures: we essentially obtain the following result - a more precise statement is Theorem 5.1: There exists a constant $C > 0$ such that for any $\mathcal{C}_b^2(H)$ function ϕ , any parameters $\tau \in (0, 1)$ and $h \in (0, 1)$, any time $N \geq 1$ and any initial condition

$x \in H$

$$\left| \frac{1}{N} \sum_{m=0}^{N-1} \left(\mathbb{E} \phi(X_m^h) - \int_H \phi(z) \mu(dz) \right) \right| \leq C \left(\tau^{1/2} + h + \frac{1}{N\tau} \right).$$

The error is divided into three parts: the first (resp. the second) is due to the time (resp. space) discretization, while the last one goes to 0 when time increases.

For the proof of this result, we need to study the Poisson equation associated with the SPDE (1.1). More precisely, we work with Galerkin approximations, and show bounds that are independent of dimension. Moreover, the strategy described above for the study of weak approximation for infinite dimensional processes require some additional regularization properties for the solution of the Kolmogorov equation. Here, we need similar properties for the solutions of Poisson equations. When compared with [3], [5] or [20], many error terms look the same: the method with Poisson equation does not really simplify the proof, it just moves some technical problems to other places along the proof. The main reason for studying only the additive noise case is the following. As soon as the equation is discretized either in time - [20] - or in space - [3] - the possible diffusion coefficients must satisfy very strict conditions: they should be decomposed as the sum of a continuous affine function, and another function such that the second order derivative is controlled with respect to a very weak norm - namely, the norm associated with a negative power of the linear operator. Moreover, the treatment of such noise requires lengthier computations. We could do so here by adding our argument with the ones in [3] and [20] but this would result only in hiding the main ideas of our work.

The paper is organized as follows: in Section 2, we make the assumptions on the coefficients of the equation, and we define the discretization method in Section 3. In Section 4, we study the asymptotic behavior of the solutions of the continuous and discrete time processes. In Section 5, we give the convergence results that we obtained. In Section 6 we show how the error is decomposed, and we present two essential tools: the Poisson equation, and an integration by parts from Malliavin calculus. Finally detailed proofs of the estimates are developed in Section 7.

2 Notations and assumptions

Let $\mathcal{D} \subset \mathbb{R}$ be a bounded, open interval; without restriction in the sequel we assume $\mathcal{D} = (0, 1)$. Let $H = L^2(\mathcal{D})$, with norm and inner product denoted by $|\cdot|_H$ and $\langle \cdot, \cdot \rangle_H$ or simply $|\cdot|$ and $\langle \cdot, \cdot \rangle$.

We consider equations in the abstract form

$$\begin{aligned} dX(t, x) &= (AX(t, x) + F(X(t, x)))dt + dW(t) \\ X(0, x) &= x. \end{aligned} \tag{2.1}$$

In the next paragraphs, we state the assumptions made on the coefficients A and F in (1.1). We also recall basic facts on the cylindrical Wiener process W , and on the mild solution of the SPDE.

2.1 Test functions

To quantify the weak approximation, we use test functions - called *admissible* - ϕ in the space $\mathcal{C}_b^2(H, \mathbb{R})$ of functions from H to \mathbb{R} that are twice continuously differentiable, bounded, with first and second order bounded derivatives.

Remark 2.1 *In the sequel, we often identify the first derivative $D\phi(x) \in \mathcal{L}(H, \mathbb{R})$ with the gradient in the Hilbert space H , and the second derivative $D^2\phi(x)$ with a linear operator on H , via the formulae:*

$$\begin{aligned} \langle D\phi(x), h \rangle &= D\phi(x).h \text{ for every } h \in H \\ \langle D^2\phi(x).h, k \rangle &= D^2\phi(x).(h, k) \text{ for every } h, k \in H. \end{aligned}$$

We then use the following notation, for an admissible test function ϕ :

$$\begin{aligned} \|\phi\|_0 &= \sup_{x \in H} |\phi(x)|_H \\ \|\phi\|_1 &= \sup_{x \in H} |D\phi(x)|_H, \\ \|\phi\|_2 &= \sup_{x \in H} |D^2\phi(x)|_{\mathcal{L}(H)}. \end{aligned}$$

2.2 Assumptions on the coefficients

2.2.1 The linear operator

We denote by $\mathbb{N} = \{0, 1, 2, \dots\}$ the set of nonnegative integers.

We suppose that the following properties are satisfied:

Assumptions 2.2 1. *The operator A is self-adjoint.*

2. *We assume that there exist a complete orthonormal system of elements of H denoted by $(e_k)_{k \in \mathbb{N}}$, and a non-decreasing sequence of real positive numbers $(\lambda_k)_{k \in \mathbb{N}}$ such that:*

$$Ae_k = -\lambda_k e_k \text{ for all } k \in \mathbb{N}.$$

3. *The sequence $(\lambda_k)_{k \in \mathbb{N}}$ goes to $+\infty$ and*

$$\sum_{k=0}^{+\infty} \frac{1}{\lambda_k^\alpha} < +\infty \Leftrightarrow \alpha > 1/2.$$

The smallest eigenvalue of $-A$ is then λ_0 .

Example 2.3 *We can choose $A = \frac{d^2}{dx^2}$, with the domain $H^2(0, 1) \cap H_0^1(0, 1) \subset L^2(0, 1)$ - corresponding to homogeneous Dirichlet boundary conditions. In this case for any $k \in \mathbb{N}$ $\lambda_k = \pi^2(k+1)^2$, and $e_k(\xi) = \sqrt{2} \sin((k+1)\pi\xi)$ - see [8].*

In the following Definition, we introduce finite dimensional subspaces of H and associated orthogonal projections; both are based on the spectral decomposition of A .

Definition 2.4 *For any $M \in \mathbb{N}$, we define H_M the subspace of H generated by e_0, \dots, e_M ,*

$$H_M = \text{Span}\{e_k; 0 \leq k \leq M\}$$

and $P_M \in \mathcal{L}(H)$ the orthogonal projection onto H_M : for any $x = \sum_{k=0}^{+\infty} x_k e_k \in H$,

$$P_M x = \sum_{k=0}^M x_k e_k.$$

The domain $D(A)$ of A is equal to

$$D(A) = \left\{ x = \sum_{k=0}^{+\infty} x_k e_k \in H, \sum_{k=0}^{+\infty} (\lambda_k)^2 |x_k|^2 < +\infty \right\}.$$

More generally, fractional powers of $-A$, are defined for $\alpha \in [0, 1]$:

$$(-A)^\alpha x = \sum_{k=0}^{\infty} \lambda_k^\alpha x_k e_k \in H,$$

with the domains

$$D((-A)^\alpha) = \left\{ x = \sum_{k=0}^{+\infty} x_k e_k \in H, |x|_\alpha^2 := \sum_{k=0}^{+\infty} (\lambda_k)^{2\alpha} |x_k|^2 < +\infty \right\}.$$

Example 2.5 *In the case when A is the Laplace operator with homogeneous Dirichlet boundary conditions on $H = L^2(\mathcal{D})$,*

$$D((-A)^{1/2}) = H_0^1(\mathcal{D}) \quad D(A) = H_0^1(\mathcal{D}) \cap H^2(\mathcal{D}).$$

When $\alpha \in [0, 1]$, it is also possible to define spaces $D((-A)^{-\alpha})$ and operators $(-A)^{-\alpha}$, with norm denoted by $|\cdot|_{-\alpha}$; in particular when $x = \sum_{k=0}^{+\infty} x_k e_k \in H$, we have $(-A)^{-\alpha} x = \sum_{k=0}^{+\infty} \lambda_k^{-\alpha} x_k e_k$ and $|x|_{-\alpha}^2 := \sum_{k=0}^{+\infty} (\lambda_k)^{-2\alpha} |x_k|^2$.

The semi-group $(e^{tA})_{t \geq 0}$ can be defined by the Hille-Yosida Theorem - see [8]. We use the following spectral formula: if $x = \sum_{k=0}^{+\infty} x_k e_k \in H$, then for any $t \geq 0$

$$e^{tA} x = \sum_{k=0}^{+\infty} e^{-\lambda_k t} x_k e_k. \quad (2.2)$$

For any $t \geq 0$, e^{tA} is a continuous linear operator in H , with operator norm $e^{-\lambda_0 t}$. The semi-group (e^{tA}) is used to define the solution $Z(t) = e^{tA} z$ of the linear Cauchy problem

$$\frac{dZ(t)}{dt} = AZ(t) \quad \text{with} \quad Z(0) = z.$$

To define solutions of more general PDEs of parabolic type, we use a mild formulation together with the Duhamel principle.

This semi-group enjoys some smoothing properties that we often use in this work. Here we recall a few important ones, which are easily obtained from the spectral formula (2.2):

Proposition 2.6 *Under Assumption 2.2, for any $\sigma \in [0, 1]$, there exists $C_\sigma > 0$ such that:*

1. for any $t > 0$ and $x \in H$,

$$|e^{tA} x|_\sigma \leq C_\sigma t^{-\sigma} e^{-\frac{\lambda_0}{2} t} |x|_H.$$

2. for any $0 < s < t$ and $x \in H$,

$$|e^{tA} x - e^{sA} x|_H \leq C_\sigma \frac{(t-s)^\sigma}{s^\sigma} e^{-\frac{\lambda_0}{2} s} |x|_H.$$

3. for any $0 < s < t$ and $x \in D(-A)^\sigma$,

$$|e^{tA} x - e^{sA} x|_H \leq C_\sigma (t-s)^\sigma e^{-\frac{\lambda_0}{2} s} |x|_\sigma.$$

2.2.2 The nonlinear operator

The nonlinear operator F is assumed to satisfy some general assumptions, like in [5]. In Example 2.10, we give the two main kind of operators that can be used in our framework.

Assumptions 2.7 *The function $F : H \rightarrow H$ is assumed to be bounded and Lipschitz continuous. We denote by L_F the Lipschitz constant of F .*

We also define for each $M \geq 0$ a function $F_M : H_M \rightarrow H_M$, with $F_M(x) = P_M F(x)$ for any $x \in H_M$. We assume that each F_M is twice differentiable, and that we have the following bounds on the derivatives, uniformly with respect to M :

- *There exists a constant C_1 such that for any $M \geq 0$, $x \in H_M$ and $h \in H_M$*

$$|DF_M(x).h|_H \leq C_1|h|_H.$$

- *There exist $\eta \in [0, 1[$ and a constant C_2 such that for any $M \geq 0$, $x \in H_M$ and any $h, k \in H_M$ we have*

$$|(-A)^{-\eta} D^2 F_M(x).(h, k)| \leq C_2|h|_H|k|_H.$$

- *Moreover, there exists a constant C_3 such that for any $M \geq 0$, $x \in H_M$ and any $h, k \in H_M$*

$$|D^2 F_M(x).(h, k)| \leq C_3|h|_{(-A)^\eta}|k|_H.$$

Remark 2.8 *Multiplicative noise with appropriate assumptions like in [3] can be considered; however proofs of the required estimates become much more technical.*

Since F is bounded, the following property is easily seen to be satisfied:

Proposition 2.9 (Dissipativity) *There exist $c > 0$ and $C > 0$ such that for any $x \in D(A)$*

$$\langle Ax + F(x), x \rangle \leq -c|x|^2 + C. \quad (2.3)$$

We remark that we have uniform control with respect to the dimension M of the bounds on $F_M := P_M \circ F$ and on its derivatives, and that (2.3) is also satisfied for F_M , with constants c and C independent from M .

Example 2.10 *We give some fundamental examples of nonlinearities for which the previous assumptions are satisfied:*

- *A function $F : H \rightarrow H$ of class C^2 , bounded and with bounded derivatives, fits in the framework, with the choice $\eta = 0$.*
- *The function F can be a **Nemytskii** operator: let $g : (0, 1) \times \mathbb{R} \rightarrow \mathbb{R}$ be a measurable, bounded, function such that for almost every $\xi \in (0, 1)$ $g(\xi, \cdot)$ is twice continuously differentiable, with uniformly bounded derivatives. Then $F(x)$ is defined for every $x \in H = L^2(0, 1)$ by*

$$F(x)(\xi) = g(\xi, x(\xi)).$$

In general, such functions are not Fréchet differentiable, but only Gâteaux differentiable, with the following expressions:

$$\begin{aligned} [DF(x).h](\xi) &= \frac{\partial g}{\partial x}(\xi, x(\xi))h(\xi) \\ [D^2F(x).(h, k)](\xi) &= \frac{\partial^2 g}{\partial x^2}(\xi, x(\xi))h(\xi)k(\xi). \end{aligned}$$

If h and k are only L^2 functions, $D^2F(x).(h, k)$ may only be L^1 ; however if h or k is L^∞ , it is L^2 . The conditions in Assumption 2.7 are then satisfied as soon as there exists $\eta < 1$ such that $D(-A)^\eta$ is continuously embedded into $L^\infty(0, 1)$ - it is the case for A given in Example 2.3, with $\eta > 1/4$. Then the finite dimensional spaces H_N are subspaces of L^∞ , and differentiability can be shown.

2.3 The cylindrical Wiener process and stochastic integration in H

In this section, we recall the definition of the cylindrical Wiener process and of stochastic integral on a separable Hilbert space H with norm $|\cdot|_H$. For more details, see [16].

We first fix a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$. A cylindrical Wiener process on H is defined with two elements:

- a complete orthonormal system of H , denoted by $(q_i)_{i \in I}$, where I is a subset of \mathbb{N} ;
- a family $(\beta_i)_{i \in I}$ of independent real Wiener processes with respect to the filtration $((\mathcal{F}_t)_{t \geq 0})$;

then W is defined by

$$W(t) = \sum_{i \in I} \beta_i(t) q_i. \quad (2.4)$$

When I is a finite set, we recover the usual definition of Wiener processes in the finite dimensional space $\mathbb{R}^{|I|}$. However the subject here is the study of some Stochastic Partial Differential Equations, so that in the sequel the underlying Hilbert space H is infinite dimensional; for instance when $H = L^2(0, 1)$, an example of complete orthonormal system is $(q_k)_{k \geq 1} = (\sqrt{2} \sin(k\pi \cdot))_{k \geq 1}$ - see Example 2.3.

A fundamental remark is that the series in (2.4) does not converge in H ; but if a linear operator $\Psi : H \rightarrow K$ is Hilbert-Schmidt, then $\Psi W(t)$ converges in $L^2(\Omega, H)$ for any $t \geq 0$.

Moreover, the resulting process does not depend on the choice of the complete orthonormal system $(q_i)_{i \in I}$.

We recall that a bounded linear operator $\Psi : H \rightarrow K$ is said to be Hilbert-Schmidt when

$$|\Psi|_{\mathcal{L}_2(H, K)}^2 := \sum_{k=0}^{+\infty} |\Psi(q_k)|_K^2 < +\infty,$$

where the definition is independent of the choice of the orthonormal basis (q_k) of H . The space of Hilbert-Schmidt operators from H to K is denoted $\mathcal{L}_2(H, K)$; endowed with the norm $|\cdot|_{\mathcal{L}_2(H, K)}$ it is an Hilbert space.

The stochastic integral $\int_0^t \Psi(s) dW(s)$ is defined in K for predictable processes Ψ with values in $\mathcal{L}_2(H, K)$ such that $\int_0^t |\Psi(s)|_{\mathcal{L}_2(H, K)}^2 ds < +\infty$ a.s; moreover when $\Psi \in L^2(\Omega \times [0, t]; \mathcal{L}_2(H, K))$, the following two properties hold:

$$\begin{aligned} \mathbb{E} \left| \int_0^t \Psi(s) dW(s) \right|_K^2 &= \mathbb{E} \int_0^t |\Psi(s)|_{\mathcal{L}_2(H, K)}^2 ds \quad (\text{It\^o isometry}), \\ \mathbb{E} \int_0^t \Psi(s) dW(s) &= 0. \end{aligned}$$

A generalization of It\^o formula also holds - see [16].

For instance, if $v = \sum_{k \in \mathbb{N}} v_k q_k \in H$, we can define

$$\langle W(t), v \rangle = \int_0^t \langle v, dW(s) \rangle = \sum_{k \in \mathbb{N}} \beta_k(t) v_k;$$

we then have the following space-time white noise property

$$\mathbb{E}\langle W(t), v_1 \rangle \langle W(s), v_2 \rangle = t \wedge s \langle v_1, v_2 \rangle.$$

Therefore to be able to integrate a process with respect to W requires some strong properties on the integrand; in our SPDE setting, the Hilbert-Schmidt properties follow from the assumptions made on the linear coefficients of the equations.

Thanks to Assumption 2.2, it is easy to show that the following stochastic integral is well-defined in H , for any $t \geq 0$:

$$W^A(t) = \int_0^t e^{(t-s)A} dW(s). \quad (2.5)$$

It is called a stochastic convolution, and it is the unique mild solution of

$$dZ(t) = AZ(t)dt + dW(t) \quad \text{with} \quad Z(0) = 0.$$

Under the second condition of Assumption 2.2, there exists $\delta > 0$ such that for any $t > 0$ we have $\int_0^t \frac{1}{s^\delta} |e^{sA}|_{\mathcal{L}_2(H)}^2 ds < +\infty$; it can then be proved that W^A has continuous trajectories - via the *factorization method*, see [16] - and that for any $1 \leq p < +\infty$

$$\mathbb{E} \sup_{t \geq 0} |W^A(t)|_H^p < +\infty. \quad (2.6)$$

We can now define solutions to equation (1.1), thanks to the assumptions made on the coefficients: the following result is classical - see [16]:

Proposition 2.11 *For every $T > 0$, $x \in H$, the equation (1.1) admits a unique mild solution $X \in L^2(\Omega, \mathcal{C}([0, T], H))$:*

$$X(t) = e^{tA}x + \int_0^t e^{(t-s)A} F(X(s)) ds + \int_0^t e^{(t-s)A} dW(s). \quad (2.7)$$

3 Definition of the discretization schemes

We will consider approximations in time and in space of the process X . In this Section, we introduce the corresponding schemes: a finite element approximation for discretization in space, and a semi-implicit Euler scheme for discretization in time. We also discuss the discretization in space using the spectral decomposition of the operator A .

3.1 Discretization in space : finite element approximation

We use the same framework as in [3] and [25]. For precise general references on Finite Element Methods, see for instance [12] and [28].

Let $(V_h)_{h \in (0,1)}$ be a family of spaces of continuous piecewise linear functions corresponding to a (quasiuniform) family of meshes (possibly not uniformly distributed) in $\mathcal{D} = (0, 1)$ such that $V_h \subset H_0^1(\mathcal{D}) = D((-A)^{1/2})$ - in other words, 0 and 1 should be included as nodes in the partition of $[0, 1]$. The parameter h denotes the mesh size, which is the length of the largest subinterval in the partition.

Let $P_h : H \rightarrow V_h$ denote the orthogonal projection onto the finite dimensional space V_h . According to the context, we also consider P_h as a linear operator in $\mathcal{L}(H)$, since $V_h \in H$.

We finally define the approximation of the operator A : it is a linear operator $A_h \in \mathcal{L}(V_h)$.

Definition 3.1 *The linear operator $A_h : V_h \rightarrow V_h$ is defined such that the following variational equality holds: for any $x_h \in V_h$ and $y_h \in V_h$*

$$\langle A_h x_h, y_h \rangle = \langle A x_h, y_h \rangle$$

We recall a few important properties of the operator V_h :

Proposition 3.2 *For any $h \in (0, 1)$, A_h is symmetric, such that $-A_h$ is positive definite.*

If N_h is the dimension of V_h , we denote by $(e_i^h)_{i=0}^{N_h-1} \subset V_h$ an orthonormal eigenbasis corresponding to $-A_h$ with eigenvalues $0 < \lambda_0^h \leq \lambda_1^h \leq \dots \leq \lambda_{N_h-1}^h$.

Then for any $h \in (0, 1)$, we have $\lambda_0^h \geq \lambda_0$.

Indeed, we have

$$\lambda_0 = \inf_{v, u \in H} \langle -Au, v \rangle \leq \inf_{u, v \in V_h} \langle -Au, v \rangle = \inf_{u, v \in V_h} \langle -A_h u, v \rangle = \lambda_0^h.$$

For any $h \in (0, 1)$, A_h generates a semi-group on V_h , which is denoted $(e^{tA_h})_{t \in \mathbb{R}^+}$. It is also not difficult to define fractional powers $(-A_h)^\alpha$ of $-A_h$, for any $\alpha \in [-1, 1]$: for any $x^h = \sum_{i=0}^{N_h-1} x_i^h e_i^h \in V_h$, we have

$$e^{tA_h} x^h = \sum_{i=0}^{N_h-1} e^{-\lambda_i^h t} x_i^h e_i^h; (-A_h)^\alpha x^h = \sum_{i=0}^{N_h-1} (\lambda_i^h)^\alpha x_i^h e_i^h.$$

The regularization estimates of Proposition 2.6 are then easily generalized to these semi-groups; moreover bounds are uniform with respect to the mesh size $h \in (0, 1)$.

We focus now on the approximations of PDEs - seen as equations in the Hilbert space H - with equations in finite dimensional spaces V_h .

We consider the spatially semidiscrete approximation of (1.1): $(X^h(t))_{t \in \mathbb{R}^+}$, is a process taking values in V_h , such that

$$dX^h(t) = A_h X^h(t) dt + F^h(X^h(t)) dt + P_h dW(t), \quad X^h(0) = P_h x = P_h X_0, \quad (3.1)$$

where the non-linear coefficient $F^h : V_h \rightarrow V_h$ satisfies $F^h(x) = P_h(F(x))$ for any $x \in V_h$.

We remark that the regularity properties of Assumption 2.7 and the dissipativity inequality (2.3) are satisfied if we replace A (resp. F) with A_h (resp. F^h).

This equation admits a unique mild solution, such that for any $0 \leq t \leq T$

$$X^h(t) = e^{tA_h} P_h x + \int_0^t e^{(t-s)A_h} F^h(X^h(s)) ds + \int_0^t e^{(t-s)A_h} P_h dW(s). \quad (3.2)$$

Notice that the stochastic integral is always well-defined, since for any $h \in (0, 1)$ the linear operator P_h has finite rank; on V_h , the noise process $P_h W$ is a standard N_h -dimensional Wiener process - as is easily seen by expanding W in a complete orthonormal system $(q_i)_{i \in \mathbb{N}}$ with $q_i = e_i^h$ for $0 \leq i \leq N_h - 1$.

To be able to state a convergence result of X^h to X , and to give an order of convergence, we now recall some important results - see [3] for more details:

Proposition 3.3 *(i) We have an equivalence of norms: there exist two constants $c, C \in (0, +\infty)$, such that for any $h \in (0, 1)$, any $\alpha \in [-1/2, 1/2]$ and any $x^h \in V_h$,*

$$c|(-A_h)^\alpha x^h| \leq |(-A)^\alpha x^h| \leq C|(-A_h)^\alpha x^h|. \quad (3.3)$$

Moreover, we have for any $h \in (0, 1)$, $\alpha \in [-1/2, 1/2]$, and $x \in H$,

$$|(-A_h)^\alpha P_h x| \leq C|(-A)^\alpha x|. \quad (3.4)$$

(ii) Let us denote by R_h the so-called Ritz projector, defined as the orthogonal projection onto V_h in $D((-A)^{1/2})$. We have the identity $R_h = (-A_h)^{-1}P_h(-A)$ on $D(A)$, and

$$|(-A)^{s/2}(I - R_h)(-A)^{-r/2}|_{\mathcal{L}(H)} \leq C_{r,s}h^{r-s} \quad \forall 0 \leq s \leq 1 \leq r \leq 2 \quad (3.5)$$

(iii) For P_h , we have the following error estimate:

$$|(-A)^{s/2}(I - P_h)(-A)^{-r/2}|_{\mathcal{L}(H)} \leq C_{r,s}h^{r-s} \quad \forall 0 \leq s \leq 1 \text{ and } 0 \leq s \leq r \leq 2. \quad (3.6)$$

As a consequence, we get the following important result:

Proposition 3.4 For any $\kappa > 0$, the linear operator on H $P_h(-A_h)^{-1/2-\kappa}P_h$ is continuous, self-adjoint and semi-definite positive. Moreover,

$$\sup_{0 < h < 1} \text{Tr}(P_h(-A_h)^{-1/2-\kappa}P_h) < +\infty.$$

The symmetry and the positivity are very important properties for our purpose: indeed, they allow to use inequalities like

$$|\text{Tr}(MN)| \leq |M|_{\mathcal{L}(H)}\text{Tr}(N),$$

for $M, N \in \mathcal{L}(H)$ such that L is symmetric and semi-definite positive.

Proof The operator is well-defined on H , and self-adjointness is clear, since $(-A_h)^{-1/2-\kappa} \in \mathcal{L}(V_h)$ is symmetric.

Now from point (i) of Proposition 3.3, the following linear operators are defined and continuous on H : $(-A)^\kappa(-A_h)^{-\kappa}P_h$, and $(-A)^{1/2}P_h(-A_h)^{-1/2}P_h$; their norms are uniformly bounded with respect to h .

By duality, the operator $P_h(-A_h)^{-1/2}P_h(-A)^{1/2}$ is well-defined on H - by unique continuous extension from the dense subspace $D((-A)^{1/2})$ - and it has the same norm as $(-A)^{1/2}P_h(-A_h)^{-1/2}P_h$.

Finally, we write that for any $0 < h < 1$

$$\begin{aligned} & \text{Tr}(P_h(-A_h)^{-1/2-\kappa}P_h) \\ &= \text{Tr}((P_h(-A_h)^{-1/2}P_h(-A)^{1/2})(-A)^{-1/2-\kappa}((-A)^\kappa(-A_h)^{-\kappa}P_h)) \\ &\leq |P_h(-A_h)^{-1/2}P_h(-A)^{1/2}|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa})|(-A)^\kappa(-A_h)^{-\kappa}P_h|_{\mathcal{L}(H)} \\ &\leq C\text{Tr}((-A)^{-1/2-\kappa}). \end{aligned}$$

◆

We now recall a few convergence results for the approximation in space, valid on time-intervals of finite length $[0, T]$:

- the strong order of convergence is $1/2$ - see for instance [56], [88]:
 $\forall 0 < r < 1/2, \exists C_{T,r} \in (0, +\infty), \forall h \in (0, 1), \text{ we have } \mathbb{E}|X^h(T) - X(T)| \leq C_{T,r}h^{1/2-r};$
- the weak order of convergence is 1 - see [3]: for any admissible test function ϕ ,
 $\forall 0 < r < 1, \exists C_{T,r} \in (0, +\infty), \forall h \in (0, 1), \text{ we have } |\mathbb{E}\phi(X^h(T)) - \mathbb{E}\phi(X(T))| \leq C_{T,r}h^{1-r}.$

To conclude this part, we introduce a notation which is useful to give some of the results in a compact way.

Definition 3.5 For $h = 0$, we set $X^0 = X$, as well as $V_0 = H$, $A_0 = A$, $P_0 = Id_H$.

3.2 Another discretization in space: spectral Galerkin projection

A tool in our proof will be an additional finite dimensional projection onto the subspaces H_M . This approximation allows to justify rigorously the required computations; even if the process X^h takes values in a finite dimensional subspace of H , it is easier to prove some estimates with a process taking values in finite dimensional subspaces which are left invariant by the action of A and of the noise. We define here the corresponding approximating processes, and give a few important convergence properties.

Let $M \in \mathbb{N}$. According to Definition 2.4, we can consider an approximate equation in the finite-dimensional subspace H_M :

$$dX^{(M)}(t) = AX^{(M)}(t)dt + F_M(X^{(M)}(t))dt + P_M dW(t), \quad X^{(M)}(0) = P_M x, \quad (3.7)$$

where $F_M = P_M \circ F$ - see also Assumption 2.7. The process $W^{(M)} := P_M W$ takes values in H_M , it is a standard Wiener process.

For any final time $T \in (0, +\infty)$, it admits a unique mild solution, taking values in $H_M \subset H$ - we recall that H_M is stable by A :

$$X^{(M)}(t) = e^{tA} P_M x + \int_0^t e^{(t-s)A} F_M(X^{(M)}(s)) ds + \int_0^t e^{(t-s)A} P_M dW(s).$$

To study the convergence of $X^{(M)}$ to X , the following inequality is useful:

$$|(I - P_M)A^{-r}|_{\mathcal{L}(H)} \leq C_r \lambda_{M+1}^{-r}, \quad 0 \leq r \leq 1. \quad (3.8)$$

We then have the following convergence results, for any $T \in (0, +\infty)$, in the stochastic case:

- the strong order of convergence is $1/4$:
 $\forall 0 < r < 1/2, \exists C_{T,r} \in (0, +\infty), \forall M \in \mathbb{N}$, we have $\mathbb{E}|X^{(M)}(T) - X(T)| \leq \frac{C_{T,r}}{\lambda_{M+1}^{1/4-r}}$;
- the weak order of convergence is $1/2$: for any admissible test function ϕ ,
 $\forall 0 < r < 1, \exists C_{T,r} \in (0, +\infty), \forall M \in \mathbb{N}$, we have $|\mathbb{E}\phi(X^{(M)}(T)) - \mathbb{E}\phi(X(T))| \leq \frac{C_{T,r}}{\lambda_{M+1}^{1/2-r}}$.

Those estimates can be proved with direct computations and the appropriate techniques from [3] and [20]. Another possibility is to check that the projectors P_M satisfy the estimates of Proposition 3.3 with $h = \lambda_{N+1}^{-1/2}$, see Example 3.4 in [56]. Once again, we define a value for $M = \infty$:

Definition 3.6 For $M = \infty$, we set $X^{(\infty)} = X$, as well as $H_\infty = H$ and $P_\infty = Id_H$.

3.3 Discretization in time

For each fixed mesh size $h \in (0, 1)$, and for $h = 0$, we now define a time approximation of the process X_h : denoting by $\tau > 0$ a time step, we use a semi-implicit Euler scheme to define, for $k \in \mathbb{N}$,

$$\begin{aligned} X_{k+1}^h(\tau, x) &= X_k^h(\tau, x) + \tau A_h X_{k+1}^h(\tau, x) + \tau P_h F(X_k^h(\tau, x)) + \sqrt{\tau} P_h \chi_{k+1} \\ X_0^h(\tau, x) &= P_h x, \end{aligned}$$

where $\chi_{k+1} = \frac{1}{\sqrt{\tau}}(W((k+1)\tau) - W(k\tau))$.

To simplify the equations, most of the time we omit the dependence of X_k^h on the time-step τ and on the initial condition x .

The previous equation can be replaced by

$$X_{k+1}^h = S_{\tau,h} X_k^h + \tau S_{\tau,h} P_h F(X_k^h) + \sqrt{\tau} S_{\tau,h} P_h \chi_{k+1}, \quad (3.9)$$

where $S_{\tau,h}$ is defined by

$$S_{\tau,h} = (I - \tau A_h)^{-1}. \quad (3.10)$$

When $h = 0$, the process is well-defined in H , since it is easily checked that $S_{\tau,0}$ is a Hilbert-Schmidt operator on H . When $h > 0$, it is well-defined in the finite-dimensional space V_h .

For the analysis of the convergence of the scheme, we need the following technical estimates on the discrete-time semi-group $(S_{\tau,h}^j)_{j \in \mathbb{N}}$ for $\tau > 0$ and $h \geq 0$:

Lemma 3.7 *For any $0 \leq \kappa \leq 1$, $h \in [0, 1)$ and $j \geq 1$*

$$|(-A_h)^{1-\kappa} S_{\tau,h}^j P_h|_{\mathcal{L}(H)} \leq \frac{1}{(j\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0 \tau)^{j\kappa}}.$$

Moreover, for any $\beta \geq 1$ and $j \geq \beta$

$$|(-A_h)^\beta S_{\tau,h}^j P_h|_{\mathcal{L}(H)} \leq \frac{\beta^\beta}{(j\tau)^\beta},$$

and for any $0 \leq \beta \leq 1$

$$|(-A_h)^{-\beta} (S_{\tau,h} - I) P_h|_{\mathcal{L}(H)} \leq 2\tau^\beta.$$

Proof. Using the notations of Proposition 3.2, we have, for any $z \in H$,

$$\begin{aligned} & |(-A_h)^{1-\kappa} S_{\tau,h}^j P_h z|_H^2 \\ &= \sum_{i=0}^{N_h} (\lambda_i^h)^{2(1-\kappa)} \frac{1}{(1 + \lambda_i^h \tau)^{2j}} \langle z, f_i^h \rangle^2 \\ &= \frac{1}{(j\tau)^{2(1-\kappa)}} \sum_{i=0}^{N_h} \langle z, f_i^h \rangle^2 (\lambda_i^h)^{2(1-\kappa)} (j\tau)^{2(1-\kappa)} \frac{1}{(1 + \lambda_i^h \tau)^{2j(1-\kappa)}} \frac{1}{(1 + \lambda_i^h \tau)^{2j\kappa}} \\ &\leq \frac{1}{(j\tau)^{2(1-\kappa)}} \sum_{i=0}^{N_h} \left(\frac{\lambda_i^h j\tau}{1 + \lambda_i^h j\tau} \right)^{2(1-\kappa)} \frac{1}{(1 + \lambda_0^h \tau)^{2j\kappa}} \langle z, f_i^h \rangle^2 \\ &\leq c |P_h z|_H^2 \frac{1}{(j\tau)^{2(1-\kappa)}} \frac{1}{(1 + \lambda_0^h \tau)^{2j\kappa}} \\ &\leq c |z|_H^2 \frac{1}{(j\tau)^{2(1-\kappa)}} \frac{1}{(1 + \lambda_0^h \tau)^{2j\kappa}}. \end{aligned}$$

Above we have used the notation $N_0 = +\infty$. To conclude, we use that for any $h \in [0, 1)$, $\lambda_0 \leq \lambda_0^h$. The proofs of the two other inequalities are similar - see [5] for the second one. ♦

Remark 3.8 *Later, we often use the following expression for X_k^h :*

$$X_k^h = S_{\tau,h}^k P_h x + \tau \sum_{l=0}^{k-1} S_{\tau,h}^{k-l} P_h F(X_l^h) + \sqrt{\tau} \sum_{l=0}^{k-1} S_{\tau,h}^{k-l} P_h \chi_{l+1}. \quad (3.11)$$

The following expression is also useful:

$$\sqrt{\tau} \sum_{l=0}^{k-1} S_{\tau,h}^{k-l} P_h \chi_{l+1} = \int_0^{t_k} S_{\tau,h}^{k-l_s} P_h dW(s), \quad (3.12)$$

where $l_s = \lfloor \frac{s}{\tau} \rfloor$ - with the notation $\lfloor \cdot \rfloor$ for the integer part.

For $h \in (0, 1)$, we finally introduce the following processes: for $0 \leq k \leq m - 1$ and $t_k \leq t \leq t_{k+1}$

$$\tilde{X}^h(t) = X_k^h + \int_{t_k}^t [A_h S_{\tau, h} X_k^h + S_{\tau, h} P_h F(X_k^h)] ds + \int_{t_k}^t S_{\tau, h} P_h dW(s). \quad (3.13)$$

The process $(\tilde{X}^h(t))_{t \in \mathbb{R}^+}$ is a natural interpolation in time of the numerical solution $(X_k^h)_{k \in \mathbb{N}}$ defined by (3.9): $\tilde{X}^h(t_k) = X_k^h$.

3.4 A priori bounds on moments

We give a few results on the processes $(X(t))_{t \geq 0}$, $(X^h(t))_{t \in \mathbb{R}^+}$ and $(X_k^h)_{k \in \mathbb{N}}$.

All the appearing constants are uniform with respect to $h \in (0, 1)$ and τ .

Lemma 3.9 *For any $p \geq 1$, there exists a constant $C_p > 0$ such that for every $h \in (0, 1)$, $t \geq 0$ and $x \in H$*

$$\mathbb{E}|X^h(t, x)|^p \leq C_p(1 + |x|^p).$$

Lemma 3.10 *For any $p \geq 1$, $\tau_0 > 0$, there exists a constant $C > 0$ such that for every $h \in (0, 1)$, $0 < \tau \leq \tau_0$, $k \in \mathbb{N}$, $t \geq 0$ and $x \in H$*

$$\mathbb{E}|X_k^h|^p \leq C(1 + |x|^p) \quad \text{and} \quad \mathbb{E}|\tilde{X}^h(t)|^p \leq C(1 + |x|^p).$$

Proof of Lemmas 3.9 and 3.10. The case $h = 0$ is treated in [5]. We thus only treat the case $h \in (0, 1)$, with similar methods.

Using the mild formulation, in the continuous-time situation we need to control the three terms of (3.1):

$$|e^{tA_h} P_h x| \leq e^{-\lambda_0^h t} |P_h x| \leq e^{-\lambda_0 t} |x|,$$

since $\lambda_0^h \geq \lambda_0$ thanks to Proposition 3.2;

$$\left| \int_0^t e^{(t-s)A_h} P_h F(X_h(s)) ds \right| \leq C \int_0^t e^{-\lambda_0^h(t-s)} ds \leq \frac{C}{\lambda_0^h} \leq \frac{C}{\lambda_0},$$

thanks to the boundedness of F ;

$$\begin{aligned} \mathbb{E} \left| \int_0^t e^{(t-s)A_h} P_h dW(s) \right|^p &\leq C_p \mathbb{E} \left[\left| \int_0^t e^{(t-s)A_h} P_h dW(s) \right|^2 \right]^{p/2} \\ &\leq C_p \left(\int_0^t \text{Tr}(e^{(t-s)A_h} P_h e^{(t-s)A_h}) ds \right)^{p/2} \\ &\leq C_p \left(\int_0^t \text{Tr}(P_h A_h^{-1/2-\kappa} P_h) |A_h^{1/2+\kappa} e^{2(t-s)A_h} P_h|_{\mathcal{L}(H)} ds \right)^{p/2} \\ &\leq C_p \left(\int_0^t \frac{1}{(t-s)^{1/2+\kappa}} e^{-\lambda_0^h(t-s)} ds \right)^{p/2} \leq C_p, \end{aligned}$$

where we have reduced the estimate to the case $p = 2$ since the stochastic integral is a Gaussian random variable, and then we have used Itô's isometry formula, Proposition 2.6 and Proposition 3.4, with any $\kappa > 0$.

The proof of the first estimate of Lemma 3.10 goes along the same way, using the discrete-time mild formulation (3.11), with also three quantities to control:

$$|S_{\tau, h}^k P_h x| \leq \frac{1}{(1 + \lambda_0 \tau)^k} |x|,$$

thanks to the first estimate of Lemma 3.7 and the boundedness of F ;

$$\begin{aligned} \left| \tau \sum_{l=0}^{k-1} S_{\tau,h}^{k-l} P_h F(X_l^h) \right| &\leq C\tau \sum_{l=0}^{k-1} \frac{1}{(1 + \lambda_0\tau)^{k-l}} \\ &\leq C \frac{\tau}{(1/(1 + \lambda_0\tau)) - 1} \leq C; \end{aligned}$$

finally as before we only need to study the case $p = 2$, and we use (3.12) to get

$$\begin{aligned} \mathbb{E} \left| \sqrt{\tau} \sum_{l=0}^{k-1} S_{\tau,h}^{k-l} P_h \chi_{l+1} \right|^2 &= \sum_{l=0}^{k-1} \tau \text{Tr}(S_{\tau,h}^{k-l} P_h S_{\tau,h}^{k-l}) \\ &\leq \text{Tr}(P_h A_h^{-1/2-\kappa} P_h) \tau \sum_{l=0}^{k-1} |S_{\tau,h}^{2(k-l)} A_h^{1/2+\kappa}|_{\mathcal{L}(H)} \\ &\leq C\tau \sum_{l=0}^{k-1} \frac{1}{((k-l)\tau)^{1/2+\kappa}} \exp\left(- (1/2 - \kappa) \frac{\log(1 + \lambda_0\tau)}{\tau} (k-l)\tau\right) \\ &\leq C \int_0^{+\infty} \frac{1}{t^{1/2+\kappa}} \exp(-ct) dt, \end{aligned}$$

for some $c > 0$.

The proof of the second estimate of Lemma 3.10 using (3.13) is then straightforward.

◆

4 Asymptotic behavior of the processes and invariant laws

First, we focus on the existence of invariant measures for the continuous and discrete time processes. We use the well-known Krylov-Bogoliubov criterion - see [17]. Tightness comes from two facts: $D((-A)^\gamma)$ is compactly embedded in H when $\gamma > 0$, and when $\gamma < 1/4$ we can control moments with the same techniques used to prove the Lemmas 3.9 and 3.10:

Lemma 4.1 *For any $0 < \gamma < 1/4$, $\tau > 0$ and any $x \in H$, there exist $C(\gamma, \tau, x) > 0$ and $C(\gamma, x) > 0$ such that for every $h \in (0, 1)$, $m \geq 1$ and $t \geq 1$*

$$\mathbb{E}|X_m^h(\tau, x)|_\gamma^2 \leq C(\gamma, \tau, x) \quad \text{and} \quad \mathbb{E}|X^h(t, x)|_\gamma^2 \leq C(\gamma, x).$$

For $h \in [0, 1)$, uniqueness of the invariant probability measure for the continuous time process $(X^h(t))_{t \in \mathbb{R}^+}$ can be deduced from the well-known Doob Theorem - see [17]. Indeed, since in equation (1.1) noise is additive and non-degenerate, the Strong Feller property and irreducibility can be easily proved. In the proof of the main Theorem 5.1, we also need speed of convergence, and thanks to a coupling argument we get the following exponential convergence result :

Proposition 4.2 *There exist $c > 0$, $C > 0$ such that for any bounded test function $\phi : H \rightarrow \mathbb{R}$, any $t \geq 0$, any $h \in [0, 1)$ and any $x_1, x_2 \in V_h$*

$$|\mathbb{E}\phi(X^h(t, x_1)) - \mathbb{E}\phi(X^h(t, x_2))| \leq C\|\phi\|_0(1 + |x_1|^2 + |x_2|^2)e^{-ct}. \quad (4.1)$$

Remark 4.3 *A proof of this result can be found in Section 6.1 in [24]. In this proof it is obvious that c and C are independent of h .*

The idea of coupling relies on the following formula: if ν_1 and ν_2 are two probability measures on a state space S , their total variation distance satisfies

$$d_{TV}(\nu_1, \nu_2) = \inf \{ \mathbb{P}(X_1 \neq X_2) \},$$

which is an infimum over random variables (X_1, X_2) defined on a same probability space, and such that $X_1 \sim \nu_1$ and $X_2 \sim \nu_2$.

Roughly speaking, the principle is to define a coupling $(Z_1(t, x_1, x_2), Z_2(t, x_1, x_2))_{t \geq 0}$ for the processes $(X(t, x_1))_{t \geq 0}$ and $(X(t, x_2))_{t \geq 0}$ such that the coupling time \mathcal{T} of Z_1 and Z_2 - i.e. the first time the processes are equal - has an exponentially decreasing tail.

This technique was first used in the study of the asymptotic behavior of Markov chains - see [7], [26], [61], [65] - and was later adapted for SDEs and more recently for SPDEs - see for instance [55], [63], [72].

Corollary 4.4 *For any $h \in [0, 1)$, the process X^h admits a unique invariant probability measure μ^h , such that for any bounded test function $\phi : H \rightarrow \mathbb{R}$, $t \geq 0$ and $x \in V_h$ we have*

$$|\mathbb{E}\phi(X^h(t, x)) - \int_{V_h} \phi d\mu^h| \leq C \|\phi\|_0 (1 + |x|^2) e^{-ct}. \quad (4.2)$$

We use the notation $\mu = \mu^0$, when $h = 0$: it is the invariant law of the non-discretized process, for which we show an approximation result.

However, the situation is more complex for the discrete time approximations: given a time-step $\tau > 0$, we do not know whether uniqueness of the invariant measure also holds for the numerical approximation $(X_k^h)_{k \in \mathbb{N}}$. In the following Remark 4.5 below, we describe a strict dissipativity assumption on the non-linear coefficient which ensures ergodicity by a straightforward argument. Without this assumption, it is not clear whether ergodicity holds for small time-steps $0 < \tau \leq \tau_{\text{ergo}}$, where τ_{ergo} can be chosen independently of $h \in [0, 1)$; the answer to this question will be the subject of future works.

Remark 4.5 *Let $h \in [0, 1)$ be fixed. A sufficient condition for the uniqueness of the invariant probability measure of the discrete time process $(X_k^h)_{k \in \mathbb{N}}$ is the strict dissipativity assumption*

$$L_F < \lambda_0,$$

where we recall that L_F denotes the Lipschitz constant of F .

Then trajectories of the processes $(X_t^h)_{t \in \mathbb{R}^+}$ and $(X_k^h)_{k \in \mathbb{N}}$ issued from different initial conditions x_1 and x_2 and driven by the same noise process are exponentially close when time increases: for any $\tau_0 > 0$, there exists $c > 0$ such that for any $0 < \tau \leq \tau_0$, $h \in [0, 1)$, $k \geq 0$ and $t \geq 0$ we have almost surely

$$\begin{aligned} |X^h(t, x_1) - X^h(t, x_2)| &\leq e^{-(\lambda_0 - L_F)t} |x_1 - x_2| \\ |X_k^h(\tau, x_1) - X_k^h(\tau, x_2)| &\leq e^{-ck\tau} |x_1 - x_2|. \end{aligned}$$

The proof of the uniqueness of the invariant law is now easy, and in particular we do not use Proposition 4.2.

Results are the same when we consider the spectral Galerkin discretization:

Proposition 4.6 *There exist $c > 0$, $C > 0$ such that for any bounded test function $\phi : H \rightarrow \mathbb{R}$, any $t \geq 0$, any $M \in \mathbb{N} \cup \{\infty\}$ and any $x_1, x_2 \in H_M$*

$$|\mathbb{E}\phi(X^{(M)}(t, x_1)) - \mathbb{E}\phi(X^{(M)}(t, x_2))| \leq C \|\phi\|_0 (1 + |x_1|^2 + |x_2|^2) e^{-ct}. \quad (4.3)$$

Moreover, for any $M \in \mathbb{N} \cup \{\infty\}$, the process $X^{(M)}$ admits a unique invariant probability measure $\mu^{(M)}$, such that for any bounded test function $\phi : H \rightarrow \mathbb{R}$, $t \geq 0$ and $x \in H_M$ we have

$$|\mathbb{E}\phi(X^{(M)}(t, x)) - \int_{H_M} \phi d\mu^{(M)}| \leq C \|\phi\|_0 (1 + |x|^2) e^{-ct}. \quad (4.4)$$

With the notations of Definitions 3.5 and 3.6, we have $\mu^{(\infty)} = \mu = \mu^0$.

As consequence of Proposition 4.6, we obtain the following Lemma:

Lemma 4.7 *For any bounded test function $\phi \in \mathcal{C}(H)$, we have*

$$\bar{\phi}_M := \int_{H_M} \phi(z) d\mu^{(M)}(z) \xrightarrow{M \rightarrow \infty} \int_H \phi d\mu =: \bar{\phi}.$$

Proof of Lemma 4.7: For any $t \geq 0$ and any fixed initial condition $x \in H$, we have

$$\begin{aligned} \int_{H_M} \phi(z) d\mu^{(M)}(z) - \int_H \phi(z) d\mu(z) &= \int_{H_M} \phi(z) d\mu^{(M)}(z) - \mathbb{E}\phi(X^{(M)}(t)) \\ &\quad + \mathbb{E}\phi(X^{(M)}(t)) - \mathbb{E}\phi(X(t)) \\ &\quad + \mathbb{E}\phi(X(t)) - \int_H \phi(z) d\mu(z). \end{aligned}$$

We thus get that for any $t > 0$

$$\limsup_{M \rightarrow +\infty} \left| \int_{H_M} \phi(z) d\mu^{(M)}(z) - \int_H \phi(z) d\mu(z) \right| \leq C \exp(-ct),$$

and it remains to take $t \rightarrow +\infty$. Notice that the constant c does not depend on dimension M . \blacklozenge

The speed of convergence in Lemma 4.7 will be given below in Remark 5.3.

5 The convergence results

We now state our main result, as well as a few important consequences.

For an admissible test function ϕ we define $\|\phi\|_{0,2} = \sup_{0 \leq j \leq 2} (\|\phi\|_j)$.

Theorem 5.1 *For any $0 < \kappa < 1/2$, τ_0 , there exists a constant $C > 0$ such that for any $\mathcal{C}_b^2(H)$ function ϕ , $h \in (0, 1)$, $N \geq 1$, $x \in H$ and $0 < \tau \leq \tau_0$*

$$\begin{aligned} &\left| \frac{1}{N} \sum_{m=0}^{N-1} \left(\mathbb{E}\phi(X_m^h) - \bar{\phi} \right) \right| \\ &\leq C \|\phi\|_{0,2} (1 + |x|^3) \left(1 + (N\tau)^{-1+\kappa} + (N\tau)^{-1} \right) \left(\tau^{1/2-\kappa} + h^{1-\kappa} + \frac{1}{N\tau} \right), \end{aligned}$$

where $\bar{\phi} = \int_H \phi(z) d\mu(z)$.

This result can be interpreted from a *statistical* point of view: $\frac{1}{N} \sum_{m=0}^{N-1} \mathbb{E}\phi(X_m^h)$ is an *estimator* of the average $\bar{\phi} = \int_H \phi(z) \mu(dz)$ of the admissible test function ϕ with respect to the invariant law μ of the SPDE. Theorem 5.1 gives an error bound on its *bias*.

Of the two factors in parenthesis in the Theorem, only the second one is important - the presence of the first one is for technical estimates which degenerate at time 0 whereas we are interested at the asymptotic behavior of the quantity. The main observation is that the orders of convergence with respect to τ and h are given by the corresponding weak

orders $1/2$ and 1 in the approximation of $X(T)$ for a fixed value of the final time $T < +\infty$ - given in [20] and [3]. The aim of this chapter is to show how the corresponding error bounds are preserved asymptotically - under appropriate conditions.

An interesting supplementary result would concern the study of the *statistical error*. In [64], two more error bounds are proved: first in the mean-square sense, and then in an almost sure statement - thanks to an argument of Borel-Cantelli type. We have not been able to treat our problem in a similar way. We claim that it is for the following reason. The right order of convergence with respect to τ in Theorem 5.1 is obtained thanks to an appropriate integration by parts formula - as explained in the Introduction; the study of the mean-square error - now in a stronger sense - implies that the use of such a technique seems impossible. To generalize the results of [64] in the infinite dimensional setting, new arguments should be found.

The additional term $\frac{1}{N\tau}$ corresponds to the bias introduced between the average in time and its limit when time increases.

From Theorem 5.1, it is easy to obtain approximation results when only one type of discretization is applied.

Results on distance between invariant laws of the various processes can now be given. As explained in Section 4, without the time-discretization ergodicity holds for the spatially discretized, time-continuous process X^h for any $h \in (0, 1)$, while as soon as discretization in time is applied it is not clear whether it holds for small enough time-steps, uniformly with respect to h .

However, as a consequence of Theorem 5.1 we obtain error bounds controlling the distance between the average of admissible test functions with respect to the possibly non unique ergodic invariant laws of the discretized process and the invariant law of the SPDE.

Proposition 5.2 *For any $0 < \kappa < 1/2$, $\tau_0 > 0$, there exists a constant $C > 0$ such that the following holds: for any $0 < \tau < \tau_0$ and $h \in (0, 1)$, assume that $\mu^{\tau, h}$ is an ergodic invariant law of $(X_k^h)_{k \in \mathbb{N}}$; then for any admissible test function ϕ , we have*

$$\left| \int_H \phi(z) d\mu(z) - \int_{V_h} \phi(z) d\mu^{\tau, h}(z) \right| \leq C \|\phi\|_{0,2} \left(\tau^{1/2-\kappa} + h^{1-\kappa} \right).$$

The proof of this result is easy - we let go N to ∞ in the estimate of Theorem 5.1, and use the convergence of the time-average for $\mu^{\tau, h}$ a.e. initial condition, see also [5].

The above result also holds for invariant laws having a finite third order moment.

Remark 5.3 *It is also possible to derive the error estimate as in Theorem 5.1 and Proposition 5.2 when discretization in space is done with the spectral approximation in dimension M instead of using a finite element method with mesh-size h . For instance, we precise the speed of convergence in : for any $0 < \kappa < 1/2$ and $\phi \in \mathcal{C}_b^2(H)$, there exists a constant C_κ such that*

$$\left| \int_H \phi d\mu - \int_{H_M} \phi_M d\mu^{(M)} \right| \leq C_\kappa \frac{1}{\lambda_{M+1}^{1/2-\kappa}}.$$

The strategy - developed in Section 6 - remains the same, where we use an auxiliary dimension variable, say L , going to ∞ for the ambient space where the Poisson equation is used, while M is fixed.

6 Description of the proof

We fix the time step τ , as well as $N \in \mathbb{N}$; we then introduce the notation $T = N\tau$. We also define, for $k \in \mathbb{N}$, $t_k = k\tau$. $\kappa > 0$ is a parameter, which is supposed to be small enough. We also control τ : for some $\tau_0 > 0$, $\tau \leq \tau_0$.

6.1 Strategy

The three key ingredients to prove Theorem 5.1 are the use of an additional finite dimensional projection onto the subspaces H_M , the use of the solution of the Poisson equation as in [64] (see Sub-section 6.2) and an integration by parts formula issued from Malliavin calculus as in [5, 20] (see Sub-Section 6.3).

We will use the Poisson equation in finite dimension, then we will use the following decomposition:

$$\begin{aligned} \frac{1}{N} \sum_{m=0}^{N-1} \mathbb{E}\phi(X_m^h) - \bar{\phi} &= \frac{1}{N} \sum_{m=0}^{N-1} \mathbb{E}\phi(P_M X_m^h) - \bar{\phi}_M \\ &+ \bar{\phi}_M - \bar{\phi} + \frac{1}{N} \sum_{m=0}^{N-1} \left(\mathbb{E}\phi(X_m^h) - \mathbb{E}\phi(P_M X_m^h) \right), \end{aligned}$$

where we recall that P_M is the orthogonal projection of H into H_M and $\bar{\phi}_M$ is define at the end of Section 4.

It is obvious the the last term converge to 0 when $M \rightarrow +\infty$. The convergence to 0 of the second term is not difficult, it has been proved in Section 4. The proof of the estimate of the first term is very technical, so for pedagogy, in Sub-Section 6.4 we introduce the decomposition of the error and identify the three terms which we control later in Sub-Section 7.1, Sub-Section 7.2 and Sub-Section 7.3.

6.2 Some results on the Poisson equation in finite dimension

Let $M \in \{1, 2, \dots\}$. Let $\phi \in \mathcal{C}_b^2(H)$. We define $\Psi^{(M)} : H_M \rightarrow \mathbb{R}$ by the unique solution of the Poisson equation

$$\mathcal{L}^{(M)}\Psi^{(M)} = \phi P_M - \bar{\phi}_M \text{ and } \int_{H_M} \Psi^{(M)} d\mu^{(M)} = 0, \quad (6.1)$$

where $\mathcal{L}^{(M)}$ is the infinitesimal generator of the SPDE (3.7) defined for functions of class \mathcal{C}^2 $\psi : H \rightarrow \mathbb{R}$ and for any $x \in H$ by

$$\mathcal{L}^{(M)}\psi(x) = \langle AP_M x + P_M F(x), D\psi(x) \rangle + \frac{1}{2} \text{Tr}(P_M D^2\psi(x)).$$

In the following, we will need to control the first and the second derivatives of Ψ . The Proposition below is the essential result that we need. It is the same kind of estimation used in [5, 20] to obtain weak order of convergence 1/2.

Proposition 6.1 *Let $M \in \{1, 2, \dots\}$. Let $\phi \in \mathcal{C}_b^2(H)$. The function $\Psi^{(M)}$ defined for any $x \in H_M$ by*

$$\Psi^{(M)}(x) = \int_0^{+\infty} \mathbb{E} \left(\phi(X^{(M)}(t, x)) - \bar{\phi}_M \right) dt$$

is of class \mathcal{C}^2 and the unique solution of (6.1). Moreover, we have the following estimates: for any $0 \leq \beta, \gamma < 1/2$ there exist $C, C_\beta > 0$ - independent of M - such that for any $x \in H_M$

$$\begin{aligned} |\Psi^{(M)}(x)| &\leq C(1 + |x|^2) \|\phi\|_0, \\ |D\Psi^{(M)}(x)|_\beta &\leq C_\beta(1 + |x|^2) \|\phi\|_{0,1} \end{aligned} \quad (6.2)$$

and

$$|(-A)^\beta D^2\Psi^{(M)}(x)(-A)^\gamma|_{\mathcal{L}(H_M)} \leq C_{\beta,\gamma}(1 + |x|^2) \|\phi\|_{0,2}, \quad (6.3)$$

where $\|\phi\|_{0,i} = \sup_{0 \leq j \leq i} (\|\phi\|_j)$.

Remark 6.2 *In fact, the result on $D\Psi$ is also true for $\beta < 1$ and the result on $D^2\Psi$ is also true for $\beta < 1$, $\gamma < 1$ and $\beta + \gamma < 1$. Moreover, all the constants are uniform with respect to $M \in \{1, 2, \dots\}$.*

A proof of this result can be found in the Appendix.

6.3 A Malliavin integration by parts formula

Let $h \in (0, 1)$ be fixed - the case $h = 0$ is not required in the calculations.

As explained in the Introduction, one of the key tools to obtain the right weak order is a transformation of some spatially irregular terms involving the stochastic integral with respect to the cylindrical Wiener process, into more suitable, deterministic ones, thanks to an integration by parts formula, issued from Malliavin calculus - see [73], [78].

The notations here are the same as in [20], where the following useful integration by parts formula is given - see Lemma 2.1 therein:

Lemma 6.3 *For any $G \in \mathbb{D}^{1,2}(V_h)$, $u \in \mathcal{C}_b^2(V_h)$ and $\Psi \in L^2(\Omega \times [0, T], \mathcal{L}_2(V_h))$ an adapted process,*

$$\mathbb{E}[Du(G) \cdot \int_0^T \Psi(s) dW^{(M)}(s)] = \mathbb{E}\left[\int_0^T \text{Tr}(\Psi(s)^* D^2u(G) \mathcal{D}_s G) ds\right], \quad (6.4)$$

where $\mathcal{D}_s G : \ell \in H \mapsto \mathcal{D}_s^\ell G \in V_h$ stands for the Malliavin derivative of G , and $\mathbb{D}^{1,2}(V_h)$ is the set of H -valued random variables $G = \sum_{i \in \mathbb{N}, i \leq N_h} G_i e_i^h$, with $G_i \in \mathbb{D}^{1,2}$ the domain of the Malliavin derivative for \mathbb{R} -valued random variables for any i .

Remark 6.4 *This Lemma remains valid if u is not assumed to be bounded but only $u \in \mathcal{C}^2(V_h)$ provided the expectations and the integral above are well defined. This is easily seen by approximation of u by bounded functions.*

Some care must be taken when controlling the Malliavin derivative of \tilde{X}^h : in general it is not possible to obtain uniform estimates with respect to time - unless for instance a strict dissipativity condition is satisfied - see Remark 4.5.

In the proof of technical estimates below, we circumvent this problem by using these derivatives only at times $t_k = k\tau$ and s such that $t_{k-l_s} \leq 1$. We also have the following estimates.

Lemma 6.5 *For any $0 \leq \beta < 1$ and $\tau_0 > 0$, there exists a constant $C > 0$ such that for every $h \in (0, 1)$, $k \geq 1$, $0 < \tau \leq \tau_0$ and $s \in [0, t_k]$*

$$|(-A_h)^\beta \mathcal{D}_s^\ell X_k^h|_{\mathcal{L}(V_h)} \leq C(1 + L_F \tau)^{k-l_s} \left(1 + \frac{1}{(1 + \lambda_0 \tau)^{(1-\beta)(k-l_s)} t_{k-l_s}^\beta}\right).$$

Moreover, if $t_k \leq t < t_{k+1}$, we have

$$|(-A_h)^\beta \mathcal{D}_s^\ell \tilde{X}^h(t)|_{\mathcal{L}(V_h)} \leq C |(-A_h)^\beta \mathcal{D}_s^\ell X_k^h|_{\mathcal{L}(V_h)}.$$

We want to emphasize that the constant in Lemma 6.5 is uniform with respect to $h \in (0, 1)$.

Proof According to the definition of $\mathcal{D}_s G$ as a linear operator in V_h , we need to control $|(-A_h)^\beta \mathcal{D}_s^\ell \tilde{X}^h(t)|$ and $|(-A_h)^\beta \mathcal{D}_s^\ell X_k^h|$, uniformly with respect to $\ell \in V_h$ with $|\ell| \leq 1$.

The second inequality is a consequence of the following equality for $s \leq t_k \leq t < t_{k+1}$, thanks to (3.13):

$$\mathcal{D}_s^\ell \tilde{X}^h(t) = \mathcal{D}_s^\ell X_k^h + (t - t_m)(\tau A_h S_{\tau,h} \mathcal{D}_s^\ell X_k^h + S_{\tau,h} P_h F(X_k^h) \cdot \mathcal{D}_s^\ell X_k^h),$$

and the conclusion follows since

$$\sup_{h \in (0,1)} |\tau A_h S_{\tau,h}|_{\mathcal{L}(V_h)} < +\infty.$$

Now we prove the first estimate, and we fix $h \in (0, 1)$. For any $k \geq 1$, $\ell \in V_h$ and $s \in [0, t_k]$, using the chain rule for Malliavin calculus and expressions (3.11) and (3.12), we have

$$\mathcal{D}_s^\ell X_k^h = S_{\tau,h}^{k-l_s} \ell + \tau \sum_{i=l_s+1}^{k-1} S_{\tau,h}^{k-i} D(P_h F)(X_i^h) \cdot \mathcal{D}_s^\ell X_i^h.$$

We recall that l_s denotes the integer part of $\frac{s}{\tau}$, so that when $i \leq l_s$ we have $\mathcal{D}_s^\ell X_i^h = 0$.

As a consequence, the discrete Gronwall Lemma ensures that for $k \geq l_s + 1$

$$|\mathcal{D}_s^\ell X_k^h| \leq (1 + L_F \tau)^{k-l_s} |\ell|.$$

Now using Lemma 3.7, we have

$$|(-A_h)^\beta \mathcal{D}_s^\ell X_k^h| \leq \frac{1}{(1 + \lambda_0 \tau)^{(1-\beta)(k-l_s)} t_{k-l_s}^\beta} |\ell| + L_F \tau \sum_{i=l_s+1}^{k-1} \frac{(1 + L_F \tau)^{l-l_s}}{(1 + \lambda_0 \tau)^{(1-\beta)(k-i)} t_{k-i}^\beta} |\ell|.$$

To conclude, we see that when $0 < \tau \leq \tau_0$

$$\tau \sum_{i=l_s+1}^{k-1} \frac{1}{(1 + \lambda_0 \tau)^{(1-\beta)(k-i)} t_{k-i}^\beta} \leq C \int_0^{+\infty} t^{-\beta} \frac{1}{(1 + \lambda_0 \tau)^{(1-\beta)\frac{t}{\tau}}} dt \leq C < +\infty.$$

◆

6.4 Strategy for the estimate of $\lim_{M \rightarrow \infty} \frac{1}{N} \sum_{m=0}^{N-1} \mathbb{E} \phi(P_M X_m^h) - \bar{\phi}_M$

Let $M \in \{1, 2, \dots\}$, we define the function $\tilde{\Psi}^{(M)}$ for $x \in H$ by

$$\tilde{\Psi}^{(M)}(x) = \Psi^{(M)}(P_M x),$$

where $\Psi^{(M)}$ is the solution of the Poisson equation (6.1). Using the identifications introduced in Remark 2.1 we have for any $x \in H$

$$\begin{aligned} D\tilde{\Psi}^{(M)}(x) &= P_M D\Psi^{(M)}(P_M x), \\ D^2\tilde{\Psi}^{(M)}(x) &= P_M D^2\Psi^{(M)}(P_M x) P_M, \end{aligned}$$

then it is easy to show that $\tilde{\Psi}^{(M)}$ and $\Psi^{(M)}$ verify the same estimates (see Proposition 6.1).

We need the continuous time interpolation of the numerical process \tilde{X}^h defined by (3.13). For all $m \in \mathbb{N}$, we can associate to \tilde{X}^h on $[t_m, t_{m+1}]$ the generator $\mathcal{L}^{\tau,m,h}$ defined for $x \in V_h$ and $\phi \in \mathcal{L}(H)$ by

$$\mathcal{L}^{\tau,m,h} \phi(x) = \langle S_{\tau,h} A_h X_m^h + S_{\tau,h} P_h F(X_m^h), D\phi(x) \rangle + \frac{1}{2} \text{Tr}(S_{\tau,h} S_{\tau,h}^* P_h D^2 \phi(x)). \quad (6.5)$$

Thanks to the Itô formula and Proposition 6.1, we have for any integer m

$$\mathbb{E} \tilde{\Psi}^{(M)}(X_{m+1}^h) - \mathbb{E} \tilde{\Psi}^{(M)}(X_m^h) = \int_{t_m}^{t_{m+1}} \mathbb{E} \mathcal{L}^{\tau,m,h} \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds.$$

We also need the markov generator \mathcal{L}^h of the finite element solution X^h to decompose this term. The generator \mathcal{L}^h is given for $x \in V_h$ by

$$\mathcal{L}^h \phi(x) = \langle A_h x + P_h F(x), D_x \phi(x) \rangle + \frac{1}{2} \text{Tr}(P_h D_{xx}^2 \phi(x)).$$

We have the following decomposition:

$$\begin{aligned} \mathbb{E} \tilde{\Psi}^{(M)}(X_{m+1}^h) - \mathbb{E} \tilde{\Psi}^{(M)}(X_m^h) &= \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{\tau, m, h} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{(M)} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \mathcal{L}^{(M)} \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds. \end{aligned}$$

Using the following equality for $x \in H$

$$\mathcal{L}^{(M)} \tilde{\Psi}^{(M)}(x) = \mathcal{L}^{(M)} \Psi^{(M)}(P_M x) + \langle P_M F(x) - P_M F(P_M x), D \Psi^{(M)}(P_M x) \rangle$$

and the definition of $\Psi^{(M)}$, we get

$$\begin{aligned} \mathbb{E} \tilde{\Psi}^{(M)}(X_{m+1}^h) - \mathbb{E} \tilde{\Psi}^{(M)}(X_m^h) &= \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{\tau, m, h} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{(M)} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} (\phi(P_M \tilde{X}^h(s)) - \bar{\phi}_M) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \langle P_M (F(\tilde{X}^h(s)) - F(P_M \tilde{X}^h(s))), D \Psi^{(M)}(P_M \tilde{X}^h(s)) \rangle ds \\ &= \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{\tau, m, h} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{(M)} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\ &\quad + \tau (\mathbb{E} \phi(P_M X_m^h) - \bar{\phi}_M) \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\phi(P_M \tilde{X}^h(s)) - \mathbb{E} \left(\phi(P_M X_m^h) \right) \right) ds \\ &\quad + \int_{t_m}^{t_{m+1}} \mathbb{E} \langle P_M (F(\tilde{X}^h(s)) - F(P_M \tilde{X}^h(s))), D \Psi^{(M)}(P_M \tilde{X}^h(s)) \rangle ds \end{aligned}$$

Then if we sum for $m = 1, \dots, N-1$ and divide by $N\tau$, we obtain

$$\begin{aligned}
& \frac{1}{N} \sum_{m=0}^{N-1} \left(\mathbb{E} \phi(P_M X_m^h) - \bar{\phi}_M \right) \\
&= \frac{1}{N\tau} \left(\mathbb{E} \Psi^{(M)}(P_M X_N^h) - \mathbb{E} \Psi^{(M)}(P_M X_1^h) \right) \\
&\quad + \frac{1}{N} \left(\phi(P_M x) - \bar{\phi}_M \right) \\
&\quad + \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\
&\quad + \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{\tau, m, h} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\
&\quad - \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \left(\mathbb{E} \phi(P_M \tilde{X}^h(s)) - \mathbb{E} \phi(P_M X_m^h) \right) ds \\
&\quad - \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \langle P_M \left(F(\tilde{X}^h(s)) - F(P_M \tilde{X}^h(s)) \right), D\Psi^{(M)}(P_M \tilde{X}^h(s)) \rangle ds \\
&:= I_1 + I_2 + I_3 + I_4 + I_5 + I_6.
\end{aligned} \tag{6.6}$$

The two first terms and the last term are easy to control. Indeed, using Proposition 6.1 and Lemma 3.10, we get for $0 < \tau < \tau_0$,

$$|I_1 + I_2| \leq C(1 + |x|^2) \frac{1}{N\tau},$$

where τ_0 is any fixed positive real number. Using the fact that F is lipschitz, Proposition 6.1 and Lemma 3.10, we get

$$\lim_{M \rightarrow \infty} I_6 \rightarrow 0.$$

The control of the three other terms will be the subject of three following Subsections. First, in Subsection 7.1, the following estimate of I_3 is shown:

Lemma 6.6 (Space-discretization error) *For any $0 < \kappa < 1/2$ and τ_0 , there exists a constant $C > 0$ such that for any $\phi \in \mathcal{C}_b^2(H)$, $x \in H$ and $0 < \tau \leq \tau_0$*

$$\begin{aligned}
\limsup_{M \rightarrow \infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \\
\leq C(1 + |x|^3) \|\phi\|_{0,2} h^{1-\kappa} (1 + (N\tau)^{-1}).
\end{aligned}$$

In Subsection 7.3, we will show the following estimate of I_4 :

Lemma 6.7 (Time-discretization error) *For any $0 < \kappa < 1/2$ and τ_0 , there exists a constant $C > 0$ such that for any $\phi \in \mathcal{C}_b^2(H)$, $M \in \{1, 2, \dots\}$, $y \in H$ and $0 < \tau \leq \tau_0$*

$$\begin{aligned}
\left| \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{\tau, m, h} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt \right| \\
\leq C \|\phi\|_{0,2} (1 + |x|^3) \tau^{1/2-\kappa} (1 + (N\tau)^{-1+\kappa} + (N\tau)^{-1}).
\end{aligned}$$

Finally, the proof of the following estimate of I_5 is detailed in Subsection 7.2:

Lemma 6.8 (Additional time-discretization error) *For any $0 < \kappa < 1/4$ and τ_0 , there exists a constant $C > 0$ such that for any $\phi \in \mathcal{C}_b^2(H)$, $M \in \{1, 2, \dots\}$, $y \in H$ and $0 < \tau \leq \tau_0$*

$$\left| \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \left(\mathbb{E}\phi(P_M \tilde{X}^h(t)) - \mathbb{E}\phi(P_M X_m^h) \right) dt \right| \leq C \|\phi\|_{0,2} \tau^{1/2-2\kappa} \left(1 + \frac{|x|}{(N\tau)^{1-\kappa}} \right).$$

The order of the respective proofs may not seem natural. We have made the choice to put the proof of the Lemma 6.7 on the time-discretization error at the end since it essentially uses the same arguments as in [5], while the others require new estimates, appearing for the first time in this context of approximations of invariant laws. We thus begin with the proof of Lemma 6.6 on the space discretization error, and go on with the proof of Lemma 6.8 concerning the additional time-discretization error induced by the use of the Poisson equation - instead of the the generators, we have the process alone.

7 Detailed proof of the estimates

We warn the reader that constants may vary from line to line during the proofs, and that in order to use lighter notations we usually forget to mention dependence on the parameters. We use the generic notation C for such constants. All constants will depend on a parameter $\kappa > 0$, which can be chosen as small as necessary.

To simplify the expressions, we have not mentioned the dependence of the error with respect to the test function ϕ . However, thanks to Proposition 6.1 it is straightforward to give this precision.

7.1 Control of the space dicretization error $\frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt$.

In this Subsection, we prove the estimate of the Lemma 6.6.

7.1.1 Strategy

To control this term, we will mix ideas described in [3] and in [5]. In [3], to prove weak convergence, the authors use estimation on u the solution of the Kolmogorov equation associated to the SPDE. We can use the same ideas because, for each $M \in \{1, 2, \dots\}$, $\tilde{\Psi}^{(M)}$, the solution of the Poisson equation, and its derivatives verify the same kind of estimations than u .

Let $M \in \{1, 2, \dots\}$ be fixed. First, we will decompose $\mathcal{L}^{(M)} - \mathcal{L}^h$ in three terms. We have for any $x \in H$

$$\begin{aligned} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(x) &= \langle (A_M - A_h)x, D\tilde{\Psi}^{(M)}(x) \rangle \\ &\quad + \langle (P_M - P_h)F(x), D\tilde{\Psi}^{(M)}(x) \rangle \\ &\quad + \frac{1}{2} Tr \left((P_M - P_h) D^2 \tilde{\Psi}^{(M)}(x) \right) \end{aligned}$$

and we obtain

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt = \frac{1}{N\tau} \sum_{m=1}^{N-1} (a^m + b^m + c^m),$$

where for $1 \leq m \leq N - 1$

$$\begin{aligned} a^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (A_M - A_h) \tilde{X}^h(t), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ b^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (P_M - P_h)F(\tilde{X}^h(t)), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ c^m &= \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left((P_M - P_h) D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right) dt. \end{aligned}$$

7.1.2 Estimate of a^m

The Ritz projection R_h can be expressed in the form $R_h = A_h^{-1}P_hA$. Using this we can write

$$\begin{aligned} &\langle (A_M - A_h) \tilde{X}^h(t), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle \\ &= \langle (A_M P_h - A_h P_h) \tilde{X}^h(t), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle \\ &= \langle \tilde{X}^h(t), (P_h A_M - A_h P_h) D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle = \langle \tilde{X}^h(t), A_h P_h (R_h P_M - I) D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle \\ &= \langle \tilde{X}^h(t), A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle + \langle \tilde{X}^h(t), A_h P_h (P_M - I) D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle. \end{aligned}$$

The idea of this decomposition is to apply the error estimates (3.5) and (3.8) for R_h and P_M respectively. We now use formula (3.13) on $\tilde{X}^h(t)$. We then need to estimate the following five terms.

$$\begin{aligned} a^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle X_m^h, A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \langle A_h S_{\tau,h} X_m^h, A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \langle S_{\tau,h} P_h F(X_m^h), A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{t_m}^t S_{\tau,h} P_h dW(s), A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \langle A_h X_m^h, (P_M - I) D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &=: a_1^{m,h} + a_2^{m,h} + a_3^{m,h} + a_4^{m,h} + a^{m,M} \end{aligned}$$

* **Estimate of $a_1^{m,h}$:** We use expressions (3.11) of X_m^h and (3.12) to decompose $a_1^{m,h}$:

$$\begin{aligned} a_1^{m,h} &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle S_{\tau,h}^m P_h x, A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \tau \sum_{\ell=0}^{k-1} \langle S_{\tau,h}^{m-\ell} P_h F(X_\ell^h), A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_0^{t_m} S_{\tau,h}^{m-l_s} P_h dW(s), A_h P_h (R_h - I) P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &=: a_{1,1}^{m,h} + a_{1,2}^{m,h} + a_{1,3}^{m,h}. \end{aligned}$$

- *Estimate of $a_{1,1}^{m,h}$:* The ideas are to "share" $(-A_h)$ between different factors and to use regularization properties of the semi-group $(S_{\tau,h}^k)_{k \in \mathbb{N}}$. Thanks to Proposition

3.3, Proposition 6.1 for $\beta = \frac{1}{2}$, Lemma 3.10 and Lemma 3.7, we get, for any small enough parameter $0 < \kappa < 1/2$,

$$\begin{aligned}
|a_{1,1}^{m,h}| &= |\mathbb{E} \int_{t_m}^{t_{m+1}} \langle (-A_h)^{1-\kappa} S_{\tau,h}^m P_h x, (-A_h)^\kappa P_h (R_h - I) \\
&\quad \times (-A)^{-1/2} P_M (-A)^{1/2} D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt| \\
&\leq \mathbb{E} \int_{t_m}^{t_{m+1}} |(-A_h)^{1-\kappa} S_{\tau,h}^m P_h|_{\mathcal{L}(H)} |x| |(-A_h)^\kappa P_h (R_h - I) (-A)^{-1/2}|_{\mathcal{L}(H)} \\
&\quad \times |P_M|_{\mathcal{L}(H)} |(-A)^{1/2} D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))| dt \\
&\leq C \frac{1}{(m\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{m\kappa}} |x| |(-A)^\kappa (R_h - I) (-A)^{-1/2}|_{\mathcal{L}(H)} \\
&\quad \times \int_{t_m}^{t_{m+1}} \mathbb{E}(1 + |\tilde{X}^h(t)|^2) dt \\
&\leq C\tau \frac{1}{(m\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{m\kappa}} (1 + |x|^3) h^{1-2\kappa}.
\end{aligned}$$

We will now use the following useful inequality: for $\tau \leq \tau_0$ and any $N \geq 1$

$$\tau \sum_{l=1}^N \frac{1}{(l\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{l\kappa}} \leq C_\kappa. \quad (7.1)$$

Indeed,

$$\begin{aligned}
\tau \sum_{l=1}^N \frac{1}{(l\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{l\kappa}} &\leq C \int_0^{t_N} \frac{1}{t^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{\kappa \frac{t}{\tau}}} dt \\
&\leq \int_0^\infty \frac{1}{t^{1-\kappa}} e^{-t \frac{\kappa}{\tau} \log(1 + \lambda_0\tau)} dt \\
&\leq \int_0^\infty \frac{1}{s^{1-\kappa}} e^{-s} ds \left(\frac{\tau}{\kappa \log(1 + \lambda_0\tau)} \right)^\kappa \\
&\leq C_\kappa.
\end{aligned}$$

Then, using (7.1), we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_{1,1}^{m,h}| \leq C \frac{1}{T} h^{1-2\kappa} (1 + |x|^3). \quad (7.2)$$

- *Estimate of $a_{1,2}^{m,h}$* : Using the same ideas than to estimate $a_{1,1}^{m,h}$, we have

$$\begin{aligned}
|a_{1,2}^{m,h}| &\leq C\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{l=0}^{m-1} |(-A_h)^{1-\kappa} S_{\tau,h}^{m-l} P_h F(X_l^h)| \\
&\quad \times |(-A_h)^\kappa P_h (R_h - I) (-A)^{-1/2}|_{\mathcal{L}(H)} |(-A)^{1/2} D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))| dt.
\end{aligned}$$

Since F is supposed to be bounded, the estimate (7.1) yields

$$|\tau (-A_h)^{1-\kappa} \sum_{l=0}^{m-1} S_{\tau,h}^{m-l} F(X_l^h)| \leq C \|F\|_0 \tau \sum_{l=1}^m \frac{1}{(l\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0\tau)^{l\kappa}} \leq C_\kappa.$$

With Lemma 3.3, Lemma 3.10 and Proposition 6.1 for $\beta = \frac{1}{2}$, we can now write

$$|a_{1,2}^{m,h}| \leq C(1 + |x|^2)h^{1-2\kappa}\tau,$$

and we get

$$\frac{1}{N\tau} \sum_{m=0}^{N-1} |a_{1,2}^{m,h}| \leq C(1 + |x|^2)h^{1-2\kappa}. \quad (7.3)$$

- *Estimate of $a_{1,3}^{m,h}$* : The analysis of this term is more complicated. We refer the reader to [5] for a discussion on the problem, and for detailed explications on the strategy of the proof - following the original idea of [20].

We recall that the problem lies in the regularity in space of the process, due to whiteness in space of the driving noise. The strategy used to control $a_{1,1}^{m,h}$ and $a_{2,1}^{m,h}$ above would only give an order of convergence 1/4, while we expect 1/2 - our constants need to be uniform with respect to the mesh size h !

We decompose $a_{1,3}^{m,h}$ into two parts, corresponding to different intervals for the stochastic integration. On one of these parts, we can work directly. On the other, a Malliavin integration by parts is performed: it allows to use appropriate regularization properties, and to obtain the correct order of convergence 1/2. We emphasize on the length of the interval where this integration by parts is applied: its maximal size is independent of τ and h , so that the possible exponential divergence when time increases of the Malliavin derivatives implies no trouble.

By using (3.12), we make the decomposition

$$\begin{aligned} a_{1,3}^{m,h} &= \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_0^{t_m} S_{\tau,h}^{m-l_s} P_h dW(s), (-A_h)P_h(R_h - I)P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &= \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_0^{(t_m-3\tau_0)\vee 0} (-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h dW(s), (-A_h)^\kappa P_h(R_h - I) \right. \\ &\quad \times \left. P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{(t_m-3\tau_0)\vee 0}^{t_m} P_M(R_h - I)P_h(-A_h)S_{\tau,h}^{m-l_s} P_h dW(s), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt. \end{aligned}$$

For the first term - which is equal to 0 when $t_m < 3\tau_0$ - we use the Cauchy-Schwarz inequality and we directly get

$$\begin{aligned} &|\mathbb{E} \left\langle \int_0^{(t_m-3\tau_0)\vee 0} (-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h dW(s), (-A_h)^\kappa P_h(R_h - I)P_M D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle| \\ &\leq (\mathbb{E} |(-A_h)^\kappa P_h(R_h - I)(-A)^{-1/2} P_M(-A)^{1/2} D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))|^2)^{1/2} \\ &\quad \times (\mathbb{E} \left| \int_0^{(t_m-3\tau_0)\vee 0} (-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h dW(s) \right|^2)^{1/2}. \end{aligned}$$

We have the following inequality - we remark that in the integral below $t_{m-l_s} \geq 1$:

$$\begin{aligned}
\mathbb{E} \left| \int_0^{(t_m-3\tau_0) \vee 0} (-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h dW(s) \right|^2 &= \int_0^{(t_m-3\tau_0) \vee 0} |(-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h|_{\mathcal{L}_2(H)}^2 ds \\
&= \int_0^{(t_m-3\tau_0) \vee 0} \text{Tr}((-A_h)^{2-2\kappa} S_{\tau,h}^{2(m-l_s)} P_h) ds \\
&\leq \int_0^{(t_m-3\tau_0) \vee 0} |S_{\tau,h}^{(m-l_s)} P_h|_{\mathcal{L}(H)} |(-A_h)^{2+1/2+\kappa} S_{\tau,h}^{(m-l_s)} P_h|_{\mathcal{L}(H)} ds \\
&\quad \times \text{Tr}(P_h (-A_h)^{-1/2-\kappa} P_h) \\
&\leq C \int_0^{(t_m-3\tau_0) \vee 0} \frac{1}{(1+\lambda_0\tau)^{m-l_s} t_{m-l_s}^{2+1/2-\kappa}} ds \\
&\leq C \int_0^{(t_m-3\tau_0) \vee 0} \frac{1}{(1+\lambda_0\tau)^{m-l_s}} ds \\
&\leq C \int_0^{+\infty} \frac{1}{(1+\lambda_0\tau)^{s/\tau}} ds \\
&\leq C,
\end{aligned}$$

when $\tau \leq \tau_0$ and thanks to Proposition 3.4 and Lemma 3.7 . Then, thanks to Proposition 3.3, Proposition 6.1 for $\beta = \frac{1}{2}$ and Lemma 3.10, we get

$$\begin{aligned}
\mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_0^{(t_m-3\tau_0) \vee 0} (-A_h)^{1-\kappa} S_{\tau,h}^{m-l_s} P_h dW(s), (-A_h)^\kappa P_h (R_h - I) P_M D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\
\leq C(1 + |x|^2) \tau h^{1-2\kappa}.
\end{aligned}$$

For the second term, we use the Malliavin integration by parts formula (Lemma 6.3) to get

$$\begin{aligned}
&\mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{(t_m-3\tau_0) \vee 0}^{t_m} P_M (R_h - I) P_h (-A_h) S_{\tau,h}^{m-l_s} P_h dW(s), D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{(t_m-3\tau_0) \vee 0}^{t_m} \text{Tr} \left(S_{\tau,h}^{m-l_s} (-A_h) P_h (R_h - I) P_M D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \mathcal{D}_s \tilde{X}^h(t) \right) ds dt.
\end{aligned}$$

Thanks to both estimates of Lemma 6.5, we have for $(t_m - 3\tau_0) \vee 0 \leq s \leq t_m \leq t < t_{m+1}$

$$|(-A)^\alpha \mathcal{D}_s^\ell \tilde{X}^h(t)| \leq C(1 + L_F \tau)^{m-l_s} \left(1 + \frac{1}{(1+\lambda_0\tau)^{(1-\alpha)(m-l_s)} t_{m-l_s}^\alpha} \right),$$

and we see that $(1 + L_F \tau)^{m-l_s}$ is bounded by a constant.

We can then control the second term of $a_{3,1}^{m,h}$ with

$$\begin{aligned}
&\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{(t_m-3\tau_0) \vee 0}^{t_m} |(-A_h)^{1-3\frac{\kappa}{2}} S_{\tau,h}^{m-l_s}|_{\mathcal{L}(H)} |(-A_h)^{3\frac{\kappa}{2}} P_h (R_h - I) (-A)^{-1/2}|_{\mathcal{L}(H)} \\
&\quad \times |(-A)^{1/2} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa/2}|_{\mathcal{L}(H)} |(-A)^\kappa \mathcal{D}_s \tilde{X}^h(t)|_{\mathcal{L}(H)} ds dt \\
&\quad \times \text{Tr}((-A)^{-1/2-\kappa/2}) \\
&\leq C \int_{(t_m-3\tau_0) \vee 0}^{t_m} t_{m-l_s}^{-1+3\frac{\kappa}{2}} \frac{1}{(1+\lambda_0\tau)^{(m-l_s)3\frac{\kappa}{2}}} \left(1 + t_{m-l_s}^{-\kappa} \frac{1}{(1+\lambda_0\tau)^{(m-l_s)(1-\kappa)}} \right) ds \\
&\quad \times \tau h^{1-3\kappa} (1 + |x|^2),
\end{aligned}$$

using Proposition 6.1, Lemmas 6.5 and 3.7.

We have

$$\int_{(t_m-3\tau_0)\vee 0}^{t_m} t_{m-l_s}^{-1+3\frac{\kappa}{2}} \frac{1}{(1+\lambda_0\tau)^{(m-l_s)3\frac{\kappa}{2}}} ds \leq \int_0^{t_m} \frac{1}{s^{1-3\frac{\kappa}{2}}} \frac{1}{(1+\lambda_0\tau)^{3\frac{\kappa}{2}s/\tau}} ds \leq C < +\infty,$$

for $\tau \leq \tau_0$, thanks to (7.1).

Therefore

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_{1,3}^{m,h}| \leq C(1+|x|^2)h^{1-3\kappa}. \quad (7.4)$$

Using (7.2), (7.3) and (7.4), we have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_1^{m,h}| \leq C(1+\frac{1}{T})h^{1-3\kappa}(1+|x|^3). \quad (7.5)$$

* **Estimate of $a_2^{m,h}$:** Since $(t-t_m)|(-A_h)S_{\tau,h}|_{\mathcal{L}(H)} \leq C$, $a_2^{m,h}$ is bounded by the same expression as $a_1^{m,h}$: by (7.5), we have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_2^{m,h}| \leq C(1+\frac{1}{T})h^{1-3\kappa}(1+|x|^3). \quad (7.6)$$

* **Estimate of $a_3^{m,h}$:** We have

$$|a_3^{m,h}| \leq \mathbb{E} \int_{t_m}^{t_{m+1}} (t-t_m)|(-A_h)^{1-\kappa}S_{\tau,h}P_h|_{\mathcal{L}(H)}|F(X_m^h)| \\ |(-A_h)^\kappa P_h(R_h-I)(-A)^{-1/2}P_M(-A)^{1/2}D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))|dt$$

Since F and $(t-t_m)|(-A_h)^{1-\kappa}S_{\tau,h}P_h|_{\mathcal{L}(H)}$ are bounded, using the same idea than to estimate $a_{1,1}^{m,h}$, we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_3^{m,h}| \leq \frac{C}{T}h^{1-2\kappa}(1+|x|^3). \quad (7.7)$$

* **Estimate of $a_4^{m,h}$:** We again use the integration by parts formula to rewrite $a_4^{m,h}$:

$$a_4^{m,h} = -\mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{t_m}^t S_{\tau,h}P_h dW(s), (-A_h)P_h(R_h-I)D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ = -\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \text{Tr}(S_{\tau,h}P_h(-A_h)P_h(R_h-I)\tilde{\Psi}^{(M)}(\tilde{X}^h(t))\mathcal{D}_s\tilde{X}^h(t)) ds dt.$$

From (3.13), for $t_m \leq s \leq t \leq t_{m+1}$ we have $\mathcal{D}_s^\ell \tilde{X}^h(t) = S_{\tau,h}P_h\ell$; as a consequence, the situation is much simpler and we do not need to use the same trick as in the control of $a_{1,3}^{m,h}$.

Then, as previously, we have

$$\begin{aligned}
|a_4^{m,h}| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \text{Tr}((-A_h)^{1-\kappa} S_{\tau,h} P_h (-A_h)^\kappa P_h (R_h - I) (-A)^{-1/2} P_M \\
&\quad \times (-A)^{1/2} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa/2} (-A)^{-1/2-\kappa/2} (-A)^\kappa S_{\tau,h}) dt \\
&\leq c |(-A_h)^{1-\kappa} S_{\tau,h} P_h|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa/2}) |(-A_h)^\kappa P_h (R_h - I) (-A)^{-1/2}|_{\mathcal{L}(H)} \\
&\quad \times \mathbb{E} \int_{t_m}^{t_{m+1}} |(-A)^{1/2} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa/2}|_{\mathcal{L}(H)} |(-A)^\kappa S_{\tau,h} P_h|_{\mathcal{L}(H)} dt \\
&\leq c(1 + |x|^2) \tau h^{1-2\kappa}.
\end{aligned}$$

Therefore

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_4^{m,h}| \leq C(1 + |x|^2) h^{1-2\kappa}. \quad (7.8)$$

* **Estimate of $a^{m,M}$:** Using Proposition 6.1, Lemma 3.10 and estimate (3.8), we have

$$\begin{aligned}
|a^{m,M}| &\leq \int_{t_m}^{t_{m+1}} \mathbb{E} \left(|(-A_h) P_h|_{\mathcal{L}(H)} |\tilde{X}^h(t)| |(P_M - I) (-A)^{-1/2+\kappa}| \right. \\
&\quad \left. \times |(-A)^{1/2+\kappa} D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))| \right) dt \\
&\leq C_h \|\phi\|_{0,1} \lambda_M^{-1/2+\kappa} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(|\tilde{X}^h(t)| (1 + |\tilde{X}^h(t)|^2) \right) dt \\
&\leq C_h \|\phi\|_{0,1} \lambda_M^{-1/2+\kappa} \tau (1 + |x|^3)
\end{aligned}$$

Then, we get

$$\lim_{M \rightarrow \infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} |a^{m,M}| = 0$$

With the previous estimates, we get

$$\limsup_{M \rightarrow +\infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} |a^m| \leq C \|\phi\|_{0,1} (1 + |x|^3) (1 + T^{-1}) h^{1-3\kappa}. \quad (7.9)$$

7.1.3 Estimate of b^m

Writing $P_M - P_h = (P_M - I) + (I - P_h)$, we get the natural decomposition

$$\begin{aligned}
b^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (P_M - I) F(P_M \tilde{X}^h(t)), D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\
&\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (I - P_h) F(P_M \tilde{X}^h(t)), D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\
&=: b^{m,M} + b^{m,h}.
\end{aligned}$$

Using the fact that F is bounded, Proposition 6.1 and Lemma 3.9, we have

$$\begin{aligned}
|b^{m,i}| &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle F(P_M \tilde{X}^h(t)), (P_i - I) (-A)^{-1/2+\kappa} (-A)^{1/2-\kappa} D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\
&\leq \int_{t_m}^{t_{m+1}} \|F\|_0 |(P_i - I) (-A)^{-1/2+\kappa}|_{\mathcal{L}(H)} \mathbb{E} |(-A)^{1/2-\kappa} D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))| dt \\
&\leq C\tau (1 + |x|^2) |(P_i - I) (-A)^{-1/2+\kappa}|_{\mathcal{L}(H)}.
\end{aligned}$$

Using (3.6) and (3.8), we get

$$|b^{m,h}| \leq C\tau(1 + |x|^2)h^{1-2\kappa}$$

and

$$|b^{m,M}| \leq C\tau(1 + |x|^2)\lambda_M^{-1/2+\kappa}.$$

Finally, we have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |b^m| \leq C(1 + |x|^2)(h^{1-2\kappa} + \lambda_M^{-1/2+\kappa})$$

and

$$\limsup_{M \rightarrow +\infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} |b^m| \leq C(1 + |x|^2)h^{1-2\kappa}.$$

7.1.4 Estimate of c^m

We use the same natural decomposition than for b^m : $c^m = c^{m,h} + c^{m,M}$, where for $i \in \{h, M\}$

$$\begin{aligned} 2|c^{m,i}| &= \left| \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left((-A)^{2\kappa} (P_i - I) (-A)^{-1/2+\kappa} (-A)^{1/2-\kappa} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa} \right. \right. \\ &\quad \left. \left. \times (-A)^{-1/2-\kappa} \right) dt \right| \\ &\leq \text{Tr} \left((-A)^{-1/2-\kappa} \right) \left| (-A)^{2\kappa} (P_i - I) (-A)^{-1/2+\kappa} \right|_{\mathcal{L}(H)} \\ &\quad \times \int_{t_m}^{t_{m+1}} \mathbb{E} \left| (-A)^{1/2-\kappa} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa} \right| dt. \end{aligned}$$

Using Assumptions 2.2, Proposition 6.1, Lemma 3.9, commutativity of A and P_M and estimates (3.8) and (3.6), we get

$$2|c^{m,h}| \leq C\tau(1 + |x|^2)\lambda_M^{-1/2+3\kappa}$$

and

$$2|c^{m,M}| \leq C\tau(1 + |x|^2)h^{1-6\kappa}.$$

Then, we have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |c^m| \leq C(1 + |x|^2)(h^{1-6\kappa} + \lambda_M^{-1/2+3\kappa})$$

and

$$\limsup_{M \rightarrow +\infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} |c^m| \leq C(1 + |x|^2)h^{1-6\kappa}.$$

7.1.5 Conclusion

With the above estimations, we get

$$\limsup_{M \rightarrow \infty} \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^{(M)} - \mathcal{L}^h \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds \leq C(1 + |x|^3)h^{1-\kappa}(1 + T^{-1}). \quad (7.10)$$

7.2 Control of the additional time-discretization error $\mathbb{E}\phi(P_M\tilde{X}(t)) - \mathbb{E}\phi(P_M X_m^h)$,
if $t_m \leq t < t_{m+1}$.

In this Subsection, we prove the estimate of Lemma 6.8.

This part of the error is due to the replacement of the continuous-time process \tilde{X} with the discrete-time process from which it is built by interpolation.

If we compare with the other parts of the error, we observe that instead of Ψ the expression involves the test function ϕ . Since ϕ is only assumed to be of class \mathcal{C}_b^2 , its derivatives do not satisfy estimates with a regularization in space like for Ψ . However, we are still able to distribute appropriately the powers of the operator $-A_h$, thus obtaining the good rate of convergence.

We define an auxiliary function $\tilde{\phi}_M : H \rightarrow \mathbb{R}$ with $\tilde{\phi}_M = \phi \circ P_M$. It is of class \mathcal{C}_b^2 and using the identifications introduced in Remark 2.1 we have for any $x \in H$

$$\begin{aligned} D\tilde{\phi}_M(x) &= P_M D\phi(P_M x), \\ D^2\tilde{\phi}_M(x) &= P_M D^2\phi(P_M x)P_M. \end{aligned}$$

Thanks to the Itô's formula, from (3.13) we get for $t_m \leq t < t_{m+1}$

$$\begin{aligned} \mathbb{E}\phi(P_M\tilde{X}^h(t)) - \mathbb{E}\phi(P_M X_m^h) &= \mathbb{E}\tilde{\phi}_M(\tilde{X}^h(t)) - \mathbb{E}\tilde{\phi}_M(\tilde{X}(t_m)) \\ &= \mathbb{E} \int_{t_m}^t \langle S_{\tau,h} A_h X_m^h, D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds \\ &\quad + \mathbb{E} \int_{t_m}^t \langle S_{\tau,h} P_h F(X_m^h), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds \\ &\quad + \mathbb{E} \int_{t_m}^t \frac{1}{2} \text{Tr}((S_{\tau,h} P_h)(S_{\tau,h} P_h)^* D^2\tilde{\phi}_M(\tilde{X}^h(s))) ds. \\ &=: E_1(t) + E_2(t) + E_3(t). \end{aligned}$$

The error is naturally divided into three terms. We first treat the easiest ones: E_2 and E_3 .

Using boundedness of the linear operator $S_{\tau,h}$, of the nonlinear coefficient F , of the orthogonal projectors P_M and P_h and of the first-order derivative of ϕ , we easily obtain that for $t_m \leq t < t_{m+1}$

$$|E_2(t)| = \left| \mathbb{E} \int_{t_m}^t \langle S_{\tau,h} P_h F(X_m^h), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds \right| \leq C\tau.$$

We now control $E_3(t)$. Using the boundedness of the second-order derivative of $\tilde{\phi}_M$, uniformly with respect to M , we have

$$\begin{aligned} |E_3(t)| &\leq C(t - t_m) \text{Tr}((S_{\tau,h} P_h)(S_{\tau,h} P_h)^*) \\ &\leq C\tau \text{Tr} [((-A_h)^{1/2+\kappa} S_{\tau,h}^2 P_h) P_h (-A_h)^{-1/2-\kappa} P_h] \\ &\leq C\tau |(-A_h)^{1/2+\kappa} S_{\tau,h}^2 P_h|_{\mathcal{L}(H)} \text{Tr}(P_h (-A_h)^{-1/2-\kappa} P_h) \\ &\leq C\tau^{1/2-\kappa}, \end{aligned}$$

where $\kappa \in (0, 1/2)$ is a small parameter, thanks to the first inequality of Lemma 3.7 and to Proposition 3.4.

The treatment of the E_1 is the most complicated amongst the three terms, due to the presence of the unbounded operator A_h . We recall that X_m^h is controlled in the norm of

$(-A_h)^\alpha$, uniformly in h , only for $\alpha < 1/4$; to obtain the correct weak order of convergence $1/2$ with respect to τ , we need a careful control. One of the ingredients is the Malliavin integration by parts.

Thanks to (3.11) and (3.12), E_1 is divided into three parts: $E_1(t) = E_{1,1}(t) + E_{1,2}(t) + E_{1,3}(t)$, with for $t_m \leq t < t_{m+1}$

$$\begin{aligned} E_{1,1}(t) &= \mathbb{E} \int_{t_m}^t \langle S_{\tau,h}^{m+1} A_h P_h x, D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds \\ E_{1,2}(t) &= \mathbb{E} \int_{t_m}^t \langle \tau A_h S_{\tau,h} \sum_{k=0}^{m-1} S_{\tau,h}^{m-k} P_h F(X_k^h), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds \\ E_{1,3}(t) &= \mathbb{E} \int_{t_m}^t \langle A_h S_{\tau,h} \int_0^{t_m} S_{\tau,h}^{m-l_r} P_h dW(r), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle ds. \end{aligned}$$

We have isolated the stochastic part in X_m^h ; then only the treatment of $E_{1,3}(t)$ is difficult.

First, using Lemma 3.7, we have if $m \geq 1$

$$\begin{aligned} |A_h S_{\tau,h}^{m+1} P_h x| &\leq |(-A_h)^\kappa S_{\tau,h} P_h|_{\mathcal{L}(H)} |(-A_h)^{1-\kappa} S_{\tau,h}^m P_h|_{\mathcal{L}(H)} |x|_H \\ &\leq C|x|_H \tau^{-\kappa} t_m^{-1+\kappa}. \end{aligned}$$

As a consequence, for $t_m \leq t < t_{m+1}$

$$|E_{1,1}(t)| \leq C|x| \frac{\tau^{1-\kappa}}{t_m^{1-\kappa}}.$$

The treatment of $E_{1,2}$ is similar: we have when $m \geq 1$

$$\begin{aligned} |\tau A_h S_{\tau,h} \sum_{k=0}^{m-1} S_{\tau,h}^{m-k} P_h F(X_k^h)| &\leq C\tau |(-A_h)^\kappa S_{\tau,h} P_h|_{\mathcal{L}(H)} \sum_{k=0}^{m-1} |(-A_h)^{1-\kappa} S_{\tau,h}^{m-k} P_h|_{\mathcal{L}(H)} |F(X_k^h)|_H \\ &\leq C\tau^{-\kappa} \tau \sum_{k=0}^{m-1} |(-A_h)^{1-\kappa} S_{\tau,h}^{m-k} P_h|_{\mathcal{L}(H)}, \end{aligned}$$

F being bounded. Now using Lemma 3.7 and inequality (7.1) we obtain for $m \geq 1$ and $t_m \leq t < t_{m+1}$

$$|E_{1,2}(t)| \leq C\tau^{-\kappa}(t - t_m) \leq C\tau^{1-\kappa}.$$

It remains to control $E_{1,3}(t)$, which contains the stochastic term, with low regularity properties. We need to use a Malliavin integration by parts formula; however due to the weak dissipativity condition the behavior of the Malliavin derivatives is bad with respect to time. The solution is to split the stochastic integral factor into two parts: for any $t_m \leq s \leq t < t_{m+1}$

$$\begin{aligned} \mathbb{E} \langle A_h S_{\tau,h} \int_0^{t_m} S_{\tau,h}^{m-l_r} dW(r), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle \\ &= \mathbb{E} \langle A_h S_{\tau,h} \int_0^{(t_m-3\tau_0) \vee 0} S_{\tau,h}^{m-l_r} P_h dW(r), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle \\ &\quad + \mathbb{E} \langle A_h S_{\tau,h} \int_{(t_m-3\tau_0) \vee 0}^{t_m} S_{\tau,h}^{m-l_r} P_h dW(r), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle \\ &=: E_{1,3,1}(s, t) + E_{1,3,2}(s, t). \end{aligned}$$

For the first error term, we directly use the Cauchy-Schwarz inequality and we have (see term $a_{1,3}^{m,h}$ of Sub-Section 7.1 for more details)

$$\begin{aligned} |E_{1,3,1}(s, t)|^2 &\leq C(E) \int_0^{(t_m-3\tau_0)\vee 0} |S_{\tau,h} A_h S_{\tau,h}^{m-l_r} P_h dW(r)|^2 (\mathbb{E} |D\tilde{\phi}_M(\tilde{X}^h(s))|^2) \\ &\leq C \int_0^{(t_m-3\tau_0)\vee 0} \text{Tr}(P_h A_h S_{\tau,h}^{(m-l_r)+1} S_{\tau,h}^{(m-l_r)+1} A_h P_h) dr \\ &\leq C \int_0^{(t_m-3\tau_0)\vee 0} \text{Tr}(P_h (-A_h)^{-1/2-\kappa} P_h) |(-A_h)^{5/2+\kappa} S_{\tau,h}^{2(m-l_r)+1} P_h|_{\mathcal{L}(H)} dr \\ &\leq C. \end{aligned}$$

For the second error term, using the Malliavin integration by parts formula, we get for any $t_m \leq s \leq t < t_{m+1}$

$$\begin{aligned} \mathbb{E} \langle A_h S_{\tau,h} \int_{(t_m-3\tau_0)\vee 0}^{t_m} S_{\tau,h}^{m-l_r} P_h dW(r), D\tilde{\phi}_M(\tilde{X}^h(s)) \rangle \\ = \mathbb{E} \int_{(t_m-3\tau_0)\vee 0}^{t_m} \text{Tr}(S_{\tau,h}^{m-l_r} A_h S_{\tau,h} P_h D^2 \tilde{\phi}_M(\tilde{X}^h(s)) \mathcal{D}_r \tilde{X}^h(s)) dr. \end{aligned}$$

We then write that

$$\begin{aligned} |\mathbb{E} \int_{(t_m-3\tau_0)\vee 0}^{t_m} \text{Tr}(S_{\tau,h}^{m-l_r} A_h S_{\tau,h} P_h D^2 \tilde{\phi}_M(\tilde{X}^h(s)) \mathcal{D}_r \tilde{X}^h(s)) dr| \\ \leq \int_{(t_m-3\tau_0)\vee 0}^{t_m} \text{Tr}((-A_h)^\kappa S_{\tau,h}^{m-l_r} S_{h,\tau} P_h) \mathbb{E}[|(-A_h)^{1-\kappa} \mathcal{D}_r \tilde{X}^h(s)|_{\mathcal{L}(H)} |D^2 \tilde{\phi}_M(\tilde{X}^h(s))|] dr. \end{aligned}$$

Since

$$\text{Tr}((-A_h)^\kappa S_{\tau,h}^{m-l_r} S_{h,\tau} P_h) \leq \text{Tr}(P_h (-A_h)^{-1/2-2\kappa} P_h) |S_{\tau,h}^{m-l_r} ((-A_h)^{1/2+2\kappa} S_{h,\tau} P_h)|_{\mathcal{L}(H)},$$

we have (see term $a_{1,3}^{m,h}$ of Sub-Section 7.1 for more details)

$$\begin{aligned} |\mathbb{E} \int_{(t_m-3\tau_0)\vee 0}^{t_m} \text{Tr}(S_{\tau,h}^{m-l_r} A_h S_{\tau,h} P_h \mathcal{D}_r \tilde{X}^h(s) D^2 \tilde{\phi}_M(\tilde{X}^h(s))) dr| \\ \leq C \tau^{-1/2-2\kappa} \int_{(t_m-3\tau_0)\vee 0}^{t_m} \frac{1}{(1+\lambda_0\tau)^{m-l_r}} (1+L_F\tau)^{m-l_r} \left(1 + \frac{1}{(1+\lambda_0\tau)^\kappa t_{m-l_r}^{1-\kappa}}\right) dr. \end{aligned}$$

Using that $(1+L_F\tau)^{m-l_r} \leq C$ for the range of r used to compute the integral, we see that

$$|E_{1,3,2}(s, t)| \leq C \tau^{-1/2-2\kappa}.$$

After integration with respect to s , we obtain

$$|E_{1,3}(t)| \leq \int_{t_m}^t (|E_{1,3,1}(s, t)| + |E_{1,3,2}(s, t)|) ds \leq C(\tau + \tau^{1/2-2\kappa}),$$

and

$$|E_1(t)| \leq C(\tau^{1/2-2\kappa} + |x| \frac{\tau^{1-\kappa}}{t_m^{1-\kappa}} + \tau^{1-\kappa}).$$

Using the bounds on E_2 and E_3 , we therefore obtain that when $m \geq 1$ and $t_m \leq t \leq t_{m+1}$

$$|\mathbb{E}\phi(P_M \tilde{X}^h(t)) - \mathbb{E}\phi(P_M X_m^h)| \leq C \tau^{1/2-2\kappa} \left(1 + \frac{|x|}{(m\tau)^{1-\kappa}}\right).$$

As a consequence, we obtain

$$\begin{aligned}
& \left| \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \left(\mathbb{E}\phi(P_M \tilde{X}^h(t)) - \mathbb{E}\phi(P_M X_m^h) \right) dt \right| \\
& \leq C\tau^{1/2-2\kappa} (1 + |x|) \frac{1}{N\tau} \int_0^{N\tau} \frac{1}{t^{1-\kappa}} dt \\
& \leq C\tau^{1/2-2\kappa} \left(1 + \frac{|x|}{(N\tau)^{1-\kappa}} \right). \tag{7.11}
\end{aligned}$$

7.3 Control of the time-discretization error:

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{\tau,m,h} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt.$$

To control this term, we will use ideas described in [5, 20] and in Sub-Section 7.1. We decompose the error into five terms:

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E} \left(\mathcal{L}^h - \mathcal{L}^{\tau,m,h} \right) \tilde{\Psi}^{(M)}(\tilde{X}^h(s)) ds = \frac{1}{N\tau} \sum_{m=1}^{N-1} (a_m + b_m + c_m + d_m + e_m),$$

where for $1 \leq m \leq N-1$

$$\begin{aligned}
a_m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (I - S_{\tau,h}) A_h X_m^h, D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt, \\
b_m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle A_h(\tilde{X}^h(t) - X_m^h), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt, \\
c_m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle (I - S_{\tau,h}) P_h F(X_m^h), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt, \\
d_m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle F^h(\tilde{X}^h(t)) - F^h(X_m^h), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt, \\
e_m &= \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}((P_h P_h^* - (S_{\tau,h} P_h)(S_{\tau,h} P_h)^*) D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))) dt. \tag{7.12}
\end{aligned}$$

The estimates are:

Lemma 7.1

$$\begin{aligned}
\frac{1}{\tau N} \sum_{m=1}^{N-1} |a_m| &\leq C(1 + |x|^3)(1 + (N\tau)^{-1})\tau^{1/2-2\kappa}, \\
\frac{1}{N\tau} \sum_{m=1}^{N-1} |b_m| &\leq C(1 + |x|^3)(1 + T^{-1})\tau^{1/2-2\kappa}, \\
\frac{1}{N\tau} \sum_{m=1}^{N-1} |c_m| &\leq C(1 + |x|^2)\tau^{1/2-\kappa}, \\
\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m| &\leq C\tau^{1/2-2\kappa}(1 + |x|^3)(1 + T^{-1+\kappa}), \\
\frac{1}{\tau N} \sum_{m=1}^{N-1} |e_m| &\leq C(1 + |x|^2)\tau^{1/2-3\kappa}.
\end{aligned}$$

7.3.1 Estimate of a_m

We have the equality of linear operators in $\mathcal{L}(V_h)$: $(I - S_{\tau,h})A_h = -\tau S_{\tau,h}A_h^2$. Then, using (3.11), we decompose the error into three terms: $a_m = a_m^1 + a_m^2 + a_m^3$, with

$$\begin{aligned} a_m^1 &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \langle S_{\tau,h} A_h^2 S_{\tau,h}^m P_h x, P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ a_m^2 &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \langle S_{\tau,h} A_h^2 \tau \sum_{l=0}^{m-1} S_{\tau,h}^{m-l} F^h(X_l^h), P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\ a_m^3 &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \langle S_{\tau,h} A_h^2 \sqrt{\tau} \sum_{l=0}^{m-1} S_{\tau,h}^{m-l} P_h \chi_{l+1}, P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt; \end{aligned}$$

The replacement of $D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \in H$ with its orthogonal projection $P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))$ is valid since the other factor in the scalar product belongs to V_h .

The main task is to control the operator A_h^2 , using the benefits of the regularization properties of the semi-group $(S_{\tau,h}^k)_{k \in \mathbb{N}}$ and of the derivatives of $\tilde{\Psi}^{(M)}$. The main difficulties appear in the control of a_m^3 , where a Malliavin integration by parts is required in order to obtain the correct weak order of convergence. The control of the other terms a_m^1 and a_m^2 is technical but much easier.

* Estimate of a_m^1

We write, for any small enough parameter $0 < \kappa < 1/2$,

$$\begin{aligned} |a_m^1| &\leq \tau \mathbb{E} \int_{t_m}^{t_{m+1}} |S_{\tau,h}(-A_h)^{1/2+2\kappa} P_h|_{\mathcal{L}(H)} |(-A_h)^{1-\kappa} S_{\tau,h}^m P_h|_{\mathcal{L}(H)} |P_h x|_{V_h} \\ &\quad \times |(-A_h)^{1/2-\kappa} P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_{V_h} dt \\ &\leq C |x|_H \tau \tau^{-1/2-2\kappa} t_m^{-1+\kappa} (1 + \lambda_0 \tau)^{-m\kappa} \int_{t_m}^{t_{m+1}} \mathbb{E} |(-A)^{1/2-\kappa} D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_H dt \\ &\leq C(1 + |x|^3) \tau \tau^{-1/2-2\kappa} t_m^{-1+\kappa} (1 + \lambda_0 \tau)^{-m\kappa}, \end{aligned}$$

thanks to Lemma 3.7, Lemma 3.10, Proposition 3.3 and Proposition 6.1.

Thanks to estimate (7.1), we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_m^1| \leq C(1 + |x|^3) \tau^{1/2-2\kappa} (N\tau)^{-1}. \quad (7.13)$$

* Estimate of a_m^2

First we write

$$\begin{aligned} |a_m^2| &\leq C\tau \mathbb{E} \int_{t_m}^{t_{m+1}} |S_{\tau,h}(-A_h)^{1/2+2\kappa}|_{\mathcal{L}(V_h)} |\tau(-A_h)^{1-\kappa} \sum_{l=0}^{m-1} S_{\tau,h}^{m-l} P_h F^h(X_l^h)| \\ &\quad \times |(-A_h)^{1/2-\kappa} P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_{V_h} dt. \quad (7.14) \end{aligned}$$

Since F is supposed to be bounded by $\|F\|_0$, the estimate (7.1) yields

$$|\tau(-A_h)^{1-\kappa} \sum_{l=0}^{m-1} S_{\tau,h}^{m-l} P_h F(X_l^h)| \leq C \|F\|_0 \tau \sum_{l=1}^m \frac{1}{(l\tau)^{1-\kappa}} \frac{1}{(1 + \lambda_0 \tau)^{l\kappa}} \leq C_\kappa.$$

With Lemma 3.10 and Proposition 6.1, we easily obtain

$$\frac{1}{N\tau} \sum_{m=0}^{N-1} |a_m^2| \leq C(1 + |x|^2)\tau^{1/2-2\kappa}. \quad (7.15)$$

* **Estimate of a_m^3**

This is where things become harder. The problem is the same than for estimate $a_{1,3}^{m,h}$ in Sub-Section 7.1. As for $a_{1,3}^{m,h}$, using (3.12), we decompose $a_m^3 = a_m^{3,1} + a_m^{3,2}$, with

$$\begin{aligned} a_m^{3,1} &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h} A_h^2 S_{\tau,h}^{m-l_s} P_h dW(s), P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt, \\ a_m^{3,2} &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{(t_m-5\tau_0) \vee 0}^{t_m} S_{\tau,h} A_h^2 S_{\tau,h}^{m-l_s} P_h dW(s), P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt. \end{aligned}$$

We remark that $a_m^{3,1} = 0$ if $t_m < 5\tau_0$. Thanks to the Cauchy-Schwarz inequality, to Proposition 6.1 (for $\beta = 0$) and Lemma 3.10, we get

$$\begin{aligned} &|\mathbb{E} \langle \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h} A_h^2 S_{\tau,h}^{m-l_s} P_h dW(s), P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle| \\ &\leq (\mathbb{E} |\int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h} A_h^2 S_{\tau,h}^{m-l_s} P_h dW(s)|_H^2)^{1/2} (\mathbb{E} |P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_H^2)^{1/2} \\ &\leq C(1 + |x|^2); \end{aligned}$$

indeed we have the following inequality for $0 < \tau \leq \tau_0$:

$$\mathbb{E} |\int_0^{(t_m-5\tau_0) \vee 0} R_\tau A_h^2 S_{\tau,h}^{m-l_s+1} P_h dW(s)|^2 \leq C.$$

The proof is easily adapted from the corresponding one in the estimate of $a_{1,3}^{m,h}$ in Sub-Section 7.1.

Then

$$\frac{1}{N\tau} \sum_{m=0}^{N-1} |a_m^{3,1}| \leq C(1 + |x|^2)\tau.$$

For $a_m^{3,2}$, we use the integration by parts formula of Lemma 6.3 to get

$$\begin{aligned} a_m^{3,2} &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{(t_m-5\tau_0) \vee 0}^{t_m} S_{\tau,h} A_h^2 S_{\tau,h}^{m-l_s} P_h dW(s), P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &= -\tau \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{(t_m-5\tau_0) \vee 0}^{t_m} \text{Tr} \left(S_{\tau,h}^{m-l_s} A_h^2 S_{\tau,h} P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \mathcal{D}_s \tilde{X}^h(t) \right) ds dt. \end{aligned}$$

Thanks to both estimates of Lemma 6.5, we have for $(t_m - 5\tau_0) \vee 0 \leq s \leq t_m \leq t < t_{m+1}$

$$|(-A_h)^\beta \mathcal{D}_s \tilde{X}^h(t)| \leq C(1 + L_F \tau)^{m-l_s} \left(1 + \frac{1}{(1 + \lambda_0 \tau)^{(1-\beta)(m-l_s)} t_{m-l_s}^\beta} \right),$$

and we see that $(1 + L_F \tau)^{m-l_s}$ is bounded by a constant.

We have

$$\begin{aligned}
& |a_m^{3,2}| \\
& \leq \tau \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{(t_m-5\tau_0) \vee 0}^{t_m} |S_{\tau,h}(-A_h)^{1/2+2\kappa}|_{\mathcal{L}(V_h)} |(-A_h)^{1-3\frac{\kappa}{2}} S_{\tau,h}^{m-l_s}|_{\mathcal{L}(V_h)} \text{Tr}((-A)^{-1/2-\frac{\kappa}{2}}) \\
& \quad \times |(-A_h)^{1/2-\kappa/2} P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa/2}|_{\mathcal{L}(H)} |(-A)^\kappa \mathcal{D}_s \tilde{X}^h(t)|_{\mathcal{L}(H)} ds dt \\
& \leq C \int_{t_m}^{t_{m+1}} \int_{(t_m-5\tau_0) \vee 0}^{t_m} t_{m-l_s}^{-1+3\frac{\kappa}{2}} \frac{1}{(1+\lambda_0\tau)^{(m-l_s)3\frac{\kappa}{2}}} \left(1 + t_{m-l_s}^{-\kappa} \frac{1}{(1+\lambda_0\tau)^{(m-l_s)(1-\kappa)}}\right) ds dt \\
& \quad \times \tau^{1/2-2\kappa} (1+|x|^2) \\
& \leq C \tau \tau^{1/2-2\kappa} (1+|x|^2),
\end{aligned}$$

by estimate (7.1), Assumption 2.2, Propositions 6.1 and 3.3, Lemmas 6.5 and 3.7.

We obtain

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_m^{3,2}| \leq C(1+|x|^2)\tau^{1/2-2\kappa}.$$

Therefore

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_m^3| \leq C(1+|x|^2)\tau^{1/2-2\kappa}. \quad (7.16)$$

With the previous estimates on a^1 , a^2 and a^3 , we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |a_m| \leq C(1+|x|^3)(1+T^{-1})\tau^{1/2-2\kappa}. \quad (7.17)$$

7.3.2 Estimate of b_m

We decompose the corresponding term into three parts: $b_m = b_m^1 + b_m^2 + b_m^3$, with

$$\begin{aligned}
b_m^1 &= \mathbb{E} \int_{t_m}^{t_{m+1}} (t-t_m) \langle A_h(I-S_{\tau,h})X_m^h, P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\
b_m^2 &= \mathbb{E} \int_{t_m}^{t_{m+1}} (t-t_m) \langle A_h S_{\tau,h} F(X_m^h), P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle dt \\
b_m^3 &= \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{t_m}^t A_h S_{\tau,h} P_h dW(s), P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt;
\end{aligned}$$

* **Estimate of b_m^1**

b_m^1 is bounded by the same expression as a_m : by (7.17) we have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |b_m^1| \leq C(1+|y|^3)(1+T^{-1})\tau^{1/2-2\kappa}. \quad (7.18)$$

* **Estimate of b_m^2**

We have

$$\begin{aligned}
|b_m^2| &\leq \tau \mathbb{E} \int_{t_m}^{t_{m+1}} |(-A_h)^{1/2+\kappa} S_{\tau,h} P_h|_{\mathcal{L}(H)} |P_h F(X_m^h)| |(-A_h)^{1/2-\kappa} P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))| dt \\
&\leq \|F\|_0 \tau^{1/2-\kappa} \tau (1+|x|^2).
\end{aligned}$$

We then have

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |b_m^2| \leq C\tau^{1/2-\kappa}(1 + |x|^2). \quad (7.19)$$

* **Estimate of b_m^3**

We again use the integration by parts formula to rewrite b_m^3 :

$$\begin{aligned} b_m^3 &= \mathbb{E} \int_{t_m}^{t_{m+1}} \left\langle \int_{t_m}^t A_h S_{\tau,h} P_h dW(s), P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right\rangle dt \\ &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \text{Tr}(S_{\tau,h} A_h P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \mathcal{D}_s \tilde{X}^h(t)) ds dt. \end{aligned}$$

From (3.13), for $t_m \leq s \leq t \leq t_{m+1}$ we have $\mathcal{D}_s^{\ell} \tilde{X}^h(t) = S_{\tau,h} P_h \ell$; as a consequence, the situation is much simpler and we do not need to use the same trick as in the control of a_m^3 .

Then we have

$$\begin{aligned} |b_m^3| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \text{Tr}(S_{\tau,h} A_h P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) S_{\tau,h} P_h) dt \\ &\leq C\tau \int_{t_m}^{t_{m+1}} |S_{\tau,h} (-A_h)^{1/2+\kappa/2} P_h|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa/2}) |(-A)^{\kappa} S_{\tau,h} P_h|_{\mathcal{L}(H)} \\ &\quad |(-A_h)^{1/2-\kappa/2} P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa/2}|_{\mathcal{L}(H)} dt \\ &\leq C(1 + |x|^2) \tau^{1/2-3\kappa/2}. \end{aligned}$$

Therefore

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |b_m^3| \leq C(1 + |x|^2) \tau^{1/2-3\kappa/2}. \quad (7.20)$$

With the previous estimates, we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |b_m| \leq C(1 + |x|^3)(1 + T^{-1}) \tau^{1/2-2\kappa}. \quad (7.21)$$

7.3.3 Estimate of c_m

This term is easy to treat: we have

$$\begin{aligned} |c_m| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} |(-A_h)^{-1/2+\kappa} (I - S_{\tau,h})|_{\mathcal{L}(V_h)} |P_h F(X_m^h)| |(-A_h)^{1/2-\kappa} P_h D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))| dt \\ &\leq C\tau^{1/2-\kappa} \tau (1 + |x|^2), \end{aligned}$$

where we have used Proposition 6.1, Assumption 2.7 and Lemma 3.7. Then we see that

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |c_m| \leq C\tau^{1/2-\kappa}(1 + |x|^2). \quad (7.22)$$

7.3.4 Estimate of d_m

The term d_m contains the error between $F^h(\tilde{X}^h(t))$ and $F^h(X_m^h)$; we recall that $F^h = P_h \circ F$. We perform an expansion with respect to an orthonormal basis $(e_i^h)_{i \in \mathbb{N}}$ of H , such that $(e_i^h)_{i=0}^{N_h-1}$ is the orthonormal basis of V_h introduced in Proposition 3.2 - the vectors e_i^h for $i \geq N_h$ do not matter.

In this orthonormal system, the cylindrical Wiener process is expanded as

$$W(t) = \sum_{i \in \mathbb{N}} \beta_i^h(t) e_i^h, \quad (7.23)$$

with a family $(\beta_i^h)_{i \in \mathbb{N}}$ of independent standard one-dimensional Wiener processes.

Let $F_i^h : H \rightarrow \mathbb{R}$ denote the function such that $F_i^h(x) = \langle F^h(x), e_i^h \rangle$. We also denote, for any $i \in \mathbb{N}$, by ∂_i^h the operator such that $\partial_i^h \phi(x) = \langle D\phi(x), e_i^h \rangle \in \mathbb{R}$, for any $x \in H$, where $\phi : H \rightarrow \mathbb{R}$ is of class \mathcal{C}^1 . Then

$$\langle F^h(\tilde{X}^h(t)) - F^h(X_m^h), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle = \sum_{i=0}^{N_h-1} (F_i^h(\tilde{X}^h(t)) - F_i^h(X_m^h)) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)).$$

The Itô formula gives for $t_m \leq t < t_{m+1}$ and $0 \leq i \leq N_h - 1$

$$\begin{aligned} F_i^h(\tilde{X}^h(t)) - F_i^h(X_m^h) &= \frac{1}{2} \int_{t_m}^t \text{Tr}(S_{\tau,h} S_{\tau,h}^* P_h D^2 F_i^h(\tilde{X}^h(s))) ds \\ &\quad + \int_{t_m}^t \langle A_h S_{\tau,h} X_m^h, D F_i^h(\tilde{X}^h(s)) \rangle ds \\ &\quad + \int_{t_m}^t \langle S_{\tau,h} F^h(X_m^h), D F_i^h(\tilde{X}^h(s)) \rangle ds \\ &\quad + \int_{t_m}^t \langle D F_i^h(\tilde{X}^h(s)), S_{\tau,h} P_h dW(s) \rangle. \end{aligned}$$

Thanks to this, d_m^j for $j \in \{1, 2, 3, 4\}$ are naturally defined, and we now control each term.

* Estimate of d_m^1

By definition, we have

$$d_m^1 = \int_{t_m}^{t_{m+1}} \mathbb{E} \frac{1}{2} \int_{t_m}^t \sum_{i=0}^{N_h-1} \text{Tr}(S_{\tau,h} S_{\tau,h}^* P_h D^2 F_i^h(\tilde{X}^h(s))) ds \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt.$$

Expanding the trace thanks to the complete orthonormal system $(e_i^h)_{i \in \mathbb{N}}$,

$$\begin{aligned} &\sum_{i=0}^{N_h-1} \text{Tr}(P_h S_{\tau,h}^* P_h D^2 F_i^h(\tilde{X}^h(s)) S_{\tau,h} P_h) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \\ &= \sum_{i=0}^{N_h-1} \sum_{j=0}^{N_h-1} \langle D^2 F_i^h(\tilde{X}^h(s)) \frac{1}{(1 + \lambda_j^h \tau)^2} e_j^h, e_j^h \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \\ &= \sum_{i=0}^{N_h-1} \sum_{j=0}^{N_h-1} \frac{1}{(1 + \lambda_j^h \tau)^2} D^2 F_i^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)). \end{aligned}$$

For any fixed $0 \leq j \leq N_h - 1$, the Cauchy-Schwarz inequality yields

$$\begin{aligned} & \left| \sum_{i=0}^{N_h-1} D^2 F_i^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right| \\ & \leq \left(\sum_{i=0}^{N_h-1} \frac{|D^2 F_i^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)|^2}{(\lambda_i^h)^{2\eta}} \right)^{1/2} \left(\sum_{i=0}^{N_h-1} (\lambda_i^h)^{2\eta} |\partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|^2 \right)^{1/2}, \end{aligned}$$

where $\eta \leq 1/2$ is defined in Assumption 2.7.

The second factor is bounded from above by

$$|(-A_h)^\eta P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))| \leq C |(-A)^\eta D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|,$$

thanks to Proposition 3.3; the right-hand side is then controlled thanks to Proposition 6.1.

To control the first factor, thanks to Assumption 2.7 we get

$$\begin{aligned} \left(\sum_{i=0}^{N_h-1} \frac{|D^2 F_i^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)|^2}{(\lambda_i^h)^{2\eta}} \right)^{1/2} &= |(-A_h)^{-\eta} P_h D^2 F(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)| \\ &\leq C |(-A)^{-\eta} D^2 F(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)| \\ &\leq C |e_j^h|_H |e_j^h|_H \leq C, \end{aligned}$$

since $(e_j^h)_j$ is an orthonormal system, and using Proposition 3.3.

Therefore we obtain

$$\begin{aligned} & \left| \sum_{i=0}^{N_h-1} \text{Tr}(S_{\tau,h} S_{\tau,h}^* P_h D^2 F_i^h(\tilde{X}^h(s))) \partial_i^h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right| \\ & \leq C(1 + |x|^2) \sum_{j=0}^{N_h-1} \frac{1}{(1 + \lambda_j^h \tau)^2} \\ & \leq C(1 + |x|^2) \tau^{-1/2-\kappa} \sum_{j=0}^{N_h-1} \frac{(\lambda_j^h \tau)^{1/2+\kappa}}{(1 + \lambda_j^h \tau)^2} \frac{1}{(\lambda_j^h)^{1/2+\kappa}} \\ & \leq C(1 + |x|^2) \tau^{-1/2-\kappa} \text{Tr}(P_h (-A_h)^{-1/2-\kappa} P_h). \end{aligned}$$

Then thanks to Proposition 3.4, we have

$$|d_m^1| \leq C(1 + |x|^2) \tau^{1/2-\kappa} \tau,$$

and

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m^1| \leq C(1 + |x|^2) \tau^{1/2-\kappa}. \quad (7.24)$$

* **Estimate of d_m^2**

Thanks to (3.11) and (3.12), we have

$$\begin{aligned}
d_m^2 &= \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle A_h S_{\tau,h} X_m^h, DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \langle A_h S_{\tau,h}^{m+1} P_h x + \tau \sum_{l=0}^{m-1} A_h S_{\tau,h}^{m-l+1} F^h(X_l^m), DF_i^h(\tilde{X}^h(s)) \rangle \\
&\quad \times \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \langle A_h \int_0^{t_m} S_{\tau,h}^{m-l_r+1} P_h dW(r), DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&:= d_m^{2,1} + d_m^{2,2}.
\end{aligned}$$

(i) For the first term, since F and DF are bounded on H and $\tau \leq \tau_0$, we have, using (7.1),

$$\begin{aligned}
&|d_m^{2,1}| \\
&= |\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \langle DF^h(\tilde{X}^h(s)) \cdot (A_h S_{\tau,h}^{m+1} P_h x + A_h \tau \sum_{l=0}^{m-1} S_{\tau,h}^{m-l+1} F^h(X_l^h)), D\Psi^{(M)}(\tilde{X}^h(t)) \rangle ds dt| \\
&\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t |(-A_h)^\kappa S_{\tau,h} P_h|_{\mathcal{L}(H)} \left(|(-A_h)^{1-\kappa} S_{\tau,h}^m P_h x| \right. \\
&\quad \left. + \tau \sum_{l=0}^{m-1} |(-A_h)^{1-\kappa} S_{\tau,h}^{m-l} P_h|_{\mathcal{L}(H)} |P_h F(X_l^h)| \right) |D\Psi^{(M)}(\tilde{X}^h(t))| ds dt \\
&\leq C \tau^{1-\kappa} \tau (1 + |x|^2) \left(t_m^{-1+\kappa} |x| + \tau \sum_{l=0}^{m-1} t_{m-l}^{-(1-\kappa)} \frac{1}{(1 + \lambda_0 \tau)^{(m-l)\kappa}} \right) \\
&\leq C \tau^{1-\kappa} (1 + |x|^3) \tau \left(\frac{1}{t_m^{1-\kappa}} + 1 \right).
\end{aligned}$$

Therefore

$$\begin{aligned}
\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m^{2,1}| &\leq C \tau^{1-\kappa} (|x|^3 + 1) \frac{\tau}{T} \sum_{m=1}^{N-1} \left(\frac{1}{t_m^{1-\kappa}} + 1 \right) \\
&\leq C \tau^{1-\kappa} (1 + |x|^3) \left(\frac{1}{T} \int_0^T \frac{1}{t^{1-\kappa}} dt + 1 \right) \\
&\leq C \tau^{1-\kappa} (1 + |x|^3) \left(1 + T^{-1+\kappa} \int_0^1 \frac{1}{s^{1-\kappa}} ds \right) \\
&\leq C \tau^{1-\kappa} (1 + |x|^3) (1 + T^{-1+\kappa}). \tag{7.25}
\end{aligned}$$

(ii) For the second term, we again use an integration by parts, after a decomposition of

the time interval - as in the estimates for a_m^3 . First,

$$\begin{aligned}
d_m^{2,2} &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle A_h \int_0^{t_m} S_{\tau,h}^{m-l_r+1} P_h dW(r), DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle A_h \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r+1} P_h dW(r), DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&+ \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i,j,m=0}^{N_h-1} \langle A_h \int_{(t_m-5\tau_0) \vee 0}^{t_m} S_{\tau,h}^{m-l_r+1} e_m^h, e_j^h \rangle d\beta_m^h(r) \partial_j^h F_i^h(\tilde{Y}(s)) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&=: d_m^{2,2,1} + d_m^{2,2,2}.
\end{aligned}$$

Recall that $(e_i^h)_{0 \leq i \leq N_h-1}$ is the orthonormal basis of V_h introduced in Proposition 3.2. See also (7.23). For $d_m^{2,2,1}$, we can work directly as for the similar part in a_m^3 and we see that

$$\begin{aligned}
&|d_m^{2,2,1}| \\
&\leq |\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle A_h \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r+1} P_h dW(r), DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt| \\
&\leq \int_{t_m}^{t_{m+1}} \int_{t_m}^t \mathbb{E} |\langle DF^h(\tilde{X}^h(s)) \cdot A_h S_{\tau,h} \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r} P_h dW(r), D\tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \rangle| ds dt \\
&\leq \int_{t_m}^{t_{m+1}} \int_{t_m}^t (\mathbb{E} |A_h S_{\tau,h} \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r} P_h dW(r)|^2)^{1/2} (\mathbb{E} |D\tilde{\Psi}^{(M)}(\tilde{X}^h(t))|^2)^{1/2} ds dt \\
&\leq C\tau^2(1 + |x|^2),
\end{aligned}$$

thanks to Lemmas 3.10, Proposition 6.1 and to the estimate proved in the control of a_m^3 :

$$\mathbb{E} |A_h S_{\tau,h} \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r} P_h dW(r)|^2 \leq \mathbb{E} |A_h^2 S_{\tau,h} \int_0^{(t_m-5\tau_0) \vee 0} S_{\tau,h}^{m-l_r} P_h dW(r)|^2 \leq C.$$

For $d_m^{2,2,2}$, we can write thanks to the Malliavin integration by parts (6.4) and with the

chain rule

$$\begin{aligned}
& d_m^{2,2,2} \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i,j,m=0}^{N_h-1} \langle A_h \int_{(t_m-5\tau_0) \vee 0}^{t_m} S_{\tau,h}^{m-l_r+1} e_m^h, e_j^h \rangle d\beta_m^h(r) \partial_j^h F_i^h(\tilde{Y}(s)) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i,j,m,n=0}^{N_h-1} \langle A_h S_{\tau,h}^{m-l_r+1} e_m^h, e_j^h \rangle \partial_j^h \partial_n^h F_i^h(\tilde{X}^h(s)) \langle \mathcal{D}_r^{e_m^h} \tilde{X}^h(s), e_n^h \rangle \\
&\quad \times \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dr ds dt \\
&\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i,j,m,n=0}^{N_h-1} \langle A_h S_{\tau,h}^{m-l_r+1} e_m^h, e_j^h \rangle \partial_j^h F_i^h(\tilde{X}^h(s)) \partial_n^h \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \\
&\quad \times \langle \mathcal{D}_r^{e_m^h} \tilde{X}^h(t), e_n^h \rangle dr ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i,m=0}^{N_h-1} D^2 F_i^h(\tilde{X}^h(s)) (A_h S_{\tau,h}^{m-l_r+1} e_m^h, \mathcal{D}_r^{e_m^h} \tilde{X}^h(s)) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dr ds dt \\
&\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i,m=0}^{N_h-1} \langle \mathcal{B}_i(s,t) A_h S_{\tau,h}^{m-l_r+1} e_m^h, \mathcal{D}_r^{e_m^h} \tilde{X}^h(t) \rangle dr ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i=0}^{N_h-1} \text{Tr} \left(P_h (\mathcal{D}_r \tilde{X}^h(s))^* D^2 F_i^h(\tilde{X}^h(s)) A_h S_{\tau,h}^{m-l_r+1} P_h \right) \\
&\quad \times \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dr ds dt \\
&\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} \sum_{i=0}^{N_h-1} \text{Tr} \left(P_h (\mathcal{D}_r \tilde{X}^h(t))^* \mathcal{B}_i(s,t) A_h S_{\tau,h}^{m-l_r+1} P_h \right) dr ds dt,
\end{aligned}$$

where we define, for each $0 \leq i \leq N_h - 1$, a linear operator on V_h by

$$\begin{aligned}
\langle \mathcal{B}_i(s,t) x_h, y_h \rangle &= \langle DF_i^h(\tilde{X}^h(s)), x_h \rangle \sum_{n=0}^{N_h-1} \partial_n^h \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \langle y_h, e_n^h \rangle \\
&= \langle DF_i^h(\tilde{X}^h(s)), x_h \rangle \langle D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \cdot e_i^h, y_h \rangle.
\end{aligned}$$

We have, for any $x_h, y_h \in V_h$,

$$\sum_{i=0}^{N_h-1} \langle \mathcal{B}_i(s,t) x_h, y_h \rangle = D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \cdot (DF^h(\tilde{X}^h(s)) \cdot x_h, y_h)$$

and, using Proposition 6.1 and Assumption 2.7,

$$\left| \sum_{i=0}^{N_h-1} \mathcal{B}_i(s,t) \right|_{\mathcal{L}(V_h)} \leq |DF(\tilde{X}^h(s))|_{\mathcal{L}(H)} |D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_{\mathcal{L}(H)};$$

so we can write, for $(t_m - 5\tau_0) \vee 0 \leq r \leq t_m$

$$\begin{aligned} & \left| \sum_{i=0}^{N_h-1} \text{Tr} \left(P_h(\mathcal{D}_r \tilde{X}^h(t))^* \mathcal{B}_i(s, t) A_h S_{\tau, h}^{m-l_r+1} P_h \right) \right| \\ & \leq |\mathcal{D}_r \tilde{X}^h(t)|_{\mathcal{L}(V_h)} \left| \sum_{i=0}^{N_h-1} \mathcal{B}_i(s, t) \right|_{\mathcal{L}(V_h)} |(-A_h)^{1-3\kappa/2} S_{\tau, h}^{m-l_r} P_h|_{\mathcal{L}(H)} |S_{\tau, h}(-A_h)^{1/2+2\kappa} P_h|_{\mathcal{L}(H)} \\ & \quad \times \text{Tr}(P_h(-A_h)^{-1/2-\kappa/2} P_h) \\ & \leq C \tau^{-1/2-2\kappa} t_{m-l_r}^{-1+3\kappa/2} \frac{1}{(1 + \lambda_0 \tau)^{(m-l_r)3\kappa/2}}, \end{aligned}$$

using Lemma 6.5 - since $(1 + L_F \tau)^{m-l_r} \leq C$ - and Lemma 3.7.

For the other term, we have to deal with the poor regularity of F at second order. We proceed as in the control of d_m^1 , and expand the trace with respect to the orthonormal basis $(e_i^h)_{i \in \mathbb{N}}$ of H .

$$\begin{aligned} & \left| \sum_{i=0}^{N_h-1} \text{Tr} \left(P_h(\mathcal{D}_r \tilde{X}^h(s))^* D^2 F_i^h(\tilde{X}^h(s)) A_h S_{\tau, h}^{m-l_r+1} P_h \right) \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) \right| \\ & \leq |\mathcal{D}_r \tilde{X}^h(s)|_{\mathcal{L}(V_h)} \sum_{i, j=0}^{N_h-1} \frac{|D^2 F_i^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)|}{(\lambda_i^h)^\eta} \frac{\lambda_j^h}{(1 + \lambda_j^h \tau)^{1+m-l_r}} (\lambda_i^h)^\eta |\partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t))| \\ & \leq |\mathcal{D}_r \tilde{X}^h(s)|_{\mathcal{L}(V_h)} |(-A_h)^\eta P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_H \sum_{j=0}^{N_h-1} |(-A_h)^{-\eta} D^2 F^h(\tilde{X}^h(s)) \cdot (e_j^h, e_j^h)| \\ & \quad \times \frac{\lambda_j^h}{(1 + \lambda_j^h \tau)^{1+m-l_r}}, \end{aligned}$$

thanks to the Cauchy-Schwarz inequality.

By using the same analysis as in the estimation of d_m^1 , we see that the above expression is bounded by

$$C |\mathcal{D}_r \tilde{X}^h(s)|_{\mathcal{L}(V_h)} |(-A_h)^\eta P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_H \sum_{j=0}^{N_h-1} \frac{\lambda_j^h}{(1 + \lambda_j^h \tau)^{1+m-l_r}};$$

but the last sum is equal to $\text{Tr}(P_h A_h S_{\tau, h}^{m-l_r+1})$, so that we see that indeed the two expressions in $d_m^{2,2}$ are bounded by the same expression.

Therefore

$$\begin{aligned} |d_m^{2,2,2}| & \leq \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_{(t_m-5\tau_0) \vee 0}^{t_m} C \tau^{-1/2-2\kappa} t_{m-l_r}^{-1+3\kappa/2} \frac{1}{(1 + \lambda_0 \tau)^{(m-l_r)3\kappa/2}} (1 + |x|^2) dr ds dt \\ & \leq C (1 + |x|^2) \tau^{1/2-2\kappa} \int_0^{t_m} t_{m-l_r}^{-1+3\kappa/2} \frac{1}{(1 + \lambda_0 \tau)^{(m-l_r)3\kappa/2}} dr \\ & \leq C (1 + |x|^2) \tau^{1/2-2\kappa}, \end{aligned}$$

as already proved - see (7.1).

Now gathering estimates for $d_m^{2,2,1}$ and $d_m^{2,2,2}$, we obtain

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m^{2,2}| \leq C (1 + |x|^2) \tau^{1/2-2\kappa}. \quad (7.26)$$

* **Estimate of d_m^3** We have

$$\begin{aligned} d_m^3 &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle S_{\tau,h} F^h(X_m^h), DF_i^h(\tilde{X}^h(s)) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) ds dt \\ &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \langle P_h D \tilde{\Psi}^{(M)}(\tilde{X}^h(t)), DF^h(\tilde{X}^h(s)) \cdot (S_{\tau,h} F^h(X_m^h)) \rangle ds dt. \end{aligned}$$

We have assumed F and DF to be bounded, so we easily get

$$|d_m^3| \leq C(1 + |x|^2) \tau^2$$

and

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m^3| \leq C(1 + |x|^2) \tau. \quad (7.27)$$

* **Estimate of d_m^4**

Finally, thanks to the integration by parts formula of Proposition 6.3, we have

$$\begin{aligned} d_m^4 &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_{i=0}^{N_h-1} \langle DF_i^h(\tilde{X}^h(s)), S_{\tau,h} P_h dW(s) \rangle \partial_i^h \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt \\ &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \text{Tr} \left((\mathcal{D}_s \tilde{X}^h(t))^* P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) DF^h(\tilde{X}^h(s)) S_{\tau,h} P_h \right) ds dt \\ &= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \text{Tr} \left(S_{\tau,h} P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) DF^h(\tilde{X}^h(s)) S_{\tau,h} \right) ds dt; \end{aligned}$$

indeed, we have $\mathcal{D}_s^\ell \tilde{X}^h(t) = S_{\tau,h} P_h \ell$ for all $\ell \in V_h$, when $t_m \leq s \leq t \leq t_{m+1}$ - see also the control of b_m^3 . Now,

$$\begin{aligned} |d_m^4| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t |(S_{\tau,h}(-A_h))^{1/2+\kappa}|_{\mathcal{L}(V_h)} |DF(\tilde{X}^h(s))|_{\mathcal{L}(H)} |S_{\tau,h}|_{\mathcal{L}(V_h)} \\ &\quad \times |D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))|_{\mathcal{L}(H)} \text{Tr}(P_h(-A_h)^{-1/2-\kappa} P_h) ds dt \\ &\leq C(1 + |x|^2) \tau^{1/2-\kappa}, \end{aligned}$$

and

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m^4| \leq C(1 + |x|^2) \tau^{1/2-\kappa}. \quad (7.28)$$

* **Estimate of d_m : conclusion** With (7.24), (7.25), (7.26), (7.27) and (7.28), we get

$$\frac{1}{N\tau} \sum_{m=1}^{N-1} |d_m| \leq C \tau^{1/2-2\kappa} (1 + |x|^3) (1 + T^{-1+\kappa}). \quad (7.29)$$

7.3.5 Estimate of e_m

Using the symmetry of the operators $P_h \in \mathcal{L}(H)$ and $S_{\tau,h} \in \mathcal{L}(V_h)$, the commutativity of P_h and $S_{\tau,h}$ and the fact that P_h is a projector, we have in $\mathcal{L}(H)$

$$P_h P_h^* - (S_{\tau,h} P_h)(S_{\tau,h} P_h)^* = 2P_h S_{\tau,h} P_h (I - S_{\tau,h}) P_h + P_h (I - S_{\tau,h}) P_h (I - S_{\tau,h}) P_h;$$

we then decompose e_m into two parts: $e_m = e_m^1 + e_m^2$, with

$$\begin{aligned} e_m^1 &:= \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}(P_h S_{\tau,h} P_h (I - S_{\tau,h}) P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))); \\ e_m^2 &:= \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}(P_h (I - S_{\tau,h}) P_h (I - S_{\tau,h}) P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))). \end{aligned}$$

* **Estimate of e_m^1**

$$\begin{aligned} &|e_m^1| \\ &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} |\text{Tr}((-A)^{-1/2-\kappa} (-A)^{2\kappa} P_h S_{\tau,h} P_h (I - S_{\tau,h}) P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa})| ds \\ &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}((-A)^{-1/2-\kappa}) |(-A)^{2\kappa} P_h S_{\tau,h} P_h (I - S_{\tau,h}) (-A_h)^{-1/2+\kappa}|_{\mathcal{L}(H)} \\ &\quad \times |(-A_h)^{1/2-\kappa} P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa}|_{\mathcal{L}(H)} ds \\ &\leq C(1 + |x|^2) \tau |(-A_h)^{2\kappa} S_{\tau,h} P_h (I - S_{\tau,h}) (-A_h)^{-1/2+\kappa}|_{\mathcal{L}(V_h)} \\ &\leq C(1 + |x|^2) \tau \tau^{-2\kappa} \tau^{1/2-\kappa} = C\tau^{1+1/2-3\kappa}. \end{aligned}$$

* **Estimate of e_m^2**

$$\begin{aligned} |e_m^2| &= \left| \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}(P_h (I - S_{\tau,h}) P_h (I - S_{\tau,h}) P_h D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t))) \right| \\ &\leq \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} |\text{Tr}((-A)^{-1/2-\kappa} (-A)^{2\kappa} P_h (I - S_{\tau,h}) P_h (I - S_{\tau,h}) \\ &\quad \times P_h (-A_h)^{-1/2+\kappa} (-A_h)^{1/2-\kappa} D^2 \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) (-A)^{1/2-\kappa})| ds \\ &\leq C(1 + |x|^2) \tau \text{Tr}((-A)^{-1/2-\kappa}) |(-A)^{2\kappa} P_h (I - S_{\tau,h}) P_h (I - S_{\tau,h}) P_h (-A_h)^{-1/2+\kappa}|_{\mathcal{L}(H)} \\ &\leq C(1 + |x|^2) \tau |(-A_h)^{2\kappa} (I - S_{\tau,h}) P_h (I - S_{\tau,h}) (-A_h)^{-1/2+\kappa}|_{\mathcal{L}(H)} \\ &\leq C(1 + |x|^2) \tau \tau^{-2\kappa} \tau^{1/2-\kappa} = C\tau^{1+1/2-3\kappa}. \end{aligned}$$

* **Estimate of e_m : conclusion**

We thus have

$$\frac{1}{\tau N} \sum_{m=1}^{N-1} |e_m| \leq C(1 + |x|^2) \tau^{1/2-3\kappa}. \quad (7.30)$$

7.3.6 Conclusion

With the above estimations, we get

$$\left| \frac{1}{N\tau} \sum_{m=1}^{N-1} \int_{t_m}^{t_{m+1}} \mathbb{E}(\mathcal{L}^h - \mathcal{L}^{\tau,m,h}) \tilde{\Psi}^{(M)}(\tilde{X}^h(t)) dt \right| \leq C(1 + |x|^3) \tau^{1/2-\kappa} (1 + T^{-1+\kappa} + T^{-1}). \quad (7.31)$$

7.4 Conclusion

With (7.31), (7.10) and (7.11), we get

$$\frac{1}{N} \sum_{m=0}^{N-1} \left(\mathbb{E}(\phi(X_m^h)) - \bar{\phi} \right) \leq C(1 + |x|^3) \tau^{1/2-\kappa} (1 + T^{-1+\kappa} + T^{-1})(1 + h^{1-\kappa}),$$

where C does not depend of T , h , τ and M .

8 Appendix

8.1 Study of the (finite-dimensional) Poisson equation

This Section is devoted to the proof of Proposition 6.1.

Let $\phi \in \mathcal{C}_b^2$. For lighter notation, we will assume in this appendix that $\bar{\phi} = 0$. We define the function u for any $t > 0$ and $x \in H$ by

$$u(t, x) = \mathbb{E}[\phi(X(t, x))], \quad (8.1)$$

which is solution of a finite dimensional Kolmogorov equation associated with the Galerkin finite dimensional approximation of (1.1):

$$\frac{du}{dt}(t, x) = Lu(t, x) = \frac{1}{2} \text{Tr}(D^2u(t, x)) + \langle Ax + F(x), Du(t, x) \rangle.$$

Since ϕ is of class \mathcal{C}^2 , bounded and with bounded derivatives, we are able to prove that with respect to x the function u is twice differentiable. Then, using the Itô formula, we can show that Ψ is solution of (6.1).

To prove Proposition 6.1, we only need to show that $u \in \mathcal{C}^2$ and that u and its two first derivatives have estimates which are integrable with respect to t . In fact, we will show the result below:

Proposition 8.1 *Let $\phi \in \mathcal{C}_b^2$ such that $\bar{\phi} = 0$ and u defined by (8.1). There exist constants C , c and $\tilde{\mu} > 0$ such that for any $0 \leq \beta, \gamma < 1/2$ there exist constants C_β and $C_{\beta, \gamma}$ such that for any $t > 0$ and $y \in H$*

$$|u(t, x)| \leq C(1 + |x|^2) \|\phi\|_0 \quad (8.2)$$

$$|Du(t, x)|_\beta \leq C_\beta(1 + \frac{1}{t^\beta})e^{-\tilde{\mu}t}(1 + |x|^2) \|\phi\|_{0,1}. \quad (8.3)$$

and

$$|(-A)^\beta D^2u(t, x)(-A)^\gamma|_{\mathcal{L}(H)} \leq C_{\beta, \gamma}(1 + \frac{1}{t^\eta} + \frac{1}{t^{\beta+\gamma}})e^{-\tilde{\mu}t}(1 + |x|^2) \|\phi\|_{0,2}, \quad (8.4)$$

where $\eta < 1$ is defined in the Assumption 2.7

Remark 8.2 *In fact the estimation (8.3), is true for $\beta < 1$.*

The proof of this result is similar to the proof done in [5].

Remark 8.3 *Since ϕ is of class \mathcal{C}^2 , bounded and with bounded derivatives, we are able to prove that with respect to y the function u is twice differentiable, and that the derivatives can be calculated in the following way:*

- For any $h \in H$, we have

$$Du(t, x).h = \mathbb{E}[D\phi(X(t, x)).\eta^{h,x}(t)], \quad (8.5)$$

where $\eta^{h,x}$ is the solution of

$$\begin{aligned} \frac{d\eta^{h,x}(t)}{dt} &= A\eta^{h,x}(t) + DF(X(t, x)).\eta^{h,x}(t), \\ \eta^{h,y}(0) &= h. \end{aligned}$$

- For any $h, k \in H$, we have

$$D^2u(t, x).(h, k) = \mathbb{E}[D^2\phi(X(t, x)).(\eta^{h,x}(t), \eta^{k,x}(t)) + D\phi(X(t, x)).\zeta^{h,k,x}(t)], \quad (8.6)$$

where $\zeta^{h,k,x}$ is the solution of

$$\begin{aligned} \frac{d\zeta^{h,k,x}(t)}{dt} &= A\zeta^{h,k,x}(t) + DF(X(t, x)).\zeta^{h,k,x}(t) + D^2F(X(t, x)).(\eta^{h,x}(t), \eta^{k,x}(t)), \\ \zeta^{h,k,x}(0) &= 0. \end{aligned}$$

Moreover, we already have the equation (8.2) (see (4.1)).

We will now show the equations (8.3) and (8.4). The singularity $t^{-\eta}$ in (8.4) is a consequence of the regularity properties satisfied by F . The proofs require several steps. First in Lemma 8.4 below we prove estimates for a finite horizon and general $0 \leq \beta, \gamma < 1/2$; then in Lemma 8.6 we study the long-time behaviour in the particular case $\beta = \gamma = 0$; we finally conclude with the proofs of Proposition 8.1.

First, we prove estimates of these quantities for $0 < t \leq 1$ - see Lemmas 4.4 and 4.5 in [20], with a difference coming from the assumptions made on the nonlinear coefficient F :

Lemma 8.4 *For any $0 \leq \beta < 1/2$, $0 \leq \gamma < 1/2$, there exist constants C_β and $C_{\beta,\gamma}$ such that for any $y \in H$ and any $0 < t \leq 1$*

$$\begin{aligned} |Du(t, x)|_\beta &\leq \frac{C_\beta}{t^\beta} \|D\phi\|_0 \\ |(-A)^\beta D^2u(t, x)(-A)^\gamma|_{\mathcal{L}(H)} &\leq C_{\beta,\gamma} \left(\frac{1}{t^\eta} + \frac{1}{t^{\beta+\gamma}} \right) (\|D\phi\|_0 + \|D^2\phi\|_0), \end{aligned}$$

where η is defined in Assumption 2.7.

Remark 8.5 *If we take another time interval $]0, T_{max}]$ instead of $]0, 1]$, the constants C_β and $C_{\beta,\gamma}$ are a priori exponentially increasing in T_{max} .*

Proof. Owing to (8.5) and (8.6), we only need to prove the following almost sure estimates, for some constants C_β and $C_{\beta,\gamma}$ - which may vary from line to line below: for any $0 < t \leq 1$

$$\begin{aligned} |\eta^{h,x}(t)| &\leq \frac{C_\beta}{t^\beta} |h|_{-\beta} \\ |\zeta^{h,k,x}(t)| &\leq C_{\beta,\gamma} \min\left(\frac{1}{t^\eta}, \frac{1}{t^{\beta+\gamma}}\right) |h|_{-\beta} |k|_{-\gamma}, \end{aligned} \quad (8.7)$$

where the parameter η is defined in Assumption 2.7.

We use mild formulations, and the regularization properties of the semi-group given in Proposition 2.6:

$$\begin{aligned} |\eta^{h,x}(t)| &= |e^{tA}h + \int_0^t e^{(t-s)A} DF(X(s, y)).\eta^{h,x}(s) ds| \\ &\leq \frac{C_\beta}{t^\beta} |h|_{-\beta} + C \int_0^t |\eta^{h,x}(s)| ds, \end{aligned}$$

and by the Gronwall Lemma we get the result.

For the second-order derivative, we moreover use the properties of F in Assumption 2.7 to get

$$\begin{aligned}
|\zeta^{h,k,x}(t)| &= \left| \int_0^t e^{(t-s)A} DF(X(s,x)) \cdot \zeta^{h,k,x}(s) ds \right. \\
&\quad \left. + \int_0^t e^{(t-s)A} D^2F(X(s,x)) \cdot (\eta^{h,x}(s), \eta^{k,x}(s)) ds \right| \\
&\leq C \int_0^t |\zeta^{h,k,x}(s)| ds + \int_0^t \frac{C_{\beta,\gamma}}{(t-s)^\eta} |\eta^{h,y}(s)| |\eta^{k,x}(s)| ds \\
&\leq C \int_0^t |\zeta^{h,k,x}(s)| ds + C_{\beta,\gamma} |h|_{-\beta} |k|_{-\gamma} t^{1-\eta-\beta-\gamma} \int_0^1 \frac{1}{(1-s)^{\eta\beta+\gamma}} ds.
\end{aligned}$$

To conclude, it remains to use the Gronwall Lemma, since for any $0 < t \leq 1$ we get $t^{1-\eta-\beta-\gamma} \leq t^{-\eta}$, thanks to the assumption $\beta + \gamma < 1$. \blacklozenge

Thanks to the dissipativity property expressed in Proposition 2.9, we can prove the result in the case $\beta = \gamma = 0$. We notice that the proof would be straightforward under a strict dissipativity assumption - since then $\eta^{h,x}(t)$ and $\zeta^{h,k,x}(t)$ would decrease exponentially in t ; in the general case $\eta^{h,x}(t)$ and $\zeta^{h,k,x}(t)$ are exponentially increasing in time so that we can not work directly. Here the result comes from the estimate (4.1) of Proposition 4.2.

Lemma 8.6 *There exist constants C and $c > 0$ such that for any $t \geq 0$ and any $y \in H$*

$$|Du(t,x)| \leq Ce^{-ct}(1 + |x|^2) \|\phi\|_0$$

and

$$|D^2u(t,x)|_{\mathcal{L}(H)} \leq Ce^{-ct} \left(1 + \frac{1}{t^\eta}\right) (1 + |x|^2) \|\phi\|_0.$$

Proof. The Bismut-Elworthy-Li formula states that if $\Phi : H \rightarrow \mathbb{R}$ is a function of class \mathcal{C}^2 with bounded derivatives and with at most quadratic growth - i.e. there exists $M(\Phi) > 0$ such that for any $x \in H$ we have $|\Phi(x)| \leq M(\Phi)(1 + |x|^2)$ - then we can calculate the first and the second order derivatives of $(t,x) \mapsto v(t,x) := \mathbb{E}\Phi(X(t,x))$ with respect to x . First, we have for any $x \in H$ and $h \in H$

$$\begin{aligned}
Dv(t,x) \cdot h &= \frac{1}{t} \mathbb{E} \left[\int_0^t \langle \eta^{h,x}(s), dW(s) \rangle \Phi(X(t,x)) \right] \\
&= \frac{2}{t} \mathbb{E} \left[\int_0^{t/2} \langle \eta^{h,x}(s), dW(s) \rangle v(t/2, X(t/2, x)) \right];
\end{aligned} \tag{8.8}$$

the second equality is a consequence of the identity $v(t,x) = \mathbb{E}v(t/2, X(t/2, x))$ obtained with the Markov property, and of the first equality applied with the function $v(t/2, \cdot)$.

Using the second formula of (8.8), we obtain a formula for the second order derivative: for any $y \in H$ and $h, k \in H$,

$$\begin{aligned}
D^2v(t,x) \cdot (h,k) &= \frac{2}{t} \mathbb{E} \left[\int_0^{t/2} \langle \zeta^{h,k,x}(s), dW(s) \rangle v(t/2, X(t/2, x)) \right] \\
&\quad + \frac{2}{t} \mathbb{E} \left[\int_0^{t/2} \langle \eta^{h,x}(s), dW(s) \rangle Dv(t/2, X(t/2, x)) \cdot \eta^{k,x}(t/2) \right].
\end{aligned} \tag{8.9}$$

We then see, using Lemmas 3.9 and 8.4 - with $\beta = \gamma = 0$ - that there exists $C > 0$ such that for any $0 < t \leq 1$, $x \in H$, $h, k \in H$

$$\begin{aligned} |Dv(t, x).h| &\leq \frac{C}{\sqrt{t}} M(\Phi)(1 + |x|^2)|h|, \\ |D^2v(t, x).(h, k)| &\leq \frac{C}{t} M(\Phi)(1 + |x|^2)|h||k|. \end{aligned} \tag{8.10}$$

Now when $t \geq 1$ the Markov property implies that $u(t, x) = \mathbb{E}u(t-1, X(1, x))$, and by (4.2) we have

$$|u(t-1, x) - \int_H \phi d\bar{\mu}| \leq Ce^{-c(t-1)}(1 + |x|^2) \|\phi\|_0.$$

If we choose $\Phi_t(x) = u(t-1, x) - \int_H \phi d\bar{\mu}$, we have $u(t, x) = \mathbb{E}\Phi_t(X(1, x)) + \int_H \phi d\bar{\mu}$, with $M(\Phi_t) \leq Ce^{-c(t-1)} \|\phi\|_0$. With (8.10) at time 1, we obtain for $t \geq 1$

$$\begin{aligned} |Du(t, x).h| &\leq C \|\phi\|_0 e^{-c(t-1)}(1 + |x|^2)|h| \\ |D^2u(t, x).(h, k)| &\leq C \|\phi\|_0 e^{-c(t-1)}(1 + |x|^2)|h||k|. \end{aligned}$$

Moreover by Lemma 8.4 we have a control when $0 \leq t \leq 1$, so that with a change of constants we get the result. \blacklozenge

We can finally prove the Proposition 8.1. The key tool is the Markov property of the process X which yields the following formula: for any $t \geq 1$

$$u(t, x) = \mathbb{E}[u(t-1, X_1(x))]. \tag{8.11}$$

To get the exponential decreasing, we use Lemma 8.6 at time $t-1$ when $t \geq 1$, while $|h|_{-\beta}$ appears from $\eta_{h,y}(1)$, and with estimates coming from Lemma 8.4.

Proof of Propositions 8.1. Using equation (8.11) and Lemma 8.6, for any $t \geq 1$ we have

$$|Du(t, x).h| \leq C \|\phi\|_0 e^{-c(t-1)} \mathbb{E}[(1 + |X(1, x)|^2)|\eta^{h,x}(1)|] \leq C \|\phi\|_0 e^{-c(t-1)}(1 + |x|^2)|h|_{-\beta},$$

where the last estimate comes from Lemmas 3.9 and 8.4.

Combining this estimate with the result of Lemma 8.4, which gives an estimate for $t \leq 1$, we obtain (8.3).

For the second order derivatives, Lemma 8.4 gives an estimate for $t \leq 1$, and for $t \geq 1$ we use (8.11) to see that

$$\begin{aligned} D^2u(t, x).(h, k) &= \mathbb{E}[D^2[u(t-1, X(1, x))].(h, k)] \\ &= \mathbb{E}D^2u(t-1, X(1, x)).(\eta^{h,x}(1), \eta^{k,x}(1)) + \mathbb{E}Du(t-1, X(1, x)).\zeta^{h,k,x}(1). \end{aligned}$$

Using Lemma 8.6, we get an exponential decreasing; thanks to Lemma 3.9 and to the estimates in the proof of Lemma 8.4 at time 1, we obtain

$$|D^2u(t, x).(h, k)| \leq \|\phi\|_0 e^{-c(t-1)}(1 + |x|^2)|h|_{-\beta}|k|_{-\gamma}.$$

Then (8.4) easily follows. \blacklozenge

8.2 Proof of some estimates

We give the detailed proofs of some estimates on the processes $(X^h(t))_{t \in \mathbb{R}^+}$ and $(X_k^h)_{k \in \mathbb{N}}$, given in Section 3.4.

We omit the reference to the parameter of the spatial discretization $h \in (0, 1)$, but it is clear from the proofs that the constants are uniform with respect to h .

Proof of Lemma 3.9. If we define $Z(t) = X(t) - W^A(t)$, we have $Z(0) = X(0) = x$, and

$$\frac{dZ(t)}{dt} = AZ(t) + F(X(t)),$$

and by Proposition 2.9

$$\begin{aligned} \frac{1}{2} \frac{d|Z(t)|^2}{dt} &= \langle AZ(t) + F(X(t)), Z(t) \rangle \\ &= \langle AZ(t) + F(Z(t)), Z(t) \rangle + \langle F(X(t)) - F(Z(t)), Z(t) \rangle \\ &\leq -c|Z(t)|^2 + C + \|F\|_0 |Z(t)| \\ &\leq -c'|Z(t)|^2 + C', \end{aligned}$$

for some new constants c', C' .

Then almost surely we have for any $t \geq 0$

$$|Z(t)| \leq C(1 + |x|).$$

Thanks to (2.6), the conclusion easily follows. \blacklozenge

Proof of Lemma 3.10. As in the proof of Lemma 3.9 above, we introduce $Z_m = X_m - w_m$, where the process (w_m) is the numerical approximation of W^A with the numerical scheme (3.9) - with $F = 0$; it is defined by

$$w_{m+1} = S_{\tau,h} w_m + \sqrt{\tau} S_{\tau,h} \chi_{m+1}.$$

Using Theorem 3.2 of [75], giving the strong order $1/4$ for the numerical scheme - when the initial condition is 0, with no nonlinear coefficient, with a constant diffusion term and under the assumptions made here - we obtain the following estimate: for any $p \geq 1$, $\tau_0 > 0$ and $0 < r < 1/2$ there exists $C > 0$ such that for any $0 < \tau \leq \tau_0$ and $m \geq 0$

$$\mathbb{E}|w_m - W^A(m\tau)|^{2p} \leq C\tau^{(1/2-r)p}. \quad (8.12)$$

Thanks to (2.6) and (8.12), we get that for any $\tau_0 > 0$, there exists $C > 0$ such that for $0 < \tau \leq \tau_0$ and $m \geq 0$

$$\mathbb{E}|w_m|^2 \leq C. \quad (8.13)$$

Now Z_m defined above satisfies $Z_0 = X_0 = x$ and

$$Z_{m+1} = S_{\tau,h} Z_m + \tau S_{\tau,h} F(X_m);$$

since, for $h \in (0, 1)$, $|S_{\tau,h}|_{\mathcal{L}(H)} \leq \frac{1}{1+\lambda_0\tau}$, we obtain the almost sure estimates

$$|Z_{m+1}| \leq \frac{1}{1+\lambda_0\tau} |Z_m| + C\tau$$

and

$$|Z_m| \leq C(1 + |x|).$$

Thanks to (8.13), we therefore obtain the result. \blacklozenge

Chapter 5

Weak approximation of SPDE: the case of polynomial nonlinearity in a bounded interval.

1 Introduction

When one considers a numerical scheme for a stochastic equation, two types of errors can be considered. The strong error measures the pathwise approximation of the true solution by a numerical one. This problem has been extensively studied in finite dimension for stochastic differential equations - see for instance [48, 69, 83] - and also more recently in infinite dimension for various types of stochastic partial differential equations (SPDEs) - see references cited in [20]. Another way to measure the error is the so-called weak order of convergence of a numerical scheme which is concerned with the approximation of the law of the solution at a fixed time. In many applications, this error is more relevant. Pioneering works by Milstein - [67, 68] - and Talay - [81] - have been followed by many articles - see references in the books cited above. Weak approximation of solution of SPDEs has been studied only recently. Weak convergence for linear stochastic partial differential equations has been studied in the papers [19, 25, 52–54, 56] while the works [2–6, 20, 40, 41, 87] treat semi-linear equations.

In this chapter, we consider a stochastic nonlinear heat equation in a bounded interval $(0, 1)$ driven by a space-time white noise :

$$\begin{aligned}dX &= (AX + F(X))dt + dW, \\ X(0) &= x,\end{aligned}\tag{1.1}$$

where $H = L^2(0, 1)$, $A = \partial_{xx}$, $D(A) = H^2(0, 1) \cap H_0^1(0, 1)$, W is a cylindrical Wiener process and the nonlinearity F is polynomial - see Subsection 2.2.2. It is well known - [10, 16] - that this equation has a unique solution. We investigate the error committed when approximating this solution by a discretization in time by an implicit split-step scheme and a discretization in space by a spectral decomposition of A - see Section 3 - and we show that this scheme has weak order 1/2 in time - see Theorem 6.1.

In the case of stochastic differential equation, it is well known that, in general, the weak order is twice the strong order - see [83]. The classical proof of this is to expand the error thanks to the solution of the Kolmogorov equation associated with the stochastic equation and to use bounds on the spatial derivatives of this solution. This strategy has been generalized to SPDEs in [20], where a semi-implicit Euler scheme is studied. The two principal tools used in [20] are the following:

- improved estimates on the derivatives of the solution of the Kolmogorov equations, with spatial regularization;
- an integration by parts formula issued from Malliavin calculus, in order to transform some stochastic expressions with insufficient spatial regularity into more suitable ones.

These tools are fundamental to treat equations with nonlinear terms. They have also been used, among others, in [87] to treat the time-discretization in a slightly more-general setting, in [3] where discretization in space with a finite element method is studied and in [5, 6] where the authors analyze approximations of the invariant measure for SPDEs.

Notice that for linear equations a specific idea simplifies the proof - so that the second tool is not used - but can not be adapted for nonlinear parabolic equations like (1.1): see [25], and in a different context [19] where the unitary group property of the Schrödinger evolution allows to treat nonlinearities. Also, in [2, 49], the authors do not use the Kolmogorov equation but duality in refined Watanabe-Sobolev space to prove weak convergence (see also [13] in the finite dimensional case).

Here, we use the approach described in [20] to prove our result. Most of the works on weak convergence for SPDEs deal with the semi-implicit Euler scheme. With our notation, it reads:

$$X_{m+1} - X_m = \delta(AX_{m+1} + F(X_m)) + W((m+1)\delta) - W(m\delta), X_0 = x,$$

where δ is the time step. Such scheme is interesting because it has an explicit form and requires only the inversion of the linear part of the equation. It is commonly used in practice.

However, fully implicit schemes - in which the nonlinearity is evaluated at X_{m+1} - have also some interests. On the practical side, it is known that they have better qualitative properties and are supposed to reflect more properly the true dynamic of the equation. On the theoretical side, it is often impossible to prove rigorous results for a semi-implicit scheme. For instance, in the case treated here, since we consider unbounded non-linearities, it is not known whether it is possible to prove that the discrete solutions of the semi-implicit scheme has bounded moments whereas it is true for the implicit one. Of course, the drawback of implicit schemes is that the inversion of the nonlinearity may be very expensive.

Here we choose to work with the split-step scheme:

$$\begin{aligned} X_{m+1/2} &= X_m + \delta F(X_{m+1/2}) \\ X_{m+1} &= X_{m+1/2} + \delta AX_{m+1} + W((n+1)\delta) - W(n\delta) \\ X_0 &= x, \end{aligned}$$

This scheme has several advantages. First, it is often possible to explicitly solve the first equation and obtain easily $X_{m+1/2}$ in terms of X_m . Then, it is not more expensive than the semi-implicit scheme. Also, as shown below, it is possible to prove bounds on the moments of the discrete solutions. From a technical point of view, we use below a continuous interpolate of the numerical solution which is very helpful for our analysis since we can use Ito formula and avoid a lot of computations. We are not able to construct such interpolate for the implicit scheme so that the proof would be much more technical.

Note also that the first step of the scheme could be replaced by the exact solution of the ordinary differential equation: $X' = f(X)$. This might be helpful in some circumstances when this solution is known explicitly. Our result and proof are still valid for this scheme.

Another problem which emerges when we work with polynomial nonlinearity is the regularity of the derivatives of the solution of the Kolmogorov equation associated with the SPDE. Since regularity of the derivative is measured in some Sobolev spaces, we cannot use the results of [10] for instance. We have to derive more subtle estimates which are proved in the appendix and are interesting on their own.

The paper is organized as follows: in Section 2, we make the assumptions on the coefficients of the equation, and we define the discretization method in Section 3. In Sections 4 and 5, we presents two tools: a priori bound on moments and integration by parts from Malliavin calculus. In Section 6, we give the convergence result that we obtained. In Section 7, we introduce the strategy and the last tool used: the regularity of the solution of the Kolmogorov equation. A detailed proof of the estimates can be found in Section 8. A proof of the regularity of the two first derivatives of the solution of the Kolmogorov equation can be found in the Appendix.

2 Notations and assumptions

We denote by H the Hilbert space $H = L^2(0, 1)$, with the norm denoted by $|\cdot|_H = |\cdot|_{L^2}$ or simply $|\cdot|$ and the inner product denoted by $\langle \cdot, \cdot \rangle_H = \langle \cdot, \cdot \rangle_{L^2}$ or simply $\langle \cdot, \cdot \rangle$. We consider equations of the form

$$\begin{aligned} dX_x(t) &= (AX_x(t) + F(X_x(t)))dt + dW(t) \\ X_x(0) &= x. \end{aligned} \tag{2.1}$$

In the next paragraphs, we state the assumptions made on the coefficients A and F ; we also recall basic facts on the cylindrical Wiener process W and on the mild solution of the SPDE.

2.1 Test functions

To quantify the weak approximation, we use test functions ϕ in the space $\mathcal{C}_b^2(H, \mathbb{R})$ of functions from H to \mathbb{R} that are twice continuously differentiable, bounded, with first and second order bounded derivatives.

Remark 2.1 *In the sequel, we often identify the first derivative $D\phi(x) \in \mathcal{L}(H, \mathbb{R})$ with the gradient in the Hilbert space H , and the second derivative $D^2\phi(x)$ with a linear operator on H , via the formulas:*

$$\begin{aligned} \langle D\phi(x), h \rangle &= D\phi(x) \cdot h \text{ for every } h \in H \\ \langle D^2\phi(x).h, k \rangle &= D^2\phi(x) \cdot (h, k) \text{ for every } h, k \in H. \end{aligned}$$

In the sequel, we use the following notations:

$$\begin{aligned} |\phi|_0 &= \sup_{x \in H} |\phi(x)|_H \\ |\phi|_1 &= \sup_{x \in H} |D\phi(x)|_H \\ |\phi|_2 &= \sup_{x \in H} |D^2\phi(x)|_{\mathcal{L}(H)} \end{aligned}$$

and

$$|\phi|_{0,i} = \sup_{0 \leq j \leq i} |\phi|_j,$$

where $i = 1, 2$.

2.2 Assumptions on the coefficients

2.2.1 The linear operator

We denote by $\mathbb{N} = \{0, 1, 2, \dots\}$ the set of nonnegative integers and $\mathbb{N}^* = \{1, 2, \dots\}$.

We define A by $A = \frac{d^2}{dx^2}$, with the domain $H^2(0, 1) \cap H_0^1(0, 1) \subset L^2(0, 1)$ - corresponding to homogeneous Dirichlet boundary conditions. Let $\lambda_k = \pi^2(k+1)^2$ and $f_k(\xi) = \sqrt{2} \sin((k+1)\pi\xi)$, for $k \in \mathbb{N}$, then the following properties are satisfied - see [8] for more details:

Lemma 2.2 1. *The family $(f_k)_{k \in \mathbb{N}}$ is a complete orthonormal system of elements of H and we have*

$$Af_k = -\lambda_k f_k \text{ for all } k \in \mathbb{N}.$$

2. *The sequence (λ_k) is a non-decreasing sequence, goes to $+\infty$ and verifies*

$$\sum_{k=0}^{+\infty} \frac{1}{\lambda_k^\alpha} < +\infty \Leftrightarrow \alpha > 1/2.$$

The smallest eigenvalue of $-A$ is then $\lambda_0 = \pi^2$.

In the following Definition, we introduce finite dimensional subspaces of H and associated orthogonal projections; both are based on the spectral decomposition of A .

Definition 2.3 *For any $M \in \mathbb{N}$, we define H_M the subspace of H generated by f_0, \dots, f_M ,*

$$H_M = \text{Span}\{f_k; 0 \leq k \leq M\}$$

and $P_M \in \mathcal{L}(H)$ the orthogonal projection onto H_M : for any $x = \sum_{k=0}^{+\infty} x_k f_k \in H$,

$$P_M x = \sum_{k=0}^M x_k f_k.$$

The domain $D(A)$ of A is equal to $D(A) = \{x = \sum_{k=0}^{+\infty} x_k f_k \in H, \sum_{k=0}^{+\infty} (\lambda_k)^2 |x_k|^2 < +\infty\}$. More generally, fractional powers of $-A$, are defined for $\alpha \in [0, 1]$:

$$(-A)^\alpha x = \sum_{k=0}^{\infty} \lambda_k^\alpha x_k f_k \in H,$$

with the domains

$$D((-A)^\alpha) = \left\{ x = \sum_{k=0}^{+\infty} x_k f_k \in H, \quad |x|_\alpha^2 := \sum_{k=0}^{+\infty} (\lambda_k)^{2\alpha} |x_k|^2 < +\infty \right\}.$$

Remark 2.4 *We have*

$$D((-A)^{1/2}) = H_0^1(\mathcal{D}) \quad D(A) = H_0^1(\mathcal{D}) \cap H^2(\mathcal{D}).$$

When $\alpha \in [0, 1]$, it is also possible to define spaces $D(-A)^{-\alpha}$ and operators $(-A)^{-\alpha}$, with norm denoted by $|\cdot|_{-\alpha}$; in particular when $x = \sum_{k=0}^{+\infty} x_k f_k \in H$, we have $(-A)^{-\alpha} x = \sum_{k=0}^{+\infty} \lambda_k^{-\alpha} x_k f_k$ and $|x|_{-\alpha}^2 := \sum_{k=0}^{+\infty} (\lambda_k)^{-2\alpha} |x_k|^2$.

The semi-group $(e^{tA})_{t \geq 0}$ can be defined by the Hille-Yosida Theorem - see [8]. We use the following spectral formula: if $x = \sum_{k=0}^{+\infty} x_k f_k \in H$, then for any $t \geq 0$

$$e^{tA} x = \sum_{k=0}^{+\infty} e^{-\lambda_k t} x_k f_k.$$

For any $t \geq 0$, e^{tA} is a continuous linear operator in H , with operator norm $e^{-\lambda_0 t}$. The semi-group (e^{tA}) is used to define the solution $Z(t) = e^{tA}z$ of the linear Cauchy problem

$$\frac{dZ(t)}{dt} = AZ(t) \quad \text{with} \quad Z(0) = z.$$

To define solutions of more general PDEs of parabolic type, we use mild formulation, and Duhamel principle.

The semi-group e^{tA} enjoys some smoothing properties that we often use in this work. Basically we need the following properties, which are easily proved using the above spectral properties.

Proposition 2.5 *For any $\sigma \in [0, 1]$, there exists $C_\sigma > 0$ such that we have:*

1. for any $t > 0$ and $x \in H$,

$$|e^{tA}x|_\sigma \leq C_\sigma t^{-\sigma} e^{-\frac{\lambda_0}{2}t} |x|_H.$$

2. for any $0 < s < t$ and $x \in H$,

$$|e^{tA}x - e^{sA}x|_H \leq C_\sigma \frac{(t-s)^\sigma}{s^\sigma} e^{-\frac{\lambda_0}{2}s} |x|_H.$$

3. for any $0 < s < t$ and $x \in D(-A)^\sigma$,

$$|e^{tA}x - e^{sA}x|_H \leq C_\sigma (t-s)^\sigma e^{-\frac{\lambda_0}{2}s} |x|_\sigma.$$

For $k \geq 1$, we denote by $|\cdot|_{L^k}$ the norm of $L^k(0, 1)$ and $|\cdot|_{L^\infty}$ the norm of $L^\infty(0, 1)$.

2.2.2 The nonlinear operator

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be defined for $y \in \mathbb{R}$ by

$$f(y) = -\alpha_{2p-1}y^{2p-1} + \sum_{\ell=0}^{2(p-1)} \alpha_\ell y^\ell, \quad (2.2)$$

where $p \in \mathbb{N}^*$, $\alpha_{2p-1} > 0$ and $\alpha_\ell \in \mathbb{R}$ for $\ell = 0, \dots, 2(p-1)$. Then the operator F is defined for every $x \in L^{2p-1}(0, 1)$ and $\xi \in (0, 1)$ by

$$F(x)(\xi) = f(x(\xi)).$$

In general, such functions are not Fréchet differentiable, but only Gâteaux differentiable, with the following expressions when it can be justified:

$$\begin{aligned} [DF(x).h](\xi) &= \frac{\partial f}{\partial x}(x(\xi))h(\xi) \\ [D^2F(x).(h, k)](\xi) &= \frac{\partial^2 f}{\partial x^2}(x(\xi))h(\xi)k(\xi). \end{aligned}$$

The following properties on f are easily seen to be satisfied:

Proposition 2.6 *f and all its derivatives have polynomial growth.*

There exist $c_1 > 0$ and $c_2 > 0$ such that for any $y \in \mathbb{R}$

$$f(y)y \leq -c_1|y|^{2p} + c_2. \quad (2.3)$$

There exists $\gamma > 0$ such that for any $y \in \mathbb{R}$

$$\frac{\partial f}{\partial y}(y) \leq \gamma. \quad (2.4)$$

For any $\varepsilon > 0$, there exist $C_\varepsilon^1 > 0$ and $C_\varepsilon^2 > 0$ such that for any $x \in \mathbb{R}$ and $y \in \mathbb{R}$

$$(f(x+y) - f(x))x \leq \varepsilon|x|^{2p} + C_\varepsilon^1|y|^{2p} + C_\varepsilon^2. \quad (2.5)$$

Our equation verifies the following dissipativity condition:

Proposition 2.7 (Dissipativity) *There exist $c_1 > 0$ and $c_2 > 0$ such that for any $x \in D(A) \cap L^{2p}(0, 1)$*

$$\langle Ax + F(x), x \rangle_{L^2} \leq -c_1|x|_{L^2}^2 + c_2. \quad (2.6)$$

2.3 The cylindrical Wiener process and stochastic integration in H

In this section, we recall the definition of the cylindrical Wiener process and of the stochastic integral on a separable Hilbert space H with norm $|\cdot|_H$. For more details, see [16].

We first fix a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$. A cylindrical Wiener process on H is defined with two elements:

- a complete orthonormal system of H , denoted by $(q_i)_{i \in I}$, where I is a subset of \mathbb{N} ;
- a family $(\beta_i)_{i \in I}$ of independent real Wiener processes with respect to the filtration $((\mathcal{F}_t)_{t \geq 0})$;

then W is defined by

$$W(t) = \sum_{i \in I} \beta_i(t)q_i. \quad (2.7)$$

We can remark that the resulting process does not depend on the choice of the complete orthonormal system $(q_i)_{i \in I}$.

When I is a finite set, we recover the usual definition of Wiener processes in the finite dimensional space $\mathbb{R}^{|I|}$. Here, $H = L^2(0, 1)$ and we can choose $(q_k)_{k \geq 1} = (\sqrt{2} \sin(k\pi \cdot))_{k \geq 1}$.

A fundamental remark is that the series in (2.7) does not converge in H ; but if a linear operator $\Psi : H \rightarrow K$ is Hilbert-Schmidt, then $\Psi W(t)$ converges in $L^2(\Omega, K)$ for any $t \geq 0$.

We recall that a bounded linear operator $\Psi : H \rightarrow K$ is said to be Hilbert-Schmidt when

$$|\Psi|_{\mathcal{L}_2(H, K)}^2 := \sum_{k=1}^{+\infty} |\Psi(q_k)|_K^2 < +\infty,$$

where the definition is independent of the choice of the orthonormal basis (q_k) of H . The space of Hilbert-Schmidt operators from H to K is denoted $\mathcal{L}_2(H, K)$; endowed with the norm $|\cdot|_{\mathcal{L}_2(H, K)}$ it is an Hilbert space. For an Hilbert-Schmidt operator $L \in \mathcal{L}(H, K)$, we have

$$|L|_{\mathcal{L}_2(H, K)}^2 = \text{Tr}(L^*L) = \text{Tr}(LL^*),$$

where for a nuclear operator $R \in \mathcal{L}(H)$, $\text{Tr}(R)$ denotes the trace of the operator R , i.e.

$$\text{Tr}(R) = \sum_{i \geq 1} (Rq_i, q_i) < +\infty.$$

It is well known that the previous properties does not depend on the choice of the Hilbertian basis. Moreover, the following properties hold for L nuclear and M bounded

$$\text{Tr}(LM) = \text{Tr}(ML)$$

and, if L is also positive,

$$\text{Tr}(LM) \leq \text{Tr}(L)|M|_{\mathcal{L}(H)}. \quad (2.8)$$

The stochastic integral $\int_0^t \Psi(s)dW(s)$ is defined in K for predictable processes Ψ with values in $\mathcal{L}_2(H, K)$ such that $\int_0^t |\Psi(s)|_{\mathcal{L}_2(H, K)}^2 ds < +\infty$ a.s; moreover when $\Psi \in L^2(\Omega \times [0, t]; \mathcal{L}_2(H, K))$, the following two properties hold:

$$\begin{aligned} \mathbb{E} \left| \int_0^t \Psi(s)dW(s) \right|_K^2 &= \mathbb{E} \int_0^t |\Psi(s)|_{\mathcal{L}_2(H, K)}^2 ds \quad (\text{It\^o isometry}), \\ \mathbb{E} \int_0^t \Psi(s)dW(s) &= 0. \end{aligned}$$

A generalization of It\^o formula also holds - see [16].

For instance, if $v = \sum_{k \in \mathbb{N}^*} v_k q_k \in H$, we can define

$$\langle W(t), v \rangle = \int_0^t \langle v, dW(s) \rangle = \sum_{k \in \mathbb{N}^*} \beta_k(t) v_k;$$

we then have the following space-time white noise property

$$\mathbb{E} \langle W(t), v_1 \rangle \langle W(s), v_2 \rangle = t \wedge s \langle v_1, v_2 \rangle.$$

Therefore to be able to integrate a process with respect to W requires some strong properties on the integrand; in our SPDE setting, the Hilbert-Schmidt properties follow from the assumptions made on the linear coefficients of the equations.

Thanks to Lemma 2.2, it is easy to show that the following stochastic integral is well-defined in H , for any $t \geq 0$:

$$W^A(t) = \int_0^t e^{(t-s)A} dW(s). \quad (2.9)$$

It is called a stochastic convolution, and it is the unique mild solution of

$$dZ(t) = AZ(t)dt + dW(t) \quad \text{with} \quad Z(0) = 0.$$

By Lemma 2.2, there exists $\delta > 0$ such that for any $t > 0$ we have $\int_0^t \frac{1}{s^\delta} |e^{sA}|_{\mathcal{L}_2(H)}^2 ds < +\infty$; it can then be proved that W^A has continuous trajectories - via the *factorization method*, see [16] - and that for any $k \in \mathbb{N}^*$

$$\mathbb{E} \sup_{t \geq 0} |W^A(t)|_H^k < +\infty. \quad (2.10)$$

We also have - see [10] and [16] - that for any $T > 0$ and $1 \leq k < +\infty$

$$\mathbb{E} \sup_{t \in [0, T]} |W^A(t)|_{L^\infty}^k < \infty. \quad (2.11)$$

We can now define solutions to Equation (2.1), thanks to the assumptions made on the coefficients: the following result is classical - see [10] or [16]:

Proposition 2.8 *For every $T > 0$, $k \in \mathbb{N}^*$ and $x \in \mathcal{C}([0, 1])$, the equation (2.1) admits a unique mild solution $X_x \in L^k(\Omega, \mathcal{C}([0, T] \times [0, 1]))$:*

$$X_x(t) = e^{tA}x + \int_0^t e^{(t-s)A}F(X_x(s))ds + \int_0^t e^{(t-s)A}dW(s), \quad t \in [0, T]. \quad (2.12)$$

3 Definition of the discretization scheme

Our main interest is the time discretisation of the process X . Nevertheless, in order to avoid to introduce infinite dimensional Kolmogorov operators, we always work on a spatial discretisation which is obtained by simple Galerkin projection. The estimates will be given below are uniformly independent of the spatial discretization. In this Section, we introduce the Galerkin approximation using the spectral decomposition of the operator A and the implicit split-step scheme we are interested in.

3.1 Discretization in space : Galerkin approximation

To justify rigorously the required computations, we need to work with a finite dimensional approximation. The first step is to consider finite dimensional projection onto the subspaces H_M of the H -valued process $(X(t))_{t \in \mathbb{R}^+}$: for any $M \in \{1, 2, \dots\}$, we define $(X^{(M)}(t))_{t \in \mathbb{R}^+}$ by the equation

$$dX^{(M)}(t) = AX^{(M)}(t)dt + P_M F(X^{(M)}(t))dt + dW^{(M)}(t), \quad (3.1)$$

with the initial condition $X^{(M)}(0) = P_M x$.

The projection P_M is defined in Definition 2.3. Then $W^{(M)} = P_M W$ is a M -dimensional Wiener process on the subspace H_M . We remark that the above equations are well-defined on H_M - which is a stable subspace of A .

The following result justifies the convergence of the Galerkin approximation: for any fixed $T \in \mathbb{R}^+$ and $0 < \kappa < 1/4$, there exists $C(T) > 0$ such that for any $t \in [0, T]$, $x \in \mathcal{C}([0, 1])$ and $M \in \{1, 2, \dots\}$, we have

$$\left(\mathbb{E}|X_x(t) - X_x^{(M)}(t)|^2\right)^{1/2} \leq C(T)(1 + |x|_{L^\infty}^{4p}) \frac{1}{\lambda_{M+1}^{-1/4+\kappa}}, \quad (3.2)$$

where p is defined in (2.2).

In the sequel, we need the useful notation

$$F_\infty = F, P_\infty = I, \quad W^{(\infty)} = W, \quad X^{(\infty)} = X.$$

3.2 Discretization in time

Let δ be the time step. Let $N \in \mathbb{N}^*$ and $T = N\delta$ be fixed. For each $M \in \{1, 2, \dots\} \cup \{\infty\}$, we now define a time approximation of the process $X^{(M)}$: thanks to an implicit split-step scheme, we define for $m = 1, \dots, N - 1$

$$\begin{aligned} X_{m+1/2}^{(M)}(\delta, x) &= X_m^{(M)}(\delta, x) + \delta P_M F(X_{m+1/2}^{(M)}(\delta, x)) \\ X_{m+1}^{(M)}(\delta, x) &= X_{m+1/2}^{(M)}(\delta, x) + \delta A X_{m+1}^{(M)}(\delta, x) + \sqrt{\delta} \chi_{m+1}^{(M)} \\ X_0^{(M)}(\delta, x) &= x, \end{aligned}$$

where $\chi_{m+1}^{(M)} = \frac{1}{\sqrt{\delta}}(W^{(M)}((m+1)\delta) - W^{(M)}(m\delta))$.

We have for $\delta < \delta_0 := \frac{1}{\gamma}$, where γ is defined in (2.9), that this scheme is well-defined - see Lemma 2.4 of Chapter 2 for more details.

To simplify the equations, most of the time we omit the dependence of $X_m^{(M)}$ on the time-step δ and on the initial condition x .

When $M = \infty$, the above expression does not make sense in H . However, defining

$$R_\delta = (I - \delta A)^{-1}, \quad (3.3)$$

this last equation can be replaced by

$$\begin{aligned} X_{m+1/2}^{(M)} &= X_m^{(M)} + \delta P_M F(X_{m+1/2}^{(M)}) \\ X_{m+1}^{(M)} &= R_\delta X_{m+1/2}^{(M)} + \sqrt{\delta} R_\delta \chi_{m+1}^{(M)}, \end{aligned} \quad (3.4)$$

which is valid, since one easily checks that R_δ is a Hilbert-Schmidt operator on H . Moreover, the expression is also valid for $M \neq \infty$, since the operators R_δ and P_M commute.

Note that in many case, we can easily compute the solution of the equation: $y = x + \delta F(y)$, where x is fixed, then we have an explicit form for the implicit split-step scheme (3.4).

Remark 3.1 *The processes $(X_m^{(M)})_{m=1, \dots, N}$ can be seen in two different ways. On the one hand, for a fixed $M \in \{1, 2, \dots\} \cup \{\infty\}$ it is given by a implicit split-step discretization of the process $(X^{(M)}(t))_{t \in [0, T]}$; on the other hand, for $M \neq \infty$, it is naturally defined as a Galerkin approximation in dimension M of the discrete time process $(X_m^{(\infty)})_{m=1, \dots, N}$.*

For the analysis of the convergence of the scheme, we need the following technical estimates:

Lemma 3.2 *For any $0 \leq \kappa \leq 1$ and $j \geq 1$,*

$$|(-A)^{1-\kappa} R_\delta^j|_{\mathcal{L}(H)} \leq c \frac{1}{(j\delta)^{1-\kappa}} \frac{1}{(1 + \mu_0 \delta)^{j\kappa}}.$$

Moreover, for any $\beta \geq 1$ and $j \geq \beta$,

$$|(-A)^\beta R_\delta^j|_{\mathcal{L}(H)} \leq c \frac{1}{(j\delta)^\beta}.$$

Proof. For any $z \in H$,

$$\begin{aligned} |(-A)^{1-\kappa} R_\delta^j z|_H^2 &= \sum_{i=0}^{+\infty} \lambda_i^{2(1-\kappa)} \frac{1}{(1 + \lambda_i \delta)^{2j}} |z_i|^2 \\ &= \frac{1}{(j\delta)^{2(1-\kappa)}} \sum_{i=0}^{+\infty} |z_i|^2 \lambda_i^{2(1-\kappa)} (j\delta)^{2(1-\kappa)} \frac{1}{(1 + \lambda_i \delta)^{2j(1-\kappa)}} \frac{1}{(1 + \lambda_i \delta)^{2j\kappa}} \\ &\leq \frac{1}{(j\delta)^{2(1-\kappa)}} \sum_{i=0}^{+\infty} \left(\frac{\lambda_i j \delta}{1 + \lambda_i j \delta} \right)^{2(1-\kappa)} \frac{1}{(1 + \lambda_0 \delta)^{2j\kappa}} |z_i|^2 \\ &\leq c |z|_H^2 \frac{1}{(j\delta)^{2(1-\kappa)}} \frac{1}{(1 + \lambda_0 \delta)^{2j\kappa}}. \end{aligned}$$

The proof of the second inequality is similar.

Remark 3.3 *Later, we often use the following expression for $X_m^{(M)}$:*

$$X_m^{(M)} = R_\delta^m P_M x + \delta \sum_{\ell=0}^{m-1} R_\delta^{m-\ell} P_M F(X_{\ell+1/2}^M) + \sqrt{\delta} \sum_{\ell=0}^{m-1} R_\delta^{m-\ell} P_M \chi_{\ell+1}. \quad (3.5)$$

The following expression is also useful:

$$\sqrt{\delta} \sum_{\ell=0}^{m-1} R_\delta^{m-\ell} P_M \chi_{\ell+1} = \int_0^{t_m} R_\delta^{m-\ell_s} P_M dW(s), \quad (3.6)$$

where $\ell_s = \lfloor \frac{s}{\delta} \rfloor$ - with the notation $\lfloor \cdot \rfloor$ for the integer part - and $t_m = m\delta$.

We finally introduce the following processes, for each $M \in \{1, 2, \dots\} \cup \{\infty\}$: for $0 \leq m \leq N-1$ and $t_m \leq t \leq t_{m+1}$

$$\tilde{X}^{(M)}(t) = X_m^{(M)} + \int_{t_m}^t [AR_\delta X_m^{(M)} + R_\delta P_M F(X_{m+1/2}^{(M)})] ds + \int_{t_m}^t R_\delta dW^{(M)}(s). \quad (3.7)$$

The process $(\tilde{X}^{(M)}(t))_{t \in \mathbb{R}^+}$ is a natural interpolation of the numerical solution $(X_m^{(M)})_{m \in \mathbb{N}}$ defined by (3.4): $\tilde{X}^{(M)}(t_m) = X_m^{(M)}$.

4 A priori bounds on moments

We work with the finite dimensional approximation, but we omit the parameter $M \in \{1, 2, \dots\} \cup \{\infty\}$. The constants appearing below are independent of M .

Let $N \in \mathbb{N}^*$ and $T = N\delta$ be fixed, we give few results on the processes $(X(t))_{t \in [0, T]}$, $(\tilde{X}(t))_{t \in [0, T]}$ and $(X_m)_{m=0, \dots, N}$.

Lemma 4.1 *For any $k \geq 1$, there exists a constant $C_k(T) > 0$ such that for every $0 \leq t \leq T$ and $x \in \mathcal{C}([0, 1])$*

$$\mathbb{E}(\sup_{s \in [0, t]} |X_x(s)|_{L^\infty}^k) \leq C_k(T)(1 + |x|_{L^\infty}^k).$$

A proof of Lemma 4.1 can be found in Chapter 6 of [10] or in [16].

Lemma 4.2 *Let $\delta_0 := \frac{1}{2}$. For any $\ell \in \mathbb{N}^*$, there exists a constant $C > 0$ such that for every $x \in \mathcal{C}([0, 1])$, $m = 0, \dots, N-1$, $t \in [t_m, t_{m+1})$ and $\delta < \delta_0$*

$$\begin{aligned} \mathbb{E} \sup_{m=0, \dots, N} |X_m|_{L^\infty}^{2\ell} &\leq C(1 + |x|_{L^\infty}^{2\ell}), \\ \mathbb{E} \sup_{m=0, \dots, N-1} |X_{m+1/2}|_{L^\infty}^{2\ell} &\leq C(1 + |x|_{L^\infty}^{2\ell}), \\ \mathbb{E} \sup_{t \in [0, T]} |\tilde{X}(t)|_{L^\infty}^{2\ell} &\leq C(1 + |x|_{L^\infty}^{2\ell}). \end{aligned}$$

A proof of Lemma 4.2 can be found in the Section 9.

5 Malliavin calculus

We work with the finite dimensional approximation, but we omit the parameter $M \in \{1, 2, \dots\}$ - the case $M = \infty$ is not required in the computations. The constants appearing below are independent of M .

As explained in the Introduction, one of the key tools to obtain the right weak order is a transformation of some spatially irregular terms involving the stochastic integral with respect to the cylindrical Wiener process, into more suitable, deterministic ones, thanks to an integration by parts formula, issued from Malliavin calculus - see [73], [78].

The notations here are the same as in [20], where the following useful integration by parts formula is given - see Lemma 2.1 therein:

Lemma 5.1 *For any $F \in \mathbb{D}^{1,2}(H)$, $u \in \mathcal{C}_b^2(H)$ and $\Psi \in L^2(\Omega \times [0, T], \mathcal{L}_2(H))$ an adapted process,*

$$\mathbb{E}[Du(F) \cdot \int_0^T \Psi(s) dW(s)] = \mathbb{E}\left[\int_0^T \text{Tr}(\Psi(s)^* D^2 u(F) \mathcal{D}_s F) ds\right], \quad (5.1)$$

where $\mathcal{D}_s F : h \in H \mapsto \mathcal{D}_s^h F \in H$ stands for the Malliavin derivative of F , and $\mathbb{D}^{1,2}(H)$ is the set of H -valued random variables $F = \sum_{i \in \mathbb{N}} F_i f_i$, with $F_i \in \mathbb{D}^{1,2}$ the domain of the Malliavin derivative for \mathbb{R} -valued random variables for any i .

Remark 5.2 *This Lemma remains valid if u is not assumed to be bounded but only $u \in \mathcal{C}^2(H)$ provided the expectations and the integral above are well defined. This is easily seen by approximation of u by bounded functions.*

Lemma 5.3 *Let $\delta_0 < \frac{1}{2\gamma}$, where γ is defined in Proposition 2.6, be fixed. For any $h \in H$, $0 < \delta \leq \delta_0$, $N \in \mathbb{N}^*$, $T = \delta N$ and $s \in [0, T]$, we have for $m \leq \ell_s$, where ℓ_s is the integer part of $\frac{s}{\delta}$,*

$$\mathcal{D}_s^h X_m = 0$$

and for $\ell_s + 1 \leq m \leq N$

$$|\mathcal{D}_s^h X_m|^2 \leq (1 + 2\lambda_0 \delta)^{-(m-\ell_s)} (1 - 2\gamma \delta)^{-(m-\ell_s-1)} |h|^2.$$

Moreover, for $\alpha > 0$, $\kappa > 0$ and $\ell_s \leq m \leq N$, we have

$$\begin{aligned} |(-A)^\alpha \mathcal{D}_s^h X_m|_H &\leq t_{m-\ell_s}^{-\alpha} (1 + \lambda_0 \delta)^{-(m-\ell_s)(1-\alpha)} |h|_H \\ &+ c\delta \sum_{\ell=\ell_s+1}^{m-1} t_{m-\ell}^{-1/4-\alpha-\kappa} (1 + 2\lambda_0 \delta)^{-1/2(\ell-\ell_s)} (1 - 2\gamma \delta)^{-1/2(\ell-\ell_s)} |h|_H |DF(X_{\ell+1/2})|_H. \end{aligned}$$

Proof. Let $N \in \mathbb{N}^*$, $T = \delta N$, $s \in [0, T]$ and $h \in H$ be fixed. Using (3.4), we have

$$\begin{cases} \mathcal{D}_s^h X_{\ell_s+1} &= R_\delta \mathcal{D}_s^h X_{\ell_s+1/2} + R_\delta h \\ \mathcal{D}_s^h X_{\ell_s+1/2} &= \mathcal{D}_s^h X_{\ell_s} + \delta DF(X_{\ell_s+1/2}) \cdot \mathcal{D}_s^h X_{\ell_s+1/2} \end{cases}$$

and, for $m = \{1, \dots, N\}$ and $m \neq \ell_s + 1$,

$$\begin{cases} \mathcal{D}_s^h X_m &= \mathcal{D}_s^h X_{m-1/2} + \delta A \mathcal{D}_s^h X_m \\ \mathcal{D}_s^h X_{m-1/2} &= \mathcal{D}_s^h X_{m-1} + \delta DF(X_{m-1/2}) \cdot \mathcal{D}_s^h X_{m-1/2} \end{cases}.$$

Using Proposition 2.6, we get for $m \neq \ell_s + 1$

$$\frac{1}{2} |\mathcal{D}_s^h X_{m-1/2}|^2 \leq \frac{1}{2} |\mathcal{D}_s^h X_{m-1}|^2 + \delta \gamma |\mathcal{D}_s^h X_{m-1/2}|^2,$$

and

$$\frac{1}{2}|\mathcal{D}_s^h X_m|^2 \leq \frac{1}{2}|\mathcal{D}_s^h X_{m-1/2}|^2 - \delta\lambda_0|\mathcal{D}_s^h X_m|^2,$$

then we obtain for $m \neq \ell_s + 1$

$$|\mathcal{D}_s^h X_m|^2 \leq (1 + 2\lambda_0\delta)^{-1}(1 - 2\gamma\delta)^{-1}|\mathcal{D}_s^h X_{m-1}|^2.$$

By induction, we obtain, for $m \leq \ell_s$

$$\mathcal{D}_s^h X_m = 0$$

and

$$\mathcal{D}_s^h X_{m-1/2} = 0.$$

We also have $\mathcal{D}_s^h X_{\ell_s+1/2} = 0$ and $\mathcal{D}_s^h X_{\ell_s+1} = R_\delta h$. Then we get, by induction, for $m \geq \ell_s + 1$

$$|\mathcal{D}_s^h X_m|^2 \leq (1 + 2\lambda_0\delta)^{-(m-\ell_s)}(1 - 2\gamma\delta)^{-(m-\ell_s-1)}|h|$$

and

$$|\mathcal{D}_s^h X_{m+1/2}|^2 \leq (1 + 2\lambda_0\delta)^{-(m-\ell_s)}(1 - 2\gamma\delta)^{-(m-\ell_s)}|h|.$$

Let $\alpha > 0$ and $\ell_s + 1 \leq m \leq N$ be fixed. Using (3.5) and above computations, we have

$$\mathcal{D}_s^h X_m = \delta \sum_{\ell=\ell_s+1}^{m-1} R_\delta^{m-\ell} DF(X_{\ell+1/2}) \cdot \mathcal{D}_s^h X_{\ell+1/2} + R_\delta^{m-\ell_s} h$$

and

$$|(-A)^\alpha \mathcal{D}_s^h X_m|_H \leq |(-A)^\alpha R_\delta^{m-\ell_s} h|_H + \delta \sum_{\ell=\ell_s+1}^{m-1} |(-A)^\alpha R_\delta^{m-\ell} DF(X_{\ell+1/2}) \cdot \mathcal{D}_s^h X_{\ell+1/2}|_H.$$

Let $\kappa > 0$, $\phi \in L^1(0, 1)$, $\psi \in L^2(0, 1)$ be fixed. We have, by duality, Sobolev inequality (see [8]) and Lemma 3.2, for $\ell = 0, \dots, m-1$

$$\begin{aligned} \langle (-A)^\alpha R_\delta^{m-\ell} \phi, \psi \rangle_{L^2} &= \langle \phi, (-A)^\alpha R_\delta^{m-\ell} \psi \rangle_{L^2} \\ &\leq |\phi|_{L^1} |(-A)^\alpha R_\delta^{m-\ell} \psi|_{L^\infty} \\ &\leq c |\phi|_{L^1} |(-A)^{1/4+\kappa+\alpha} R_\delta^{m-\ell} \psi|_{L^2} \\ &\leq c t_{m-\ell}^{-1/4-\kappa-\alpha} |\phi|_{L^1} |\psi|_{L^2}, \end{aligned}$$

then we get, for $\ell = \ell_s + 1, \dots, m-1$

$$\delta |(-A)^\alpha R_\delta^{m-\ell} DF(X_{\ell+1/2}) \cdot \mathcal{D}_s^h X_{\ell+1/2}|_H \leq c \delta t_{m-\ell}^{-1/4-\alpha-\kappa} |DF(X_{\ell+1/2}) \cdot \mathcal{D}_s^h X_{\ell+1/2}|_{L^1} \quad (5.2)$$

$$\leq c \delta t_{m-\ell}^{-1/4-\alpha-\kappa} |DF(X_{\ell+1/2})|_H |\mathcal{D}_s^h X_{\ell+1/2}|_H. \quad (5.3)$$

Using Lemma 3.2 and above computations, we obtain

$$\begin{aligned} |(-A)^\alpha \mathcal{D}_s^h X_m|_H &\leq t_{m-\ell_s}^{-\alpha} (1 + \lambda_0\delta)^{-(m-\ell_s)(1-\alpha)} |h|_H \\ &\quad + c \delta \sum_{\ell=\ell_s+1}^{m-1} t_{m-\ell}^{-1/4-\alpha-\kappa} (1 + 2\lambda_0\delta)^{-1/2(\ell-\ell_s)} (1 - 2\gamma\delta)^{-1/2(\ell-\ell_s)} |h|_H |DF(X_{\ell+1/2})|_H. \end{aligned}$$

Lemma 5.4 *Let $\delta_0 < \frac{1}{2\gamma}$, where γ is defined in Proposition 2.6, be fixed. For any $h \in H$, $0 < \delta \leq \delta_0$, $N \in \mathbb{N}^*$, $T = N\delta$ and $s \in [0, T]$, we have for $t \leq t_{\ell_s}$, where ℓ_s is the integer part of $\frac{s}{\delta}$,*

$$\mathcal{D}_s^h \tilde{X}(t) = 0,$$

for $t_{\ell_s} < t \leq t_{\ell_s+1}$

$$\mathcal{D}_s^h \tilde{X}(t) = R_\delta h$$

and for $t \geq t_{\ell_s+1}$ and m the integer part of $\frac{t}{\delta}$

$$|\mathcal{D}_s^h \tilde{X}(t)|_H^2 \leq c(1 + 2\lambda_0\delta)^{-(m-\ell_s)}(1 - 2\gamma\delta)^{-(m-\ell_s-1)}|h|_H^2.$$

Moreover, for $\alpha > 0$, $\kappa > 0$, $m \geq \ell_s + 1$ and $t_m \leq t \leq t_{m+1}$, we have

$$\begin{aligned} |(-A)^\alpha \mathcal{D}_s^h \tilde{X}(t)|_H &\leq ct_{m-\ell_s}^{-\alpha} (1 + \lambda_0\delta)^{-(m-\ell_s)(1-\alpha)} |h|_H \\ &+ c\delta \sum_{\ell=\ell_s+1}^m t_{m-\ell}^{-1/4-\alpha-\kappa} (1 + 2\lambda_0\delta)^{-1/2(\ell-\ell_s)} (1 - 2\gamma\delta)^{-1/2(\ell-\ell_s)} |h|_H |DF(X_{\ell+1/2})|_H \\ &+ c\delta^{3/4-\alpha-\kappa} (1 + 2\lambda_0\delta)^{-1/2(m-\ell_s)} (1 - 2\gamma\delta)^{-1/2(m-\ell_s)} |DF(X_{m+1/2})|_H |h|_H. \end{aligned}$$

Proof. Using Lemma 5.3 and the definition of \tilde{X} (3.7), the proof of the three first results are obvious. Moreover, we have for any $h \in H$, $s \in [0, T]$, $m \geq \ell_s + 1$ and $t_m \leq t \leq t_{m+1}$

$$\mathcal{D}_s^h \tilde{X}(t) = \mathcal{D}_s^h X_m + (t - t_m)AR_\delta \mathcal{D}_s^h X_m + (t - t_m)R_\delta DF(X_{m+1/2}) \cdot \mathcal{D}_s^h X_{m+1/2}.$$

Then, using computations done in Lemma 5.3, we get for $\alpha > 0$ and $\kappa > 0$

$$\begin{aligned} |(-A)^\alpha \mathcal{D}_s^h \tilde{X}(t)| &\leq c|(-A)^\alpha \mathcal{D}_s^h X_m| + \delta|(-A)^\alpha R_\delta DF(X_{m+1/2}) \cdot \mathcal{D}_s^h X_{m+1/2}| \\ &\leq c|(-A)^\alpha \mathcal{D}_s^h X_m| + \delta^{3/4-\alpha-\kappa} |DF(X_{m+1/2})| |\mathcal{D}_s^h X_{m+1/2}| \\ &\leq ct_{m-\ell_s}^{-\alpha} (1 + \lambda_0\delta)^{-(m-\ell_s)(1-\alpha)} |h| \\ &+ c\delta \sum_{\ell=\ell_s+1}^{m-1} t_{m-\ell}^{-1/4-\alpha-\kappa} (1 + 2\lambda_0\delta)^{-1/2(\ell-\ell_s)} (1 - 2\gamma\delta)^{-1/2(\ell-\ell_s)} |h| |DF(X_{\ell+1/2})| \\ &+ c\delta^{3/4-\alpha-\kappa} (1 + 2\lambda_0\delta)^{-1/2(m-\ell_s)} (1 - 2\gamma\delta)^{-1/2(m-\ell_s)} |DF(X_{m+1/2})| |h| \end{aligned}$$

6 Result

We now give our main result which states that our scheme is of weak order 1/2:

Theorem 6.1 *Let $\delta_0 < \frac{1}{2\gamma}$, where γ is defined in Proposition 2.6, be fixed. For any $N \in \mathbb{N}^*$ and $0 < \kappa < 1/4$, there exists $C(T) > 0$ such that for any $m \in \{0, \dots, N\}$, $M \in \{1, 2, \dots\}$, $x \in \mathcal{C}([0, 1])$ and $\delta < \delta_0$, we have*

$$|\mathbb{E}(\phi(X_m^{(M)})) - \mathbb{E}(\phi(X_x(m\delta)))| \leq C(T)(1 + |x|_{L^\infty}^{20p})|\phi|_{0,2} \left(\delta^{1/2-\kappa} + \frac{1}{\lambda_{M+1}^{1/4-\kappa}} \right),$$

where $T = \delta N$ and $p \in \mathbb{N}$ is defined in (2.2). For the semi-discrete solution with $M = \infty$, we deduce:

$$|\mathbb{E}(\phi(X_m)) - \mathbb{E}(\phi(X_x(m\delta)))| \leq C(T)(1 + |x|_{L^\infty}^{20p})|\phi|_{0,2} \delta^{1/2-\kappa}.$$

The error estimate in space is not optimal since it is deduced from the strong order estimate (3.2). As already mentionned, the aim of this chapter is the study of the weak convergence of the discretization in time. It is of order 1/2 as in the case of Lipschitz linearity - see [20]. To study the weak convergence in time, we introduce a discretization in space for technical reasons.

7 Structure of the proof of the weak approximation result

Let $\delta_0 < \frac{1}{2\gamma}$, where γ is defined in Proposition 2.6, be fixed. We also fix the time step $\delta \leq \delta_0$ and $N \in \mathbb{N}$. We use the notation $T = N\delta$ and $\kappa > 0$ is a parameter, which is supposed to be small enough.

7.1 Strategy

We start with the following decomposition

$$\begin{aligned} \mathbb{E}(\phi(X_m^{(M)})) - \mathbb{E}(\phi(X_x(m\delta))) &= \mathbb{E}(\phi(X_m^{(M)})) - \mathbb{E}(\phi(X_x^{(M)}(m\delta))) \\ &\quad + \mathbb{E}(\phi(X_x^{(M)}(m\delta))) - \mathbb{E}(\phi(X_x(m\delta))). \end{aligned}$$

By (3.2), we directly have for $\kappa > 0$

$$|\mathbb{E}(\phi(X_x^{(M)}(m\delta))) - \mathbb{E}(\phi(X_x(m\delta)))| \leq C(T)(1 + |x|_{L^{4p}}^{4p})|\phi|_{0,1} \frac{1}{\lambda_{M+1}^{1/4-\kappa}}.$$

The proof of the estimate of the first term is very technical, so for pedagogy we first introduce the decomposition of the error, and identify the term which we control later in Section 8. Some crucial estimates on the derivatives of the semi-group with respect to the initial conditions are given below in Sub-Section 7.3 and proved in the Appendix.

7.2 Strategy for the estimate of $\mathbb{E}(\phi(X_m^{(M)})) - \mathbb{E}(\phi(X_x^{(M)}(m\delta)))$

In the following, we work with the finite dimensional approximation, but we omit the parameter $M \in \{1, 2, \dots\}$. The constants appearing below are independent of M .

Let L , the Kolmogorov operator associated with the finite dimensional approximation of (2.1), be defined for $\phi \in C^\infty$ and $x \in H$ by

$$L\phi(x) = \frac{1}{2}\text{Tr}(D^2\phi(x)) + \langle D\phi(x), Ax + F(x) \rangle. \quad (7.1)$$

We also define, for $x \in H$ and $t \geq 0$,

$$u(t, x) = \mathbb{E}[\phi(X_x(t))], \quad (7.2)$$

which is solution of a finite dimensional Kolmogorov equation associated with the finite dimensional approximation of (2.1):

$$\frac{du}{dt}(t, x) = Lu(t, x).$$

The weak error at time $T = N\delta$ can be decomposed as a telescoping sum - where, to simplify, the dependence of the numerical approximation in δ and x is not written:

$$\begin{aligned} \mathbb{E}[\phi(X_x(T))] - \mathbb{E}[\phi(X_N)] &= u(T, x) - \mathbb{E}[u(0, X_N)] \\ &= \sum_{m=0}^{N-1} (\mathbb{E}[u(T - t_m, X_m)] - \mathbb{E}[u(T - t_{m+1}, X_{m+1})]) \\ &= u(T, x) - \mathbb{E}[u(T - \delta, X_1)] + \sum_{m=1}^{N-1} (A^m + B^m + C^m + D^m), \end{aligned} \quad (7.3)$$

where for $1 \leq m \leq N - 1$

$$\begin{aligned}
 A^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), (I - R_\delta)F(\tilde{X}(t)) \rangle dt \\
 B^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), A\tilde{X}(t) - AR_\delta X_m \rangle dt \\
 C^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), R_\delta(F(\tilde{X}(t)) - F(X_{m+1/2})) \rangle dt \\
 D^m &= -\frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left((I - R_\delta R_\delta^*) D^2 u(T-t, \tilde{X}(t)) \right) dt.
 \end{aligned} \tag{7.4}$$

This follows from the use of the Kolmogorov equation and of the Itô formula.

7.3 Bounds on the derivatives of the transition semigroup

In the following, we will need to control the first and the second derivatives of u . The Proposition below is the essential result that we need. Similar estimates are used in [5, 20] to obtain weak order of convergence $1/2$.

Proposition 7.1 *Let p be defined in (2.2). For any $0 \leq \alpha < 1/2$, $0 < t \leq T$ and $x \in \mathcal{C}([0, 1])$, we have*

$$|Du(t, x)|_\alpha \leq C(T)(1 + t^{-\alpha})(1 + |x|_{L^\infty}^{8p})|\phi|_{0,1}. \tag{7.5}$$

Moreover, for any $0 \leq \alpha < 1/2$, $0 \leq \beta < 1/2$, $0 < t \leq T$ and $x \in \mathcal{C}([0, 1])$, we have

$$|(-A)^\alpha D^2 u(t, x)(-A)^\beta|_{\mathcal{L}(H)} \leq C(T)(1 + t^{-(\alpha+\beta)})(1 + |x|_{L^\infty}^{16p})|\phi|_{0,2}. \tag{7.6}$$

A proof of this result can be found in the Appendix.

8 Proof of the estimates

We need to control the terms given in (7.4), according to the decomposition (7.3).

We warn the reader that constants may vary from line to line during the proofs, and that in order to use lighter notations we usually forget to mention dependence on the parameters. We use the generic notation C for such constants. All constants will depend on a parameter $\kappa > 0$, which can be chosen as small as necessary.

To simplify the expressions, we have not mentioned the dependence of the error with respect to the test function ϕ . However, thanks to Proposition 7.1 it is straightforward to give this precision.

We recall that we work with the finite dimensional approximation, but we omit the parameter $M \in \{1, 2, \dots\}$. The constants appearing below are independent of M .

8.1 Estimate of $u(T, x) - \mathbb{E}[u(T - \delta, X_1)]$

The Markov property gives

$$u(T, x) = \mathbb{E}[\phi(X_x(T))] = \mathbb{E}[u(T - \delta, X_x(\delta))].$$

Using Lemmas 4.1 and 4.2 and Proposition 7.1, we get for $0 < \kappa < 1/2$

$$|u(T, x) - \mathbb{E}[u(T - \delta, X_1)]| \leq C(T)(1 + (T - \delta)^{-1/2+\kappa})(\mathbb{E}|X_x(\delta) - X_1|_{-1/2+\kappa}^2)^{1/2}(1 + |x|_{L^\infty}^{8p}).$$

Using (3.5) and (2.12), we can write

$$\begin{aligned} X_x(\delta) - X_1 &= e^{A\delta}x - R_\delta x + \int_0^\delta e^{(\delta-s)A}F(X_x(s))ds - \delta R_\delta F(X_{1/2}) \\ &\quad + \int_0^\delta e^{A(\delta-s)}dW(s) - \int_0^\delta R_\delta dW(s). \end{aligned} \quad (8.1)$$

We have

$$|(-A)^{-1/2+\kappa}(e^{A\delta} - R_\delta)|_{\mathcal{L}(H)} \leq \delta^{1/2-\kappa} \sup_{x \geq \lambda_0} x^{-1/2+\kappa}(e^x - (1+x)^{-1}).$$

Hence:

$$|(-A)^{-1/2+\kappa}(e^{A\delta} - R_\delta)x|_H \leq C\delta^{1/2-\kappa}|x|_H.$$

Since f has polynomial growth, we have for any $x \in \mathcal{C}([0, 1])$, $|F(x)|_H^2 \leq C(1 + |x|_{L^\infty}^{4p})$. Moreover, $|e^{sA}|_{\mathcal{L}(H)} \leq 1$ for $s \geq 0$, $|R_\delta|_{\mathcal{L}(H)} \leq 1$ and $|(-A)^{-1/2+\kappa}|_{\mathcal{L}(H)} \leq c$, then we get, by Lemmas 4.1 and 4.2,

$$\mathbb{E} \left| (-A)^{-1/2+\kappa} \int_0^\delta e^{(\delta-s)A}F(X_x(s))ds - \delta R_\delta F(X_{1/2}) \right|_H^2 \leq C\delta^2(1 + |x|_{L^\infty}^{4p}).$$

Using Proposition 2.5 and Lemma 2.2, we get

$$\begin{aligned} \mathbb{E} \left| (-A)^{-1/2+\kappa} \int_0^\delta e^{(\delta-s)A}dW(s) \right|_H^2 &= \mathbb{E} \int_0^\delta |(-A)^{-1/2+\kappa}e^{(\delta-s)A}|_{\mathcal{L}_2(H)}^2 ds \\ &\leq \text{Tr} \left((-A)^{-1/2-\kappa} \right) \int_0^\delta |(-A)^{3\kappa}e^{(\delta-s)A}|_H |e^{(\delta-s)A}|_H ds \\ &\leq c \int_0^\delta \frac{1}{(\delta-s)^{3\kappa}} ds \\ &\leq c\delta^{1-3\kappa}. \end{aligned}$$

The last term is controlled in the same way: $\mathbb{E} |(-A)^{-1/2+\kappa} \int_0^\delta R_\delta dW(s)|^2 \leq c\delta^{1-3\kappa}$. Therefore we have

$$|u(T, x) - \mathbb{E}[u(T - \delta, X_1)]| \leq C(T)(1 + (T - \delta)^{-1/2+\kappa})\delta^{1/2-3/2\kappa}(1 + |x|_{L^\infty}^{8p}).$$

We thus understand that to obtain weak order 1/2 requires to be careful in the estimate. Here we used Proposition 7.1 with $\alpha = 1/2 - \kappa$ instead of $\alpha = 0$; otherwise looking at $\mathbb{E}|X(\delta, x) - X_1|^2$ is not sufficient. The control of the other terms must be done in the same spirit.

8.2 Estimate of A^m

We can not use directly Cauchy-Schwarz inequality and Proposition 7.1 for $\alpha = 0$. We first rewrite and bound A^m by:

$$\begin{aligned} |A^m|_H &= \left| \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \delta A R_\delta F(\tilde{X}(t)) \rangle dt \right|_H \\ &= \left| \mathbb{E} \int_{t_m}^{t_{m+1}} \delta \langle (-A)^{1/2-\kappa} Du(T-t, \tilde{X}(t)), (-A)^{1/2+\kappa} R_\delta F(\tilde{X}(t)) \rangle dt \right|_H \\ &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \delta |Du(T-t, \tilde{X}(t))|_{1/2-\kappa} |(-A)^{1/2+\kappa} R_\delta|_{\mathcal{L}(H)} |F(\tilde{X}(t))|_H dt, \end{aligned}$$

where $0 < \kappa < 1/2$. We now use Cauchy-Schwarz inequality, Proposition 7.1 and Lemmas 3.2 and 4.2 to obtain:

$$|A^m| \leq C(T)\delta^{1/2-\kappa}(1 + |x|_{L^\infty}^{12p}) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1/2+\kappa}) dt$$

and

$$\begin{aligned} \sum_{m=1}^{N-1} |A^m| &\leq C(T)\delta^{1/2-\kappa}(1 + |x|_{L^\infty}^{12p})(T + \int_0^T (T-t)^{-1/2+\kappa} dt) \\ &\leq C(T)\delta^{1/2-\kappa}(1 + |x|_{L^\infty}^{12p}). \end{aligned}$$

8.3 Estimate of B^m

Using expression (3.7), we decompose B^m :

$$\begin{aligned} B^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), A(I - R_\delta)X_m \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \langle Du(T-t, \tilde{X}(t)), A^2 R_\delta X_m \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} (t - t_m) \langle Du(T-t, \tilde{X}(t)), AR_\delta F(X_{m+1/2}) \rangle dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t AR_\delta dW(s) \rangle dt. \\ &:= B_1^m + B_2^m + B_3^m + B_4^m. \end{aligned}$$

8.3.1 Estimate of B_1^m

Using $I - R_\delta = -\delta AR_\delta$ and expressions (3.5) and (3.6), we get

$$\begin{aligned} B_1^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \delta \langle Du(T-t, \tilde{X}(t)), A^2 R_\delta R_\delta^m x \rangle dt \\ &\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \delta \langle Du(T-t, \tilde{X}(t)), A^2 R_\delta \delta \sum_{\ell=0}^{m-1} R_\delta^{m-\ell} F(X_{\ell+1/2}) \rangle dt \\ &\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \delta \langle Du(T-t, \tilde{X}(t)), \int_0^{t_m} A^2 R_\delta^{m-\ell_s+1} dW(s) \rangle dt \\ &:= B_{1,1}^m + B_{1,2}^m + B_{1,3}^m. \end{aligned}$$

We will now study each term, the most complicated is the last.

1. **Estimate of $B_{1,1}^m$.** We have

$$\begin{aligned} |B_{1,1}^m| &\leq \delta \mathbb{E} \int_{t_m}^{t_{m+1}} |Du(T-t, \tilde{X}(t))|_{1/2-\kappa} |(-A)^{1/2+2\kappa} R_\delta|_{\mathcal{L}(H)} |(-A)^{1-\kappa} R_\delta^m x|_H dt \\ &\leq C(T)\delta^{1/2-2\kappa}(1 + |x|_{L^\infty}^{8p}) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1/2+\kappa}) dt \frac{1}{t_m^{1-\kappa}} |x|_H, \end{aligned}$$

by Proposition 7.1 and Lemmas 3.2 and 4.2. Then, it follows easily

$$\begin{aligned} \sum_{m=1}^{N-1} |B_{1,1}^m| &\leq C(T)(1 + |x|_{L^\infty}^{8p+1})\delta^{1/2-2\kappa} \sum_{m=1}^{N-1} \frac{1}{t_m^{1-\kappa}} \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1/2+\kappa}) dt \\ &\leq C(T)(1 + |x|_{L^\infty}^{8p+1})\delta^{1/2-2\kappa}. \end{aligned}$$

2. **Estimate of $B_{1,2}^m$.** By Proposition 7.1, Cauchy-Schwarz inequality and Lemmas 3.2 and 4.2, we can write

$$\begin{aligned}
|B_{1,2}^m| &\leq \delta \mathbb{E} \int_{t_m}^{t_{m+1}} |Du(T-t, \tilde{X}(t))|_{1/2-\kappa} |(-A)^{1/2+2\kappa} R_\delta|_{\mathcal{L}(H)} \\
&\quad \times \delta \sum_{\ell=0}^{m-1} |(-A)^{1-\kappa} R_\delta^{m-\ell}|_{\mathcal{L}(H)} |F(X_{\ell+1/2})|_H dt \\
&\leq C(T) \int_{t_m}^{t_{m+1}} (1+(T-t)^{-1/2+2\kappa}) dt \delta^{1/2-2\kappa} (1+|x|_{L^\infty}^{12p}) \delta \sum_{\ell=1}^m \frac{1}{t_\ell^{1-\kappa}} \\
&\leq C(T) \int_{t_m}^{t_{m+1}} (1+(T-t)^{-1/2+\kappa}) dt \delta^{1/2-2\kappa} (1+|x|_{L^\infty}^{12p}) \int_0^T \frac{1}{t^{1-\kappa}} dt
\end{aligned}$$

and we obtain

$$\sum_{m=1}^{N-1} |B_{1,2}^m| \leq C(T) (1+|x|_{L^\infty}^{12p}) \delta^{1/2-2\kappa}.$$

3. **Estimate of $B_{1,3}^m$.** The analysis of this term is more complicated. As in [20] the problem lies in the regularity in space of the process, due to whiteness in space of the driving noise. The strategy used to control $B_{1,1}^m$ and $B_{1,2}^m$ above would only give an order of convergence 1/4, while we expect 1/2. To obtain the correct order of convergence 1/2 we use a Malliavin integration by parts.

By Malliavin integration by parts formula (Lemma 5.1), Proposition 7.1 and Lemmas 2.2, 3.2 and 4.2, we get

$$\begin{aligned}
&|\mathbb{E} \int_{t_m}^{t_{m+1}} \delta \langle Du(T-t, \tilde{X}(t)), \int_0^{t_m} A^2 R_\delta^{m-\ell_s+1} dW(s) \rangle dt| \\
&= |\mathbb{E} \int_{t_m}^{t_{m+1}} \int_0^{t_m} \text{Tr} \left(\delta R_\delta^{m-\ell_s+1} (-A)^2 D^2 u(T-t, \tilde{X}(t)) \mathcal{D}_s \tilde{X}^h(t) \right) ds dt| \\
&\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \int_0^{t_m} |(-A)^{1/2-\kappa} D^2 u(T-t, \tilde{X}(t)) (-A)^{1/2-\kappa} | \text{Tr}((-A)^{-1/2-\kappa}) \\
&\quad \times |(-A)^{2\kappa} \mathcal{D}_s \tilde{X}(t)| |\delta (-A)^{1/2+4\kappa} R_\delta|_{\mathcal{L}(H)} |(-A)^{1-3\kappa} R_\delta^{m-\ell_s}|_{\mathcal{L}(H)} ds dt \\
&\leq C(T) \delta^{1/2-4\kappa} (1+|x|_{L^\infty}^{16p}) \int_{t_m}^{t_{m+1}} (1+(T-t)^{-1+\kappa}) \int_0^{t_m} \frac{\left(\mathbb{E} |(-A)^{2\kappa} \mathcal{D}_s \tilde{X}(t)|^2 \right)^{1/2}}{(1+\lambda_0 \delta)^{3\kappa(m-\ell_s)} t_{m-\ell_s}^{1-3\kappa}} ds dt.
\end{aligned}$$

Using Lemma 5.4, we get for $\kappa < 1/4$

$$\begin{aligned}
\int_0^{t_m} \frac{|(-A)^{2\kappa} \mathcal{D}_s \tilde{X}(t)|}{(1 + \lambda_0 \delta)^{3\kappa(m-\ell_s)} t_{m-\ell_s}^{1-3\kappa}} ds &\leq c \int_0^{t_m} \frac{1}{t_{m-\ell_s}^{1-\kappa} (1 + \lambda_0 \delta)^{(m-\ell_s)(1+\kappa)}} ds \\
&+ c \int_0^{t_m} \frac{1}{t_{m-\ell_s}^{1-3\kappa}} e^{\gamma \delta(m-\ell_s)} ds \\
&\times \delta \sum_{\ell=\ell_s+1}^{m-1} \frac{1}{t_{m-\ell}^{1/4+3\kappa}} (1 + \sup_{\ell=0, \dots, m-1} |X_{\ell+1/2}|^{4p}) \\
&+ c \delta^{3/4-3\kappa} e^{\gamma T} \int_0^{t_m} \frac{1}{t_{m-\ell_s}^{1-3\kappa}} ds (1 + |X_{m+1/2}|^{4p}) \\
&\leq c \int_0^T \frac{1}{t^{1-\kappa}} dt \\
&+ C(T) \int_0^T \frac{1}{s^{1-3\kappa}} ds \int_0^T \frac{1}{t^{1/4+3\kappa}} dt (1 + \sup_{\ell=0, \dots, m} |X_{\ell+1/2}|^{4p}) \\
&+ C(T) \int_0^T \frac{1}{t^{1-3\kappa}} dt (1 + \sup_{\ell=0, \dots, m} |X_{\ell+1/2}|^{4p}) \\
&\leq C(T) (1 + \sup_{\ell=0, \dots, m-1} |X_{\ell+1/2}|_{L^\infty}^{4p}),
\end{aligned}$$

then we obtain

$$\begin{aligned}
|\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_0^{t_m} A^2 R_\delta^{m-\ell_s+1} dW(s) \rangle dt| \\
\leq C(T) \delta^{1/2-4\kappa} (1 + |x|_{L^\infty}^{20p}) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+\kappa}) dt.
\end{aligned}$$

Finally, we have

$$\sum_{m=1}^{N-1} |B_{1,3}^m| \leq C(T) \delta^{1/2-4\kappa} (1 + |x|_{L^\infty}^{20p})$$

and

$$\sum_{m=1}^{N-1} |B_1^m| \leq C(T) \delta^{1/2-4\kappa} (1 + |x|_{L^\infty}^{20p}).$$

8.3.2 Estimate of B_2^m

The estimate of B_2^m is similar to the estimate of B_1^m , then we have

$$\left| \sum_{m=1}^{N-1} B_2^m \right| \leq C(T) \delta^{1/2-4\kappa} (1 + |x|_{L^\infty}^{20p}).$$

8.3.3 Estimate of B_3^m

We have

$$\begin{aligned}
|B_3^m| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} |(-A)^{1/2-\kappa} Du(T-t, \tilde{X}(t))|_H |(-A)^{1/2+\kappa} R_\delta|_{\mathcal{L}(H)} \delta |F(X_{m+1/2})|_H dt \\
&\leq C(T) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1/2+\kappa}) dt \delta^{1/2-\kappa} (1 + |x|_{L^\infty}^{12p})
\end{aligned}$$

by Proposition 7.1, Lemmas 4.2 and 3.2 and Cauchy Schwarz inequality. We then have

$$\sum_{m=1}^{N-1} |B_3^m| \leq C(T)\delta^{1/2-\kappa}(1 + |x|_{L^\infty}^{12p}).$$

8.3.4 Estimate of B_4^m

We again use the integration by parts formula to rewrite B_4^m :

$$\begin{aligned} B_4^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t AR_\delta dW(s) \rangle dt \\ &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \text{Tr}(D^2u(T-t, \tilde{X}(t))\mathcal{D}_s\tilde{X}(t)AR_\delta) ds dt \end{aligned}$$

From Lemma 5.4, for $t_m \leq s \leq t \leq t_{m+1}$ we have $\mathcal{D}_s^l \tilde{X}(t) = R_\delta \ell$. Then, as previously, we have

$$\begin{aligned} |B_4^m| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} (t-t_m) |(-A)^{1/2+\kappa/2} R_\delta|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa/2}) |(-A)^\kappa R_\delta|_{\mathcal{L}(H)} \\ &\quad \times |(-A)^{1/2-\kappa/2} D^2u(T-t, \tilde{X}(t))(-A)^{1/2-\kappa/2}| dt \\ &\leq C(T)(1 + |x|_{L^\infty}^{16p}) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+\kappa}) dt \delta^{1/2-\frac{3}{2}\kappa} \end{aligned}$$

and

$$\sum_{m=1}^{N-1} |B_4^m| \leq C(T)(1 + |x|_{L^\infty}^{16p}) \delta^{1/2-\frac{3}{2}\kappa}.$$

8.3.5 Estimate of B^m : Conclusion

Finally, we have

$$\sum_{m=1}^{N-1} |B^m| \leq C(T)(1 + |x|_{L^\infty}^{20p}) \delta^{1/2-\kappa}.$$

8.4 Estimate of C^m

Let $t_m \leq t < t_{m+1}$ and $i \in \mathbb{N}$ be fixed, the Itô formula give us

$$\begin{aligned} F_i(\tilde{X}(t)) &= F_i(X_m) + \int_{t_m}^t \langle DF_i(\tilde{X}(s)), AR_\delta X_m \rangle ds \\ &\quad + \int_{t_m}^t \langle DF_i(\tilde{X}(s)), R_\delta F(X_{m+1/2}) \rangle ds \\ &\quad + \int_{t_m}^t \langle DF_i(\tilde{X}(s)), R_\delta dW(s) \rangle + \frac{1}{2} \int_{t_m}^t \text{Tr}(R_\delta R_\delta^* D^2 F_i(\tilde{X}(s))) ds. \end{aligned}$$

The Taylor expansion at the first order give us

$$F_i(X_{m+1/2}) = F_i(X_m) + \delta \int_0^1 \langle DF_i(X_m + \theta(X_{m+1/2} - X_m)), F(X_{m+1/2}) \rangle d\theta.$$

We can now rewrite C^m :

$$\begin{aligned}
C^m &= \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{i \in \mathbb{N}} \partial_i u(T-t, \tilde{X}(t)) \delta \int_0^1 \langle R_\delta D F_i(x_m + \theta(X_{m+1/2} - X_m)), F(X_{m+1/2}) d\theta \rangle dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{i \in \mathbb{N}} \partial_i u(T-t, \tilde{X}(t)) \int_{t_m}^t \langle R_\delta D F_i(\tilde{X}(s)), A R_\delta X_m ds \rangle dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{i \in \mathbb{N}} \partial_i u(T-t, \tilde{X}(t)) \int_{t_m}^t \langle R_\delta D F_i(\tilde{X}(s)), R_\delta F(X_{m+1/2}) \rangle ds dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{i \in \mathbb{N}} \partial_i u(T-t, \tilde{X}(t)) \int_{t_m}^t \langle R_\delta D F_i(\tilde{X}(s)), R_\delta dW(s) \rangle dt \\
&\quad - \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \sum_{i \in \mathbb{N}} \partial_i u(T-t, \tilde{X}(t)) \int_{t_m}^t \text{Tr} \left(R_\delta^3 D^2 F_i(\tilde{X}(s)) \right) ds dt \\
&:= C_1^m + C_2^m + C_3^m + C_4^m + C_5^m.
\end{aligned}$$

We now estimate each term.

8.4.1 Estimate of C_1^m

To bound this term, we use the Cauchy-Schwarz inequality, Lemma 4.2 and Proposition 7.1 where $\alpha = 0$. We get

$$\begin{aligned}
|C_1^m| &\leq \delta \int_{t_m}^{t_{m+1}} \int_0^1 \left(\mathbb{E} |Du(T-t, \tilde{X}(t))|^2 \right)^{1/2} \left(\mathbb{E} |DF(X_m + \theta(X_{m+1/2} - X_m))|^4 \right)^{1/4} \\
&\quad \times \left(\mathbb{E} |F(X_{m+1/2})|^4 \right)^{1/4} d\theta dt \\
&\leq C(T) \delta^2 (1 + |x|_{L^\infty}^{16p})
\end{aligned}$$

and

$$\left| \sum_{m=1}^{N-1} C_1^m \right| \leq C(T) \delta (1 + |x|_{L^\infty}^{16p}).$$

8.4.2 Estimate of C_2^m

Using (3.5) and (3.6), we have the following decomposition for C_2^m :

$$\begin{aligned}
C_2^m &= - \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t \langle R_\delta D F(\tilde{X}(s)), A R_\delta^{m+1} x \rangle ds \rangle dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t \langle R_\delta D F(\tilde{X}(s)), \delta \sum_{\ell=0}^{m-1} A R_\delta R_\delta^{m-\ell} F(X_{\ell+1/2}) \rangle ds \rangle dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t \langle R_\delta D F(\tilde{X}(s)), \int_0^{t_m} A R_\delta R_\delta^{m-\ell_r} dW(r) \rangle ds \rangle dt \\
&:= C_{2,1}^m + C_{2,2}^m + C_{2,3}^m.
\end{aligned}$$

We will now study each term, the most complicated is the last.

1. Estimate of $C_{2,1}^m$.

Using Cauchy-Schwarz inequality, Lemmas 3.2 and 4.2 and Proposition 7.1, we get

$$\begin{aligned}
|C_{2,1}^m| &= |\mathbb{E} \int_{t_m}^{t_{m+1}} \langle Du(T-t, \tilde{X}(t)), \int_{t_m}^t \langle R_\delta DF(\tilde{X}(s)), (-A)^\kappa R_\delta (-A)^{1-\kappa} R_\delta^m x \rangle ds \rangle dt| \\
&\leq \int_{t_m}^{t_{m+1}} \int_{t_m}^t \left(\mathbb{E} |Du(T-t, \tilde{X}(t))|^2 \right)^{1/2} |R_\delta| \left(\mathbb{E} |DF(\tilde{X}(s))|^2 \right)^{1/2} |(-A)^\kappa R_\delta| |(-A)^{1-\kappa} R_\delta^m x| ds dt \\
&\leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{1-\kappa} \delta \frac{1}{t_m^{1-\kappa}}.
\end{aligned}$$

Then, we have

$$\begin{aligned}
\sum_{m=1}^{N-1} |C_{2,1}^m| &\leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{1-\kappa} \delta \sum_{m=1}^{N-1} \frac{1}{t_m^{1-\kappa}} dt \\
&\leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{1-\kappa} \int_0^T \frac{1}{t^{1-\kappa}} dt \\
&\leq C(T) T^\kappa (1 + |x|_{L^\infty}^{12p}) \delta^{1-\kappa}.
\end{aligned}$$

2. Estimate of $C_{2,2}^m$.

Using Cauchy-Schwarz inequality, Lemmas 4.2 and 3.2 and Proposition 7.1, we get

$$\begin{aligned}
|C_{2,2}^m| &\leq \int_{t_m}^{t_{m+1}} \int_{t_m}^t \left(\mathbb{E} |Du(T-t, \tilde{X}(t))|^4 \right)^{1/4} |R_\delta| \left(\mathbb{E} |DF(\tilde{X}(s))|^4 \right)^{1/4} |(-A)^\kappa R_\delta| \\
&\quad \times \delta \sum_{\ell=0}^{m-1} |(-A)^{1-\kappa} R_\delta^{m-\ell}| \left(\mathbb{E} |F(X_{\ell+1/2})|^2 \right)^{1/2} dr ds dt \\
&\leq C(T) (1 + |x|_{L^\infty}^{16p}) \int_{t_m}^{t_{m+1}} \int_{t_m}^t ds dt \delta^{-\kappa} \delta \sum_{\ell=0}^{m-1} \frac{1}{t_{m-\ell}^{1-\kappa}} \\
&\leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta \delta^{1-\kappa}
\end{aligned}$$

and

$$\sum_{m=1}^{N-1} |C_{2,2}^m| \leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1-\kappa}.$$

3. Estimate of $C_{2,3}^m$.

We use the integration by parts formula of Lemma 5.1 to get

$$\begin{aligned}
C_{2,3}^m &= -\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_{i,j,k} \partial_i u(T-t, \tilde{X}(t)) R_\delta \partial_j F_i(\tilde{X}(s)) \langle AR_\delta^{m+1-\ell_r} f_k, f_j \rangle d\beta_k(r) ds dt \\
&= -\mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_{i,j,k,n} \partial_{i,n}^2 u(T-t, \tilde{X}(t)) \langle \mathcal{D}_r^k \tilde{X}(t), f_n \rangle R_\delta \partial_j F_i(\tilde{X}(s)) \langle AR_\delta^{m+1-\ell_r} f_k, f_j \rangle dr ds dt \\
&\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_{i,j,k,n} \partial_i u(T-t, \tilde{X}(t)) R_\delta \partial_{j,n}^2 F_i(\tilde{X}(s)) \langle \mathcal{D}_r^k \tilde{X}(s), f_n \rangle \langle AR_\delta^{m+1-\ell_r} f_k, f_j \rangle dr ds dt \\
&:= C_{2,3,1}^m + C_{2,3,2}^m.
\end{aligned}$$

Using the Cauchy-Schwarz inequality, Lemmas 4.2, 3.2 and 5.4 and Proposition 7.1,

we get

$$\begin{aligned}
& |C_{2,3,2}^m| \\
&= \left| \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_i \text{Tr} \left[\mathcal{D}_r \tilde{X}(s) R_\delta D^2 F_i(\tilde{X}(s)) A R_\delta^{m+1-\ell_r} \right] \partial_i u(T-t, \tilde{X}(t)) dr ds dt \right| \\
&\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \text{Tr}((-A)^{-1/2-\kappa}) |\mathcal{D}_r \tilde{X}(s)| |R_\delta| |D^2 F(\tilde{X}(s))| |(-A)^{1/2+2\kappa} R_\delta| \\
&\quad \times |(-A)^{1-\kappa} R_\delta^{m-\ell_r}| |Du(T-t, \tilde{X}(t))| dr ds dt \\
&\leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{3/2-2\kappa} \int_0^{t_m} \frac{1}{t_{m-\ell_r}^{1-\kappa}} dr ds dt \\
&\leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{3/2-2\kappa}.
\end{aligned}$$

We used that for $0 \leq r \leq t_m \leq s < t_{m+1}$ and $\ell \in H$, $|\mathcal{D}_r^\ell \tilde{X}(s)| \leq ce^{\gamma T} |\ell|$. For the other term, we have

$$\begin{aligned}
C_{2,3,1}^m &= - \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_{i,k} \langle \mathcal{B}_i(s, t) A R_\delta^{m+1-\ell_r} f_k, \mathcal{D}_r^k \tilde{X}(t) \rangle dr ds dt \\
&= \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \int_0^{t_m} \sum_i \text{Tr} \left[\mathcal{D}_r \tilde{X}(t) \mathcal{B}_i(s, t) A R_\delta^{m+1-\ell_r} \right] dr ds dt,
\end{aligned}$$

where we define a linear operator on H by

$$\begin{aligned}
\langle \mathcal{B}_i(s, t) h, k \rangle &= \langle R_\delta D F_i(\tilde{X}(s)), h \rangle \sum_n \partial_{i,n}^2 u(T-t, \tilde{X}(t)) \langle k, f_n \rangle \\
&= \langle R_\delta D F_i(\tilde{X}(s)) \rangle \langle D^2 u(T-t, \tilde{X}(t)) \cdot h, k \rangle.
\end{aligned}$$

We have

$$\sum_i \langle \mathcal{B}_i(s, t) h, k \rangle = D^2 u(T-t, \tilde{X}(t)) \cdot (R_\delta D F(\tilde{X}(s)) \cdot h, k),$$

then, using the same ideas than above,

$$\begin{aligned}
& \mathbb{E} \left| \sum_i \text{Tr} \left[\mathcal{D}_r \tilde{X}(t) \mathcal{B}_i(s, t) A R_\delta^{m+1-\ell_r} \right] \right| \\
&\leq \mathbb{E} \left(|\mathcal{D}_r \tilde{X}(t)| |R_\delta| |D F(\tilde{X}(s))| |D^2 u(T-t, \tilde{X}(t))| |(-A)^{1-\kappa} R_\delta^{m-\ell_r}| \right. \\
&\quad \left. \times |(-A)^{1/2+2\kappa} R_\delta| |\text{Tr}((-A)^{-1/2-\kappa})| \right) \\
&\leq C(T) (1 + |x|_{L^\infty}^{20(p-1)}) t_{m-\ell_r}^{-1+\kappa} \delta^{-1/2-2\kappa},
\end{aligned}$$

and

$$|C_{2,3,1}^m| \leq C(T) (1 + |x|_{L^\infty}^{20p}) \delta^{3/2-2\kappa}.$$

Finally, we have

$$\sum_{m=1}^{N-1} |C_{2,3}^m| \leq C(T) (1 + |x|_{L^\infty}^{20p}) \delta^{1/2-2\kappa}.$$

8.4.3 Estimate of C_3^m

To bound this term, we need the Cauchy-Schwarz inequality, Lemma 4.2 and Proposition 7.1 where $\alpha = 0$. We get

$$\begin{aligned} |C_3^m| &\leq \int_{t_m}^{t_{m+1}} \int_{t_m}^t \left(\mathbb{E} |Du(T-t, \tilde{X}(t))|^2 \right)^{1/2} |R_\delta| \left(\mathbb{E} |DF(\tilde{X}(s))|^4 \right)^{1/4} |R_\delta| \left(\mathbb{E} |F(X_{m+1/2})|^4 \right)^{1/4} ds dt \\ &\leq C(T) \delta^2 (1 + |x|_{L^\infty}^{16p}) \end{aligned}$$

and

$$\left| \sum_{m=1}^{N-1} C_3^m \right| \leq C(T) \delta (1 + |x|_{L^\infty}^{16p}).$$

8.4.4 Estimate of C_4^m

Thanks to a Malliavin integration by parts, we can write

$$\begin{aligned} C_4^m &= - \sum_{i,j,k} \mathbb{E} \int_{t_m}^{t_{m+1}} \partial_i u(T-t, \tilde{X}(t)) \int_{t_m}^t R_\delta \partial_k F_i(\tilde{X}(s)) \langle R_\delta f_j, f_k \rangle d\beta_j(s) dt \\ &= - \sum_{i,j,k,n} \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \partial_{i,n}^2 u(T-t, \tilde{X}(t)) \langle \mathcal{D}_s^j \tilde{X}(t), f_n \rangle R_\delta \partial_k F_i(\tilde{X}(s)) \langle R_\delta f_j, f_k \rangle ds dt \\ &\quad - \sum_{i,j,k,n} \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \partial_i u(T-t, \tilde{X}(t)) R_\delta \partial_{k,n}^2 F_i(\tilde{X}(s)) \langle \mathcal{D}_s^j \tilde{X}(s), f_n \rangle \langle R_\delta f_j, f_k \rangle ds dt \\ &= - \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \text{Tr} \left(\mathcal{D}_s \tilde{X}(t) \mathcal{B}_i(s, t) R_\delta \right) ds dt \\ &\quad - \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \text{Tr} \left(R_\delta^2 D^2 F_i(\tilde{X}(s)) \mathcal{D}_s \tilde{X}(s) \right) \partial_i u(T-t, \tilde{X}(t)) ds dt, \end{aligned}$$

where we define a linear operator on H by

$$\begin{aligned} \langle \mathcal{B}_i(s, t) h, k \rangle &= \langle R_\delta D F_i(\tilde{X}(s)), h \rangle \sum_n \partial_{i,n}^2 u(T-t, \tilde{X}(t)) \langle k, f_n \rangle \\ &\quad \langle R_\delta D F_i(\tilde{X}(s)), h \rangle \langle D^2 u(T-t, \tilde{X}(t)) \cdot f_i, k \rangle. \end{aligned}$$

We have $\sum_i \langle \mathcal{B}_i(s, t) h, k \rangle = D^2 u(T-t, \tilde{X}(t)) \cdot (R_\delta D F(\tilde{X}(s)) \cdot h, k)$ and for $t_m \leq s \leq t < t_{m+1}$,

$$\mathcal{D}_s^h \tilde{X}(t) = R_\delta h,$$

so we can write

$$\left| \sum_i \text{Tr} \left(\mathcal{D}_s \tilde{X}(t) \mathcal{B}_i(s, t) R_\delta \right) \right| \leq \text{Tr}((-A)^{-1/2-\kappa}) |(-A)^{1/2+\kappa} R_\delta| |R_\delta|^2 |D^2 u(T-t, \tilde{X}(t))| |DF(\tilde{X}(s))|$$

and

$$\left| \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \text{Tr} \left(\mathcal{D}_s \tilde{X}(t) \mathcal{B}_i(s, t) R_\delta \right) ds dt \right| \leq C(T) (1 + |x|_{L^\infty}^{20p}) \delta^{3/2-\kappa},$$

by Lemma 4.2 and Proposition 7.1 Using the same ideas, we have

$$\left| \mathbb{E} \int_{t_m}^{t_{m+1}} \int_{t_m}^t \sum_i \text{Tr} \left(R_\delta^2 D^2 F_i(\tilde{X}(s)) \mathcal{D}_s \tilde{X}(s) \right) ds dt \right| \leq C(T) (1 + |x|_{L^\infty}^{12p}) \delta^{3/2-\kappa}$$

and

$$\left| \sum_{m=1}^{N-1} C_4^m \right| \leq C(T) \delta^{1/2-\kappa} (1 + |x|_{L^\infty}^{20p}).$$

8.4.5 Estimate of C_5^m

The control of this term is easy. Indeed, using Lemmas 3.2 and 2.2, we have for $i \in \mathbb{N}$

$$\begin{aligned} \left| \text{Tr} \left(R_\delta^3 D^2 F_i(\tilde{X}(s)) \right) \right| &\leq \text{Tr}((-A)^{-1/2-\kappa}) |(-A)^{1/2+\kappa} R_\delta|_{\mathcal{L}(H)} |R_\delta|_{\mathcal{L}(H)}^2 |D^2 F(\tilde{X}(s))|_H \\ &\leq C \delta^{-1/2-\kappa} (1 + |\tilde{X}(s)|_{L^{4p}}^{4p}). \end{aligned}$$

Then, using Cauchy-Schwarz inequality, Proposition 7.1 and Lemma 4.2, we obtain

$$|C_5^m| \leq C(T) \delta \delta^{1/2-\kappa} (1 + |x|_{L^\infty}^{12p})$$

and

$$\left| \sum_{m=1}^{N-1} C_5^m \right| \leq C(T) \delta^{1/2-\kappa} (1 + |x|_{L^\infty}^{12p}).$$

8.4.6 Estimate of C^m

Finally, we get

$$\sum_{m=1}^{N-1} |C^m| \leq C(T) (1 + |x|_{L^\infty}^{20p}) \delta^{1/2-\kappa}.$$

8.5 Estimate of D^m

We have, using the symmetry of R_δ ,

$$\frac{1}{2}I - \frac{1}{2}R_\delta R_\delta^* = R_\delta(I - R_\delta)^* + \frac{1}{2}(I - R_\delta)(I - R_\delta)^*,$$

and

$$\begin{aligned} D^m &= \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left((I - R_\delta R_\delta^*) D^2 u(T-t, \tilde{X}(t)) \right) dt \\ &= \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left((I - R_\delta)(I - R_\delta)^* D^2 u(T-t, \tilde{X}(t)) \right) dt \\ &\quad + \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr} \left(R_\delta(I - R_\delta)^* D^2 u(T-t, \tilde{X}(t)) \right) dt \\ &:= D_1^m + D_2^m. \end{aligned}$$

8.5.1 Estimate of D_1^m .

Using $I - R_\delta = -\delta A R_\delta$, Lemmas 3.2, 4.2 and 2.2 and Proposition 7.1, we have

$$\begin{aligned} |D_1^m| &\leq \frac{1}{2} \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}((-A)^{-1/2-\kappa} (I - R_\delta)^2 (-A)^{-1/2+3\kappa}) \\ &\quad \times |(-A)^{1/2-\kappa} D^2 u(T-t, \tilde{X}(t)) (-A)^{1/2-\kappa}|_{\mathcal{L}(H)} dt \\ &\leq C(T) |(-A)^{-1/2+3\kappa} (I - R_\delta)|_{\mathcal{L}(H)} |I - R_\delta|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa}) \\ &\quad \times \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+2\kappa}) \mathbb{E}(1 + |\tilde{X}(t)|_{L^\infty}^{16p}) dt \\ &\leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1/2-3\kappa} \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+2\kappa}) dt. \end{aligned}$$

Then

$$\sum_{m=1}^{N-1} |D_1^m| \leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1/2-3\kappa}. \quad (8.2)$$

8.5.2 Estimate of D_2^m .

Using Lemmas 3.2 and 2.2 and Proposition 7.6, we have

$$\begin{aligned}
 |D_2^m| &\leq \mathbb{E} \int_{t_m}^{t_{m+1}} \text{Tr}((-A)^{-1/2+\kappa} R_\delta (I - R_\delta) (-A)^{-1/2+\kappa}) \\
 &\quad \times |(-A)^{1/2-\kappa} D^2 u(T-t, \tilde{X}(t)) (-A)^{1/2-\kappa}|_{\mathcal{L}(H)} dt \\
 &\leq C(T) (1 + |x|_{L^\infty}^{16p}) |(-A)^{-1/2+\kappa} (I - R_\delta) (-A)^{2\kappa}|_{\mathcal{L}(H)} \text{Tr}((-A)^{-1/2-\kappa}) \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+2\kappa}) dt \\
 &\leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1/2-3\kappa} \int_{t_m}^{t_{m+1}} (1 + (T-t)^{-1+2\kappa}) dt.
 \end{aligned}$$

Then

$$\sum_{m=1}^{N-1} |D_2^m| \leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1/2-3\kappa}. \quad (8.3)$$

8.5.3 Estimate of D^m : conclusion

With (8.2) and (8.3), we get

$$\sum_{m=1}^{N-1} |D^m| \leq C(T) (1 + |x|_{L^\infty}^{16p}) \delta^{1/2-3\kappa}. \quad (8.4)$$

8.6 Conclusion

With the above estimate, we get

$$|\mathbb{E}(\phi(X_x(T))) - \mathbb{E}(\phi(X_N))| \leq C(T) (1 + |x|_{L^\infty}^{20p}) \delta^{1/2-\kappa}.$$

9 Appendix: Bounds on moments of the scheme

To prove Lemma 4.2, we introduce a process $(Z_m)_{m \in \mathbb{N}}$ defined for any $m \in \mathbb{N}$ by $Z_m = X_m - w_m$, where the process $(w_m)_{m \in \mathbb{N}}$ is the numerical approximation of W^A - defined in (2.9) - with the numerical schema (3.5) - with $F = 0$ - and use bounds on moments of $(w_m)_{m \in \mathbb{N}}$ to obtain bounds of moments for $(Z_m)_{m \in \mathbb{N}}$ and then for $(X_m)_{m \in \mathbb{N}}$. Therefore, we first show the following Lemma:

Lemma 9.1 *Let $\delta > 0$, $N \in \mathbb{N}^*$ and $T = N\delta$ be fixed. Let $(w_m)_{m=0, \dots, N}$ be the numerical approximation of W^A on $[0, T]$ with the numerical schema (3.5) - with $F = 0$; it is defined by $w_0 = 0$ and for $m = 0, \dots, N-1$ by*

$$w_{m+1} = R_\delta w_m + \sqrt{\delta} R_\delta \chi_{m+1}.$$

We have for $\ell \in \mathbb{N}^*$

$$\mathbb{E} \sup_{m=0, \dots, N-1} |w_m|_{L^\infty}^\ell \leq \infty. \quad (9.1)$$

Proof. To prove Lemma 9.1, we will proceed as follows. First we define a continuous interpolation of the discrete scheme $(w_m)_{m=0, \dots, N-1}$. Let \tilde{X} be defined on $[0, T]$ by

$$\tilde{W}(t) = w_m + (t - t_m) A R_\delta w_m + \int_{t_m}^t R_\delta dW(s) \quad t \in [t_m, t_{m+1}).$$

In the following, we set

$$\tilde{W}(t)(\xi) = \tilde{W}(t, \xi), \quad 0 \leq t \leq T, \quad \xi \in (0, 1).$$

Then, we show the following result: For any $0 < \kappa < 1/2$, there exists $C(T) > 0$ such that for every $\xi \in (0, 1)$, $\eta \in (0, 1)$, $t \in [0, T]$ and $s \in [0, T]$

$$\mathbb{E} |\tilde{W}(t, \xi) - \tilde{W}(t, \eta)|^2 \leq C(T) |\eta - \xi|^{1-\kappa} \quad (9.2)$$

and

$$\mathbb{E} |\tilde{W}(t, \eta) - \tilde{W}(s, \eta)|^2 \leq C(T) |t - s|^{1/2-\kappa}. \quad (9.3)$$

Finally, we use Kolomogorov's test - see chapter 3 of [16] - to prove

$$\mathbb{E} \sup_{t \in [0, T]} |\tilde{W}(t)|_{L^\infty}^\ell < \infty$$

and (9.1) follows.

Let us prove (9.2). First, we remark that we can show by induction for $m = 1, \dots, N$ that $w_m = \sum_{\ell=1}^m \int_0^\delta R_\delta^\ell dW(s)$. Let $\eta \in (0, 1)$, $\xi \in (0, 1)$, $m = 0, \dots, N-1$ and $t_m \leq t < t_{m+1}$ be fixed. We have

$$\begin{aligned} \tilde{W}(t, \xi) - \tilde{W}(t, \eta) &= \sum_{\ell=1}^m \sum_{k=0}^{\infty} (f_k(\xi) - f_k(\eta)) (1 + \lambda_k \delta)^{-\ell} (1 + (t - t_m) \lambda_k (1 + \lambda_k \delta)^{-1}) \int_0^\delta d\beta_k(s) \\ &\quad + \sum_{k=0}^{\infty} (f_k(\xi) - f_k(\eta)) (1 + \lambda_k \delta)^{-1} \int_0^{t-t_m} d\beta_k(s) \end{aligned}$$

then for any $0 < \kappa < 1/2$

$$\begin{aligned} \mathbb{E} |\tilde{W}(t, \xi) - \tilde{W}(t, \eta)|^2 &\leq c \sum_{k=0}^{\infty} |f_k(\xi) - f_k(\eta)|^2 \delta \frac{1}{2\lambda_k \delta (1 + \lambda_k \delta / 2)} \left(1 + \frac{\lambda_k \delta}{1 + \lambda_k \delta}\right)^2 \\ &\quad + \sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} \frac{\lambda_k^{1/2+\kappa}}{(1 + \lambda_k \delta)^2} |f_k(\xi) - f_k(\eta)|^2 \delta. \end{aligned}$$

As for any $\beta \in [0, 1]$ there exists $c_\beta > 0$ such that for all $x \geq 0$ and $y \geq 0$

$$|\sin x - \sin y| \leq c_\beta |x - y|^\beta,$$

we get for $\beta = \frac{1}{2} - \frac{\kappa}{2}$

$$\begin{aligned} \mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(t, \eta)|^2 &\leq c|\xi - \eta|^{1-2\kappa} \left(\sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} + \sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} \frac{\lambda_k \delta}{1 + \lambda_k \delta} \right) \\ &\leq C|\xi - \eta|^{1/4}, \end{aligned}$$

by Lemma 2.2.

Let us prove (9.3). Let $\xi \in (0, 1)$ and $0 \leq s < t \leq T$ be fixed. Let us first assume that $t_m \leq s < t \leq t_{m+1}$. We have

$$\tilde{W}(t, \xi) - \tilde{W}(s, \xi) = (t - s)AR_\delta \sum_{\ell=1}^m \int_0^\delta R_\delta^\ell dW(s)(\xi) + \int_0^{t-s} R_\delta dW(s)(\xi),$$

then for $0 < \kappa < 1/2$

$$\begin{aligned} \mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(s, \xi)|^2 &\leq (t - s)^2 \sum_{k=0}^{\infty} \frac{\lambda_k^2}{(1 + \lambda_k \delta)^2} \frac{e^{2m \ln(1 + \lambda_k \delta)} - 1}{2\lambda_k \delta (1 + \lambda_k \delta/2)} e^{-2m \ln(1 + \lambda_k \delta)} \delta |f_k(\xi)|^2 \\ &\quad + (t - s) \sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} \frac{\lambda_k^{1/2+\kappa}}{(1 + \lambda_k \delta)^2} \delta |f_k(\xi)|^2. \end{aligned}$$

As for any $\beta \in [0, 1]$ there exists $c_\beta > 0$ such that for all $x \geq 0$ and $y \geq 0$

$$|e^x - e^y| \leq c_\beta |x - y|^\beta, \tag{9.4}$$

we get for $\beta = \frac{\kappa}{2}$

$$\begin{aligned} \mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(s, \xi)|^2 &\leq |t - s|^{1/2-\kappa} \left(\sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa/2} \frac{(\lambda_k \delta)^{3/2+\kappa}}{(1 + \lambda_k \delta)^2} T^{\kappa/2} + \sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} \right) \\ &\leq C(T)|t - s|^{1/2-\kappa}, \end{aligned}$$

by Lemma 2.2 and $|t - s| \leq \delta$.

Let us now assume that $0 \leq s < t_m \leq t < t_{m+1}$. We set $n = \lfloor \frac{s}{\delta} \rfloor$ and we write

$$\mathbb{E}|\tilde{W}(t, \xi) - \tilde{X}(s, \xi)|^2 \leq \mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(t_m, \xi)|^2 + \mathbb{E}|\tilde{W}(t_m, \xi) - \tilde{W}(t_{n+1}, \xi)|^2 + \mathbb{E}|\tilde{W}(t_{n+1}, \xi) - \tilde{W}(s, \xi)|^2.$$

We already showed that for any $0 < \kappa < 1/2$

$$\mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(t_m, \xi)|^2 \leq C(T)|t - t_m|^{1/2-\kappa}$$

and

$$\mathbb{E}|\tilde{W}(t_{n+1}, \xi) - \tilde{W}(s, \xi)|^2 \leq C(T)|t_{n+1} - s|^{1/2-\kappa}.$$

Moreover, we have

$$\tilde{W}(t_m, \xi) - \tilde{W}(t_{n+1}, \xi) = \sum_{\ell=2}^m \int_0^\delta R_\delta^\ell dW(s)(\xi)$$

and

$$\begin{aligned} \mathbb{E}|\tilde{W}(t_m, \xi) - \tilde{W}(t_{n+1}, \xi)|^2 &\leq C \sum_{k=0}^{\infty} \frac{1}{(1 + \lambda_k \delta)^{2n}} \frac{e^{2(m-n-1)\ln(1+\lambda_k \delta)} - 1}{2\lambda_k(1 + \lambda_k \delta/2)} e^{-2(m-n-1)\ln(1+\lambda_k \delta)} \\ &\leq C |t_m - t_{n+1}|^{1/2-\kappa} \sum_{k=0}^{\infty} \lambda_k^{-1/2-\kappa} \\ &\leq C |t_m - t_{n+1}|^{1/2-\kappa} \end{aligned}$$

by Lemma 2.2 and inequality (9.4) where $\beta = \frac{1}{2} - \kappa$. Using

$$(a + b)^4 \leq c(a^4 + b^4), \quad a \geq 0, \quad b \geq 0,$$

it is easy to prove (9.3).

It follows from (9.3) and (9.2) that for any $0 < \kappa < 1/4$ there exists $C > 0$ such that

$$\mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(s, \eta)|^2 \leq C \left(|t - s|^2 + |\xi - \eta|^2 \right)^{1/4-\kappa}.$$

Since $\tilde{W}(t, \xi) - \tilde{W}(s, \eta)$ is a Gaussian random variable, we have for $\ell = 1, 2, \dots$ that there exists $C > 0$ such that

$$\mathbb{E}|\tilde{W}(t, \xi) - \tilde{W}(s, \eta)|^{2\ell} \leq C \left(|t - s|^2 + |\xi - \eta|^2 \right)^{\ell(1/4-\kappa)}.$$

Kolmogorov's test now implies that \tilde{W} has a Hölder continuous on $[0, T] \times (0, 1)$ versions for any $\alpha \in [0, 1/4)$. Moreover, we have

$$\mathbb{E} \sup_{t \in [0, T]} |\tilde{W}(t)|_{L^\infty}^\ell < \infty$$

and (9.1) follows.

We can now prove Lemma 4.2.

Proof of Lemma 4.2. Let $\delta > 0$ be fixed. We introduce $Z_m = X_m - w_m$ and $Z_{m+1/2} = X_{m+1/2} - w_m$, where the process (w_m) is the numerical approximation of W^A with the numerical schema (3.5) - with $F = 0$; it is defined by

$$w_{m+1} = R_\delta w_m + \sqrt{\delta} R_\delta \chi_{m+1}.$$

We have $Z_0 = X_0 = x$ and for any $m \in [0, \dots, N - 1]$

$$\begin{aligned} Z_{m+1/2} &= Z_m + \delta F(X_{m+1/2}) \\ Z_{m+1} &= R_\delta Z_{m+1/2}. \end{aligned}$$

Let $\ell \in \mathbb{N}^*$ and $m = 0, \dots, N - 1$ be fixed. By a maximum principle, we have for any $x \in \mathcal{C}([0, 1])$, $|R_\delta x|_{L^\infty} \leq |x|_{L^\infty}$. Then, we obtain the almost sure estimate

$$|Z_{m+1}|_{L^\infty} \leq |Z_{m+1/2}|_{L^\infty}.$$

Moreover, using Properties (2.5) and (2.3), we get for any $\xi \in (0, 1)$

$$\begin{aligned} |Z_{m+1/2}(\xi)|^2 &\leq |Z_m(\xi)|^2 + 2\delta f(Z_{m+1/2}(\xi))Z_{m+1/2}(\xi) \\ &\quad + 2\delta \left(f(X_{m+1/2}(\xi)) - f(Z_{m+1/2}(\xi)) \right) Z_{m+1/2}(\xi) \\ &\leq |Z_m(\xi)|^2 - \delta(2c - \varepsilon)|Z_{m+1/2}(\xi)|^{2p} + \delta c_1 + \delta C_\varepsilon^1 |w_m(\xi)|^{2p} + \delta C_\varepsilon^2 \\ &\leq |Z_m(\xi)|^2 - \delta(2c - \varepsilon)|Z_{m+1/2}(\xi)|^2 + \delta c_1 + \delta C_\varepsilon^1 |w_m(\xi)|^{2p} + \delta C_\varepsilon^2. \end{aligned}$$

Then, with $\varepsilon = c$, we get

$$|Z_{m+1}|_{L^\infty}^2 \leq |Z_{m+1/2}|_{L^\infty}^2 \leq (1 + c\delta)^{-1} |Z_m|_{L^\infty}^2 + (1 + c\delta)^{-1} \delta C (1 + |w_m|_{L^\infty}^{2p})$$

and

$$|Z_{m+1}|_{L^\infty}^{2\ell} \leq (1 + c\delta)^{-\ell} (1 + \delta\varepsilon_1) |Z_m|_{L^\infty}^{2\ell} + (1 + c\delta)^{-1} \delta C (1 + |w_m|_{L^\infty}^{2p\ell}).$$

We take ε_1 such that $1 + \delta\ell\varepsilon_1 < (1 + c\delta)^\ell$ and we get, by induction on m ,

$$|Z_{m+1}|_{L^\infty}^{2\ell} \leq \mathbb{E}|x|_{L^\infty}^{2\ell} + C(T) \left(1 + \sup_{n=0, \dots, N} |w_n|_{L^\infty}^{2p\ell}\right)$$

Finally, using Lemma 9.1, we obtain

$$\mathbb{E} \sup_{m=0, \dots, N} |Z_m|_{L^\infty}^{2\ell} \leq C(T) (1 + |x|_{L^\infty}^{2\ell}).$$

We also have

$$\mathbb{E} \sup_{m=0, \dots, N-1} |Z_{m+1/2}|_{L^\infty}^{2\ell} \leq C(T) (1 + |x|_{L^\infty}^{2\ell}).$$

Using Lemma 9.1, we can conclude that

$$\mathbb{E} \sup_{m=0, \dots, N} |X_m|_{L^\infty}^{2\ell} \leq C(T) (1 + |x|_{L^\infty}^{2\ell})$$

and

$$\mathbb{E} \sup_{m=0, \dots, N-1} |X_{m+1/2}|_{L^\infty}^{2\ell} \leq C(T) (1 + |x|_{L^\infty}^{2\ell}).$$

Moreover, using for $t \in [t_m, t_{m+1})$ that

$$\tilde{X}(t) = X_m + (t - t_m) A R_\delta X_m + \frac{t - t_m}{\delta} R_\delta (X_{m+1/2} - X_m) + \int_{t_m}^t R_\delta dW(s)$$

and above estimates, we get

$$\mathbb{E} \sup_{t \in [0, T]} |\tilde{X}(t)|_{L^\infty}^{2\ell} \leq C(T) (1 + |x|_{L^\infty}^{2\ell}).$$

10 Appendix: Smoothing properties of the transition semigroup

10.1 Introduction

In this Appendix, we want to prove Proposition 7.1. We recall that we work with the Galerkin finite dimensional approximation, but we omit the parameter M . The constants appearing below are independent of M . Moreover, the constants C and $C(T)$ may vary from line to line. We also recall that the transition semigroup P_t associated to the solution of (2.1) is given by

$$P_t \phi(x) = \mathbb{E}(\phi(X_x(t))) = u(t, x), \quad t \geq 0, \quad x \in H, \quad \phi \in \mathcal{C}_b^2(H). \quad (10.1)$$

As F and its derivatives are not bounded and we have not bound on exponential moments of $X_x(t)$, we can not use directly usual method - see appendix of [20] and section

5 of [5]. For that purpose, we use here a similar method as in [14] and [15]. We introduce a Kolmogorov operator with a suitable potential term

$$\tilde{N}\phi(x) = L\phi(x) - Kg(x)\phi(x), \quad x \in H, \quad (10.2)$$

where $K > 0$ is sufficiently large, L is the Kolmogorov operator defined by (7.1), g is defined for $x \in L^{4p}(0, 1)$ by

$$g(x) = 1 + |x|_{L^{4p}}^{4p},$$

and p is defined in equation (2.2). We also introduce the corresponding semigroup S_t given by the Feynman-Kac formula,

$$S_t\phi(x) = \mathbb{E}\left(e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t))\right), \quad \phi \in \mathcal{C}_b^2(H), \quad t \geq 0, \quad x \in H. \quad (10.3)$$

Thanks to the exponential factor and estimates on the derivative $X_x(t)$, we are able to find an estimate for $|DS_t\phi(x)|$. Then, using the identity

$$P_t\phi = S_t\phi + K \int_0^t S_{t-s}(gP_s\phi) ds, \quad t \geq 0, \quad \phi \in \mathcal{C}_b^2(H), \quad (10.4)$$

we obtain estimates for $DP_t\phi(x)$. This arguments will be iterated to get a bound on second order derivative of P_t .

Throughout this appendix, we use the following notation: for $x \in \mathcal{C}([0, 1])$, $h \in H$ and $0 \leq t \leq T$, $\eta_x^h(t) := DX_x(t) \cdot h$ is the first derivative of $X_x(t)$ in the direction h and $\xi_x^h(t) = D^2X_x(t) \cdot (h, h)$ is the second derivative of $X_x(t)$ in the direction h .

We end this section by giving some estimates. We shall often use the classical interpolary estimate,

$$|x|_\beta \leq |x|_\alpha^{\frac{\gamma-\beta}{\gamma-\alpha}} |x|_\gamma^{\frac{\beta-\alpha}{\gamma-\alpha}}, \quad \alpha < \beta < \gamma, \quad x \in D((-A)^\gamma) \quad (10.5)$$

and the Agmon estimate

$$|x|_{L^\infty} \leq |x|_{L^2}^{1/2} |x|_{1^{1/2}}^{1/2}, \quad x \in D((-A)^{1/2}). \quad (10.6)$$

10.2 Estimate of $DP_t\phi(x)$

We shall proceed in three steps to bound $DP_t\phi(x)$. In section 10.2.1, we give two estimates of $\eta_x^h(t)$, the derivative of $X_x(t)$ in the direction $h \in H$. In section 10.2.2 we use these estimates to bound $DS_t\phi(x)$, where the semigroup S_t is defined in (10.3). Finally in section 10.2.3, we obtain the required estimate for $DP_t\phi(x)$ using the identity (10.4).

10.2.1 Estimate of $\eta_x^h(t)$

First, we will show the following Lemma.

Lemma 10.1 *For any $\alpha \in [-1/2, 0)$, there exists $c > 0$ such that*

$$e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} |\eta_x^h(t)|_\alpha^2 + \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |\eta_x^h(s)|_{1/2+\alpha}^2 ds \leq |h|_\alpha^2, \quad (10.7)$$

for all $0 \leq t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$. Moreover, we have

$$|\eta_x^h(t)|_{L^2}^2 \leq e^{\gamma t} |h|_{L^2}^2 \quad (10.8)$$

for all $0 \leq t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$.

Proof. Let $0 \leq t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. Let us first notice that $\eta_x^h(t)$ fulfills the equation

$$\begin{cases} \frac{d}{dt}\eta_x^h(t) &= A\eta_x^h(t) + DF(X_x(t)) \cdot \eta_x^h(t), \\ \eta_x^h(0) &= h. \end{cases} \quad (10.9)$$

Multiplying both sides of the first identity in (10.9) by $(-A)^{2\alpha}\eta_x^h(t)$ and integrating in $[0, 1]$ yields

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\eta_x^h(t)|_\alpha^2 + |\eta_x^h(t)|_{1/2+2\alpha}^2 &= |\langle DF(X_x(t)) \cdot \eta_x^h(t), (-A)^{2\alpha}\eta_x^h(t) \rangle|_{L^1} \\ &\leq |(-A)^{2\alpha}\eta_x^h(t)|_{L^\infty} |DF(X_x(t))|_{L^2} |\eta_x^h(t)|_{L^2}. \end{aligned}$$

Since $H^1(0, 1) \subset L^\infty(0, 1)$, we have, for $\alpha \in (-1/2, 0)$ and by the interpolary estimate (10.5),

$$|(-A)^{2\alpha}\eta_x^h(t)|_{L^\infty} \leq c|\eta_x^h(t)|_{1/2+2\alpha} \leq c|\eta_x^h(t)|_\alpha^{-2\alpha} |\eta_x^h(t)|_{1/2+2\alpha}^{1+2\alpha}$$

and

$$|\eta_x^h(t)|_{L^2} \leq |\eta_x^h(t)|_\alpha^{1+2\alpha} |\eta_x^h(t)|_{1/2+2\alpha}^{-2\alpha}. \quad (10.10)$$

Therefore, it results, for $\alpha \in (-1/2, 0)$,

$$\begin{aligned} \frac{d}{dt} |\eta_x^h(t)|_\alpha^2 + |\eta_x^h(t)|_{1/2+2\alpha}^2 &\leq c|DF(X_x(t))|_{L^2} |\eta_x^h(t)|_\alpha |\eta_x^h(t)|_{1/2+2\alpha} \\ &\leq c|DF(X_x(t))|_{L^2}^2 |\eta_x^h(t)|_\alpha^2 + \frac{1}{2} |\eta_x^h(t)|_{1/2+2\alpha}^2. \end{aligned}$$

Since $H^1(0, 1) \subset L^\infty(0, 1)$, we immediately have for $\alpha = -1/2$,

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\eta_x^h(t)|_{-1/2}^2 + |\eta_x^h(t)|_{L^2}^2 &\leq c|\eta_x^h(t)|_{-1/2} |DF(X_x(t))|_{L^2} |\eta_x^h(t)|_{L^2} \\ &\leq c|DF(X_x(t))|_{L^2}^2 |\eta_x^h(t)|_{-1/2}^2 + \frac{1}{2} |\eta_x^h(t)|_{L^2}^2 \end{aligned}$$

Then, (10.7) follows by integrating in time $\frac{d}{dt} \left(e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} |\eta_x^h(t)|_\alpha^2 \right)$. For $\alpha = 0$, by (2.4), we have

$$\frac{d}{dt} |\eta_x^h(t)|_{L^2}^2 + |\eta_x^h(t)|_{1/2}^2 \leq \gamma |\eta_x^h(t)|_{L^2}^2. \quad (10.11)$$

Then, by Grönwall Lemma, we get (10.8).

Now, we can show the following Lemma.

Lemma 10.2 *For any $0 < \varepsilon \leq \frac{1}{2}$ and $T > 0$, there exists $C(T) > 0$ such that for any $0 < t \leq T$, $h \in H$ and $x \in \mathcal{C}([0, 1])$*

$$e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} |\eta_x^h(t)|_{L^2}^2 \leq C(T)(1 + t^{-1+2\varepsilon}) |h|_{-1/2+\varepsilon}^2, \quad (10.12)$$

where c is defined in Lemma 10.1

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$, $0 < \varepsilon \leq 1/2$ and $h \in H$ be fixed. Using (10.11), we have

$$\begin{aligned} \frac{d}{dt} \left(e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} t |\eta_x^h(t)|_{L^2}^2 \right) &= e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} |\eta_x^h(t)|_{L^2}^2 \\ &\quad + e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} t \frac{d}{dt} |\eta_x^h(t)|_{L^2}^2 \\ &\quad - c |DF(X_x(t))|_{L^2}^2 e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} t |\eta_x^h(t)|_{L^2}^2 \\ &\leq e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} |\eta_x^h(t)|_{L^2}^2 \\ &\quad + \gamma e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} t |\eta_x^h(t)|_{L^2}^2. \end{aligned}$$

Integrating by time and using the Hölder inequality, Lemma 10.1 and inequality (10.10) with $\alpha = -1/2 + \varepsilon$, yields

$$\begin{aligned}
& e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} t |\eta_x^h(t)|_{L^2}^2 \\
& \leq \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |\eta_x^h(s)|_{L^2}^2 ds + \gamma \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} s |\eta_x^h(s)|_{L^2}^2 ds \\
& \leq \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |\eta_x^h(s)|_{-1/2+\varepsilon}^{4\varepsilon} |\eta_x^h(s)|_{\varepsilon}^{2(1-2\varepsilon)} ds \\
& \quad + \gamma \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} s |\eta_x^h(s)|_{L^2}^2 ds \\
& \leq \left(\int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |\eta_x^h(s)|_{\varepsilon}^2 ds \right)^{1-2\varepsilon} \left(\int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |\eta_x^h(s)|_{-1/2+\varepsilon}^2 ds \right)^{2\varepsilon} \\
& \quad + \gamma \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} s |\eta_x^h(s)|_{L^2}^2 ds \\
& \leq t^{2\varepsilon} |h|_{-1/2+\varepsilon}^2 + \gamma \int_0^t e^{-c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} s |\eta_x^h(s)|_{L^2}^2 ds.
\end{aligned}$$

Then, using Grönwall Lemma and dividing by t , we have (10.12).

10.2.2 Estimate of $DS_t\phi(x)$

We shall use the following notation

$$\|\phi\|_{0, L^{4p}} := \sup_{x \in L^{4p}(0,1)} \frac{|\phi(x)|}{1 + |x|_{L^{4p}}^{4p}}.$$

If we want to use equation (10.4) to have an estimate of $P_t\phi(x)$, we need to have an estimate of $DS_t\phi$ for $\phi \in \mathcal{C}_b^1(H)$ and another for $\phi \in \mathcal{C}^0(H)$ such that $\|\phi\|_{0, L^{4p}} < +\infty$.

Lemma 10.3 *Let $0 < \varepsilon \leq 1/2$ be fixed. If K is chosen sufficiently large then for any $\phi \in \mathcal{C}_b^1(H)$, we have for any $0 < t \leq T$ and $x \in \mathcal{C}([0, 1])$*

$$|DS_t\phi(x)|_{1/2-\varepsilon} \leq C(T) |\phi|_{0,1} \left(1 + |x|_{L^\infty}^{4p} \right) (1 + t^{-1/2+\varepsilon}).$$

Proof. Let $h \in H$, $x \in \mathcal{C}([0, 1])$, $0 < t \leq T$ and $\phi \in \mathcal{C}_b^1(H)$ be fixed. We have

$$\begin{aligned}
DS_t\phi(x) \cdot h &= \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} D\phi(X_x(t)) \cdot \eta_x^h(t) \right) \\
&\quad - K \mathbb{E} \left(\int_0^t Dg(X_x(s)) \cdot \eta_x^h(s) ds e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \right).
\end{aligned} \tag{10.13}$$

Using Cauchy-Schwarz inequality, we have

$$|Dg(X_x(t)) \cdot \eta_x^h(t)| \leq C \left(1 + |X_x(t)|_{L^{8p}}^{4p} \right) |\eta_x^h(t)|_{L^2}. \tag{10.14}$$

Then, choosing K sufficiently large and using Lemmas 10.1 and 4.1, we get for $0 < \varepsilon \leq 1/2$

$$\begin{aligned}
|DS_t\phi(x) \cdot h| &\leq |\phi|_{0,1} \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} |\eta_x^h(t)|_{L^2} \right) \\
&\quad + C |\phi|_0 \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^\infty}^{4p}) |\eta_x^h(s)|_{L^2} e^{-K \int_0^s g(X_x(\tau)) d\tau} ds \right) \\
&\leq C(T) |\phi|_{0,1} (1 + t^{-1/2+\varepsilon}) |h|_{-1/2+\varepsilon} \\
&\quad + C(T) |\phi|_0 \int_0^t (1 + \mathbb{E} |X_x(s)|_{L^\infty}^{4p}) (1 + s^{-1/2+\varepsilon}) ds |h|_{-1/2+\varepsilon} \\
&\leq C(T) (1 + t^{-1/2+\varepsilon}) (1 + |x|_{L^\infty}^{4p}) |\phi|_{0,1} |h|_{-1/2+\varepsilon}.
\end{aligned}$$

The conclusions follows.

Lemma 10.4 *Let $0 < \varepsilon \leq 1/2$ be fixed. If K is chosen sufficiently large then for any $\phi \in \mathcal{C}_b^0(H)$ such that $\|\phi\|_{0,L^{4p}} < \infty$, we have for $x \in \mathcal{C}([0,1])$ and $0 < t \leq T$*

$$|DS_t\phi(x)|_{1/2-\varepsilon} \leq C(T) \|\phi\|_{0,L^{4p}} \left(1 + |x|_{L^\infty}^{8p}\right) (1 + t^{-1+\varepsilon}).$$

Proof. Let $0 < t \leq T$, $h \in H$ and $x \in \mathcal{C}([0,1])$ be fixed. We know from [17] that for any $\phi \in \mathcal{C}_b(H)$, $S_t\phi$ is differentiable in any direction $h \in H$ and its derivative $DS_t\phi(x) \cdot h$ is given by the generalized Bismut-Elworthy formula

$$\begin{aligned} DS_t\phi(x) \cdot h &= \frac{1}{t} \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \int_0^t \langle \eta_x^h(s), dW(s) \rangle \right) \\ &\quad + K \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \int_0^t \left(1 - \frac{s}{t}\right) Dg(X_x(s)) \cdot \eta_x^h(s) ds \right) \end{aligned}$$

Hence, we can write by Cauchy-Schwarz inequality

$$\begin{aligned} |DS_t\phi(x) \cdot h| &\leq \frac{1}{t} \|\phi\|_{0,L^{4p}} \left(\mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} (1 + |X_x(t)|_{L^{4p}}^{8p}) \right) \right)^{1/2} \\ &\quad \times \left(\mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} \left(\int_0^t \langle \eta_x^h(s), dW(s) \rangle \right)^2 \right) \right)^{1/2} \\ &\quad + K \|\phi\|_{0,L^{4p}} \left(\mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} (1 + |X_x(t)|_{L^{4p}}^{8p}) \right) \right)^{1/2} \\ &\quad \times \left(\mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} \left(\int_0^t Dg(X_x(s)) \cdot \eta_x^h(s) ds \right)^2 \right) \right)^{1/2} \\ &:= I_1 + I_2. \end{aligned}$$

Let us estimate I_1 . We have, by Lemma 4.1,

$$\mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} (1 + |X_x(t)|_{L^{4p}}^{8p}) \right) \leq C(T) (1 + |x|_{L^\infty}^{8p}).$$

We set

$$q(t) = e^{-\frac{K}{2} \int_0^t g(X_x(s)) ds} \int_0^t \langle \eta_x^h(s), dW(s) \rangle.$$

Then

$$dq(t) = -\frac{K}{2} g(X_x(t)) q(t) dt + e^{-\frac{K}{2} \int_0^t g(X_x(s)) ds} \langle \eta_x^h(t), dW(t) \rangle$$

and consequently, by the Itô formula,

$$\begin{aligned} q(t)^2 &= -K \int_0^t g(X_x(s)) q(s)^2 ds + 2 \int_0^t e^{-\frac{K}{2} \int_0^s g(X_x(\tau)) d\tau} \langle \eta_x^h(s), dW(s) \rangle \\ &\quad + \int_0^t e^{-K \int_0^s g(X_x(\tau)) d\tau} |\eta_x^h(s)|_{L^2}^2 ds. \quad (10.15) \end{aligned}$$

So, by Proposition 10.2 and for K large enough, we obtain for $0 < \varepsilon \leq 1/2$

$$\begin{aligned} \mathbb{E}(q(t)^2) &\leq \mathbb{E} \int_0^t e^{-K \int_0^s g(X_x(\tau)) d\tau} |\eta_x^h(s)|_{L^2}^2 ds \\ &\leq C(T) |h|_{-1/2+\varepsilon}^2 \int_0^t (1 + s^{-1+2\varepsilon}) ds \\ &\leq C(T) |h|_{-1/2+\varepsilon}^2 t^{2\varepsilon}. \end{aligned}$$

Consequently,

$$|I_1| \leq C(T)t^{-1+\varepsilon} \|\phi\|_{0,L^{4p}} \left(1 + |x|_{L^\infty}^{4p}\right) |h|_{-1/2+\varepsilon}.$$

Let us estimate I_2 . Thanks to (10.14), Cauchy-Schwarz inequality, Lemmas 4.1 and 10.2, we have

$$\begin{aligned} & \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} \left(\int_0^t Dg(X_x(s)) \cdot \eta_x^h(s) ds \right)^2 \right) \\ & \leq C \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^{8p}}^{8p}) ds \int_0^t e^{-K \int_0^s g(X_x(\tau)) d\tau} |\eta_x^h(s)|_{L^2}^2 ds \right) \\ & \leq C(T) |h|_{-1/2+\varepsilon}^2 t^{1+2\varepsilon} (1 + |x|_{L^\infty}^{8p}). \end{aligned}$$

Finally, we obtain that

$$|DS_t \phi(x) \cdot h| \leq C(T) (1 + |x|_{L^\infty}^{8p}) (1 + t^{-1+\varepsilon}) \|\phi\|_{0,L^{4p}} |h|_{-1/2+\varepsilon}$$

and the conclusion follows.

10.2.3 Estimate of $DP_t \phi(x)$

Lemma 10.5 *Assume that $\phi \in \mathcal{C}_b^1(H)$ and $0 < \varepsilon \leq 1/2$. Then we have for $x \in \mathcal{C}([0, 1])$ and $0 < t \leq T$*

$$|DP_t \phi(x)|_{1/2-\varepsilon} \leq C(T) (1 + t^{-1/2+\varepsilon}) |\phi|_{0,1} (1 + |x|_{L^\infty}^{8p}).$$

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. First, we write that

$$DP_t \phi(x) \cdot h = DS_t \phi(x) \cdot h + K \int_0^t DS_{t-s} (gP_s \phi)(x) \cdot h ds,$$

where in the definition we choose K such that Lemma 10.3 and Lemma 10.4 hold. We estimate the first term using Lemma 10.3. Since

$$\|gP_s \phi\|_{0,L^{4p}} = \sup_{x \in L^{4p}(0,1)} \frac{(1 + |x|_{L^{4p}}^{4p}) |P_s \phi(x)|}{1 + |x|_{L^{4p}}^{4p}} \leq |\phi|_0,$$

we use Lemma 10.4 to estimate the second term. We obtain

$$\begin{aligned} |DP_t \phi(x) \cdot h| & \leq C(T) |\phi|_{0,1} (1 + |x|_{L^\infty}^{4p}) (1 + t^{-1/2+\varepsilon}) |h|_{-1/2+\varepsilon} \\ & \quad + C(T) |\phi|_0 (1 + |x|_{L^\infty}^{8p}) \int_0^t (1 + (t-s)^{-1+\varepsilon}) ds |h|_{-1/2+\varepsilon} \end{aligned}$$

and the conclusion follows.

10.3 Estimate of $D^2 P_t \phi(x)$

As to estimate $DP_t \phi(x)$, we shall proceed in three steps to bound $D^2 P_t \phi(x)$. In section 10.3.1, we estimate $\xi_x^h(t)$, the second derivative of $X_x(t)$ in the direction (h, h) for $h \in H$. In section 10.3.2, we use this estimate to bound $D^2 S_t \phi(x)$, where the semigroup S_t is defined in (10.3). Finally in section 10.2.3, we obtain the required estimate for $DP_t \phi(x)$ using the identity (10.4).

10.3.1 Estimate of $\xi_x^h(t)$

Lemma 10.6 *There exists $C(T) > 0$ such that for any $0 < t \leq T$, $h \in H$ and $x \in \mathcal{C}([0, 1])$*

$$|\xi_x^h(t)|_{L^2}^2 \leq C(T)(1 + \sup_{t \in [0, T]} |X_x(t)|_{L^\infty}^{4p})|h|_{L^2}^4. \quad (10.16)$$

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. Let us first notice that $\xi_x^h(t)$ fulfills the equation

$$\begin{cases} \frac{d}{dt} \xi_x^h(t) &= A\xi_x^h(t) + DF(X_x(t)) \cdot \xi_x^h(t) + D^2F(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) \\ \xi_x^h(0) &= 0. \end{cases}$$

Multiplying both sides of the first identity in the above equality by $\xi_x^h(t)$ and integrating in $[0, 1]$ yields

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |\xi_x^h(t)|_{L^2}^2 + |\xi_x^h(t)|_{1/2}^2 &\leq \gamma |\xi_x^h(t)|_{L^2}^2 + |D^2F(X_x(t))|_{L^\infty} |\eta_x^h(t)|_{L^2}^2 |\xi_x^h(t)|_{L^\infty} \\ &\leq \gamma |\xi_x^h(t)|_{L^2}^2 + |D^2F(X_x(t))|_{L^\infty} |\eta_x^h(t)|_{L^2}^2 |\xi_x^h(t)|_{L^2}^{1/2} |\xi_x^h(t)|_{1/2}^{1/2} \\ &\leq \gamma |\xi_x^h(t)|_{L^2}^2 + C |D^2F(X_x(t))|_{L^\infty}^{4/3} |\eta_x^h(t)|_{L^2}^{8/3} |\xi_x^h(t)|_{L^2}^{2/3} + \frac{1}{4} |\xi_x^h(t)|_{1/2}^2 \end{aligned}$$

by (2.4) and Agmon estimate (10.6). Then, by (10.8), we get

$$\begin{aligned} \frac{d}{dt} |\xi_x^h(t)|_{L^2}^2 &\leq 2\gamma |\xi_x^h(t)|_{L^2}^2 + C |D^2F(X_x(t))|_{L^\infty}^{4/3} |\eta_x^h(t)|_{L^2}^{8/3} |\xi_x^h(t)|_{L^2}^{2/3} \\ &\leq 2\gamma |\xi_x^h(t)|_{L^2}^2 + C |D^2F(X_x(t))|_{L^\infty}^2 |\eta_x^h(t)|_{L^2}^4 + \frac{1}{3} |\xi_x^h(t)|_{L^2}^{2/3} \\ &\leq \tilde{\gamma} |\xi_x^h(t)|_{L^2}^2 + C(T)(1 + \sup_{0 \leq t \leq T} |X_x(t)|_{L^\infty}^{4p})|h|_{L^2}^4. \end{aligned}$$

Using Grönwall Lemma, we obtain (10.17).

Lemma 10.7 *Let c be defined in Lemma 10.1. For any $0 < \varepsilon \leq 1/2$, there exist $c_1(T) \geq c$ and $C(T) > 0$ such that for any $0 < t \leq T$, $h \in H$ and $x \in \mathcal{C}([0, 1])$*

$$|\xi_x^h(t)|_{L^2} e^{-c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} \leq C(T)(1 + \sup_{t \in [0, T]} |X_x(t)|_{L^\infty}^{4p})(1 + t^{-1/4+\varepsilon})|h|_{-1/2+\varepsilon}^2. \quad (10.17)$$

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. We recall that $\xi_x^h(t)$ fulfills the equation

$$\begin{cases} \frac{d}{dt} \xi_x^h(t) &= A\xi_x^h(t) + DF(X_x(t)) \cdot \xi_x^h(t) + D^2F(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) \\ \xi_x^h(0) &= 0. \end{cases}$$

We rewrite this equation in the integral form

$$\xi_x^h(t) = \int_0^t e^{A(t-s)} DF(X_x(s)) \cdot \xi_x^h(s) ds + \int_0^t D^2F(X_x(s)) \cdot (\eta_x^h(s), \eta_x^h(s)) ds.$$

Let $\psi \in L^1(0, 1)$, we have for any $\kappa > 0$ and $t > 0$ that there exists $c_\kappa > 0$ such that

$$|e^{tA}\psi|_{L^2} \leq c_\kappa t^{-1/4-\kappa} |\psi|_{L^1}. \quad (10.18)$$

Indeed, let $\psi \in L^1(0, 1)$ and $\Phi \in L^2(0, 1)$ be fixed, we have by duality, Sobolev inequality (see [8]) and Proposition 2.5,

$$\begin{aligned} \langle e^{tA}\psi, \Phi \rangle &= \langle \psi, e^{tA}\Phi \rangle \\ &\leq |\psi|_{L^1} |e^{tA}\Phi|_{L^\infty} \\ &\leq c_\kappa |\psi|_{L^1} |(-A)^{1/4+\kappa} e^{tA}\Phi|_{L^2} \\ &\leq c_\kappa t^{-1/4-\kappa} |\psi|_{L^1} |\Phi|_{L^2} \end{aligned}$$

for any $t > 0$, and the inequality (10.18) follows.

Then, by inequality (10.18), Lemma 10.2 and Cauchy-Schwarz inequality, we get, for any $\varepsilon > 0$

$$\begin{aligned} &|\xi_x^h(t)|_{L^2} e^{-2c \int_0^t |DF(X_x(\tau))|_{L^2}^2 d\tau} \\ &\leq \int_0^t (t-s)^{-1/4-\varepsilon/2} |\xi_x^h(s)|_{L^2} e^{-2c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |DF(X_x(s))|_{L^2} ds \\ &\quad + C(T) \int_0^t (t-s)^{-1/4-\varepsilon/2} (1+s^{-1+2\varepsilon}) ds \sup_{t \in [0, T]} |D^2F(X_x(t))|_{L^\infty} |h|_{-1/2+\varepsilon}^2 \\ &\leq \left(\int_0^t (t-s)^{-1/2-\varepsilon} ds \right)^{1/2} \left(\int_0^t |\xi_x^h(s)|_{L^2}^2 e^{-4c \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} |DF(X_x(s))|_{L^2}^2 ds \right)^{1/2} \\ &\quad + C(T) t^{-1/4+\varepsilon} \sup_{t \in [0, T]} |D^2F(X_x(t))|_{L^\infty} |h|_{-1/2+\varepsilon}^2 \end{aligned}$$

where c is defined in Proposition 10.1. We square the above inequality and by Grönwall Lemma we obtain

$$\begin{aligned} &|\xi_x^h(t)|_{L^2}^2 e^{-4c \int_0^t |DF(X_x(s))|_{L^2}^2 ds} \\ &\leq C(T) \sup_{t \in [0, T]} |D^2F(X_x(t))|_{L^\infty}^2 |h|_{-1/2+\varepsilon}^4 \\ &\quad \times \left(t^{-1/2+2\varepsilon} + T^{1/2-\varepsilon} \int_0^t s^{-1/2+2\varepsilon} |DF(X_x(s))|_{L^2}^2 e^{T^{1/2-\varepsilon} \int_0^s |DF(X_x(\tau))|_{L^2}^2 d\tau} ds \right). \end{aligned}$$

Then,

$$|\xi_x^h(t)|_{L^2}^2 e^{-(4c+T^{1/2}+1) \int_0^t |DF(X_x(s))|_{L^2}^2 ds} \leq C(T) \left(1 + \sup_{t \in [0, T]} |X_x(t)|_{L^\infty}^{4p} \right) |h|_{-1/2+\varepsilon}^4 (t^{-1/2+2\varepsilon} + 1)$$

and the conclusion follows.

10.3.2 Estimate of $D^2S_t\phi(x)$

In this sub-section, we shall prove an estimate of $D^2S_t\phi(x)$ for $\phi \in \mathcal{C}_b^2(H)$.

Lemma 10.8 *Let $0 < \varepsilon \leq 1/2$ be fixed. If $K := K(T)$ is chosen sufficiently large then for any $\phi \in \mathcal{C}_b^2(H)$, we have for any $0 < t \leq T$ and $x \in \mathcal{C}([0, 1])$*

$$|(-A)^{1/2-\varepsilon} D^2S_t\phi(x)(-A)^{1/2-\varepsilon}| \leq C(T) |\phi|_{0,2} (1 + |x|_{L^\infty}^{8p}) (1 + t^{-1+2\varepsilon}).$$

Proof. We choose K such that we can use Lemmas 10.2 and 10.7. Let $0 < \varepsilon \leq 1/2$, $\phi \in \mathcal{C}_b^2(H)$, $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. By differentiation of (10.13), we

have

$$\begin{aligned}
D^2 S_t \phi(x) \cdot (h, h) &= \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} D^2 \phi(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) \right) \\
&\quad + \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} D \phi(X_x(t)) \cdot \xi_x^h(t) \right) \\
&\quad - 2K \mathbb{E} \left(\int_0^t Dg(X_x(s)) \cdot \eta_x^h(s) ds e^{-K \int_0^t g(X_x(s)) ds} D \phi(X_x(t)) \cdot \eta_x^h(t) \right) \\
&\quad - K \mathbb{E} \left(\int_0^t D^2 g(X_x(s)) \cdot (\eta_x^h(s), \eta_x^h(s)) ds e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \right) \\
&\quad - K \mathbb{E} \left(\int_0^t Dg(X_x(s)) \cdot \xi_s^h(s) ds e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \right) \\
&\quad + K^2 \mathbb{E} \left(\left(\int_0^t Dg(X_x(s)) \cdot \eta_x^h(s) ds \right)^2 e^{-K \int_0^t g(X_x(s)) ds} \phi(X_x(t)) \right) \\
&=: I_1 + I_2 + I_3 + I_4 + I_5 + I_6.
\end{aligned}$$

The first term is estimated as follows

$$\begin{aligned}
|I_1|_{L^2} &\leq \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} |\eta_x^h(s)|_{L^2}^2 \right) |\phi|_{0,2} \\
&\leq C(T) (1 + t^{-1+2\varepsilon}) |h|_{-1/2+\varepsilon}^2 |\phi|_{0,2},
\end{aligned}$$

by Lemma 10.2. For the second term we have

$$\begin{aligned}
|I_2|_{L^2} &\leq |\phi|_{0,1} \mathbb{E} \left(e^{-K \int_0^t g(X_x(s)) ds} |\xi_x^h(t)|_{L^2} \right) \\
&\leq |\phi|_{0,1} C(T) |h|_{-1/2+\varepsilon}^2 (1 + t^{-1/4+\varepsilon}) \left(1 + \mathbb{E} \left(\sup_{t \in [0, T]} |X_x(t)|_{L^\infty}^{4p} \right) \right) \\
&\leq |\phi|_{0,1} C(T) |h|_{-1/2+\varepsilon}^2 (1 + t^{-1/4+\varepsilon}) (1 + |x|_{L^\infty}^{4p})
\end{aligned}$$

by Lemmas 10.7 and 4.1. Concerning the third term, we write

$$\begin{aligned}
|I_3|_{L^2} &\leq \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^\infty}^{4p}) |\eta_x^h(s)|_{L^2} e^{-K/2 \int_0^s g(X_x(\tau)) d\tau} ds e^{-K/2 \int_0^t g(X_x(s)) ds} |\eta_x^h(t)|_{L^2} \right) |\phi|_{0,1} \\
&\leq C(T) |\phi|_{0,1} |h|_{-1/2+\varepsilon}^2 (1 + |x|_{L^\infty}^{4p}) \int_0^t (1 + s^{-1/2+\varepsilon}) ds (1 + t^{-1/2+\varepsilon}) \\
&\leq C(T) |\phi|_{0,1} |h|_{-1/2+\varepsilon}^2 (1 + |x|_{L^\infty}^{4p}),
\end{aligned}$$

thanks to Lemmas 4.1 and 10.2. Using Lemmas 4.1 and 10.2, we have

$$\begin{aligned}
|I_4|_{L^2} &\leq C \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^\infty}^{4p}) |\eta_x^h(s)|_{L^2}^2 e^{-K \int_0^s g(X_x(\tau)) d\tau} ds \right) |\phi|_0 \\
&\leq C(T) |\phi|_0 |h|_{-1/2+\varepsilon}^2 (1 + |x|_{L^\infty}^{4p}).
\end{aligned}$$

Using Lemmas 4.1 and 10.7, we have

$$\begin{aligned}
|I_5|_{L^2} &\leq C \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^\infty}^{4p}) |\xi_s^h(s)|_{L^2} e^{-K \int_0^s g(X_x(\tau)) d\tau} ds \right) |\phi|_0 \\
&\leq C(T) (1 + |x|_{L^\infty}^{8p}) |\phi|_0 |h|_{-1/2+\varepsilon}^2.
\end{aligned}$$

For I_6 , we have

$$\begin{aligned}
|I_6|_{L^2} &\leq C \mathbb{E} \left(\int_0^t (1 + |X_x(s)|_{L^\infty}^{8p}) |\eta_x^h(s)|_{L^2}^2 e^{-K \int_0^s g(X_x(\tau)) d\tau} ds \right) |\phi|_0 \\
&\leq C(T) (1 + |x|_{L^\infty}^{8p}) |\phi|_0 |h|_{-1/2+\varepsilon}^2,
\end{aligned}$$

by Lemmas 4.1 and 10.2.

Finally, we have

$$|D^2 S_t \phi(x) \cdot (h, h)|_{L^2} \leq C(T)(1 + t^{-1+2\varepsilon})|h|_{-1/2+\varepsilon}^2(1 + |x|_{L^\infty}^{8p})|\phi|_{0,2}$$

and the conclusion follows.

10.3.3 Estimate of $D^2 P_t \phi(x)$

Lemma 10.9 *Let $\phi \in \mathcal{C}_b^2(H)$ be fixed. Then, we have for $x \in \mathcal{C}([0, 1])$, $h \in H$ and $0 < t \leq T$*

$$|D^2 P_t \phi(x) \cdot (h, h)| \leq C(T)|\phi|_{0,2}(1 + |x|_{L^\infty}^{2p})|h|_{L^2}^2.$$

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. Differentiate (10.1) two times yields

$$D^2 P_t \phi(x) \cdot (h, h) = \mathbb{E} \left(D^2 \phi(X_x(t)) \cdot (\eta_x^h(t), \eta_x^h(t)) \right) + \mathbb{E} \left(D \phi(X_x(t)) \cdot \xi_x^h(t) \right).$$

Then, by Lemmas 4.1, 10.1 and 10.6, we get

$$|D^2 P_t \phi(x) \cdot (h, h)| \leq |\phi|_2 |\eta_x^h(t)|_{L^2}^2 + |\phi|_1 \mathbb{E} |\xi_x^h(t)|_{L^2} \leq C(T)|\phi|_{0,2}(1 + |x|_{L^\infty}^{2p})|h|_{L^2}^2.$$

Lemma 10.10 *Let $\phi \in \mathcal{C}_b^2(H)$ and $0 < \varepsilon \leq 1/2$ be fixed. We have for $x \in \mathcal{C}([0, 1])$ and $0 < t \leq T$*

$$|(-A)^{1/2-\varepsilon} D^2 P_t \phi(x) (-A)^{1/2-\varepsilon}| \leq C(T)(1 + t^{-1+2\varepsilon})|\phi|_{0,2}(1 + |x|_{L^\infty}^{16p}).$$

Proof. Let $0 < t \leq T$, $x \in \mathcal{C}([0, 1])$ and $h \in H$ be fixed. Differentiate (10.4) two times yields

$$D^2 P_t \phi(x) \cdot (h, h) = D^2 S_t \phi(x) \cdot (h, h) + K \int_0^t D^2 S_{t-s}(g P_s \phi)(x) \cdot (h, h) ds.$$

The first term is estimate by Lemma 10.8,

$$|D^2 S_t \phi(x) \cdot (h, h)| \leq C(T)(1 + t^{-1+2\varepsilon})|h|_{-1/2+\varepsilon}^2(1 + |x|_{L^\infty}^{8p})|\phi|_{0,2}.$$

For the second one, we have

$$\begin{aligned}
& \int_0^t D^2 S_{t-s}(gP_s\phi)(x) \cdot (h, h) ds \\
&= \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} D^2 g(X_x(t-s)) \cdot (\eta_x^h(t-s), \eta_x^h(t-s)) P_s \phi(X_x(t-s)) \right) ds \\
&+ 2 \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} Dg(X_x(t-s)) \cdot \eta_x^h(t-s) DP_s \phi(X_x(t-s)) \cdot \eta_x^h(t-s) \right) ds \\
&+ \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} g(X_x(t-s)) D^2 P_s \phi(X_x(t-s)) \cdot (\eta_x^h(t-s), \eta_x^h(t-s)) \right) ds \\
&+ \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} Dg(X_x(t-s)) \cdot \xi_x^h(t-s) P_s \phi(X_x(t-s)) \right) ds \\
&+ \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} g(X_x(t-s)) DP_s \phi(X_x(t-s)) \cdot \xi_x^h(t-s) \right) ds \\
&- 2K \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} \int_0^{t-s} Dg(X_x(\tau)) \cdot \eta_x^h(\tau) d\tau Dg(X_x(t-s)) \cdot \eta_x^h(t-s) P_s \phi(X_x(t-s)) \right) ds \\
&- 2K \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} \int_0^{t-s} Dg(X_x(\tau)) \cdot \eta_x^h(\tau) d\tau g(X_x(t-s)) DP_s \phi(X_x(t-s)) \cdot \eta_x^h(t-s) \right) ds \\
&- K \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} \int_0^{t-s} D^2 g(X_x(\tau)) \cdot (\eta_x^h(\tau), \eta_x^h(\tau)) d\tau g(X_x(t-s)) P_s \phi(X_x(t-s)) \right) ds \\
&- K \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} \int_0^{t-s} Dg(X_x(\tau)) \cdot \xi_x^h(\tau) d\tau g(X_x(t-s)) P_s \phi(X_x(t-s)) \right) ds \\
&- K \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} \left(\int_0^{t-s} Dg(X_x(\tau)) \cdot \eta_x^h(\tau) d\tau \right)^2 g(X_x(t-s)) P_s \phi(X_x(t-s)) \right) ds \\
&:= \sum_{i=1}^{10} S_i.
\end{aligned}$$

The first term is estimated as follows

$$\begin{aligned}
|S_1|_{L^2} &\leq C \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} (1 + |X_x(t-s)|_{L^\infty}^{4p}) |\eta_x^h(t-s)|_{L^2}^2 \right) |\phi|_0 \\
&\leq C(T) |\phi|_0 (1 + |x|_{L^\infty}^{4p}) |h|_{-1/2+\varepsilon}^2 \int_0^t (t-s)^{-1+2\varepsilon} ds \\
&\leq C(T) |\phi|_0 (1 + |x|_{L^\infty}^{4p}) |h|_{-1/2+\varepsilon}^2,
\end{aligned}$$

by Lemmas 4.1 and 10.2. For the second term, using Lemmas 4.1, 10.2 and 10.5, we have

$$\begin{aligned}
|S_2|_{L^2} &\leq C(T) \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} (1 + |X_x(t-s)|_{L^\infty}^{12p}) |\eta_x^h(t-s)|_{L^2}^2 \right) ds |\phi|_{0,1} \\
&\leq C(T) |\phi|_{0,1} |h|_{-1/2+\varepsilon}^2 (1 + |x|_{L^\infty}^{12p}).
\end{aligned}$$

Concerning the third term, we write

$$\begin{aligned}
|S_3|_{L^2} &\leq C(T) |\phi|_{0,2} \int_0^t \mathbb{E} \left((1 + |X_x(t-s)|_{L^\infty}^{6p}) e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} |\eta_x^h(t-s)|_{L^2}^2 \right) ds \\
&\leq C(T) |\phi|_{0,2} (1 + |x|_{L^\infty}^{6p}) |h|_{-1/2+\varepsilon}^2 |h|_{-1/2+\varepsilon}^2,
\end{aligned}$$

by Lemmas 4.1, 10.2 and 10.9. For S_4 , we have, using Lemmas 4.1 and 10.7,

$$\begin{aligned}
|S_4|_{L^2} &\leq C \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} (1 + |X_x(t-s)|_{L^\infty}^{4p}) |\xi_x^h(t-s)|_{L^2} \right) ds |\phi|_0 \\
&\leq C(T) (1 + |x|_{L^\infty}^{8p}) |\phi|_0 |h|_{-1/2+\varepsilon}^2.
\end{aligned}$$

Concerning S_5 , we have, by Lemmas 4.1, 10.7 and 10.5,

$$\begin{aligned} |S_5|_{L^2} &\leq C(T) \int_0^t \mathbb{E} \left(e^{-K \int_0^{t-s} g(X_x(\tau)) d\tau} (1 + |X_x(t-s)|_{L^\infty}^{12p}) |\xi_x^h(t-s)|_{L^2} \right) ds |\phi|_{0,1} \\ &\leq C(T) (1 + |x|_{L^\infty}^{16p}) |\phi|_{0,1} |h|_{-1/2+\varepsilon}^2. \end{aligned}$$

For S_6 , we have

$$\begin{aligned} |S_6|_{L^2} &\leq C \int_0^t \left(\int_0^{t-s} \mathbb{E} \left((1 + |X_x(\tau)|_{L^\infty}^{8p}) |\eta_x^h(\tau)|_{L^2}^2 e^{-K \int_0^\tau g(X_x(v)) dv} \right) d\tau \right)^{1/2} \\ &\quad \times \left(\mathbb{E} \left((1 + |X_x(t-s)|_{L^\infty}^{8p}) |\eta_x^h(t-s)|_{L^2}^2 e^{-K \int_0^{t-s} g(X_x(v)) dv} \right) \right)^{1/2} ds |\phi|_0 \\ &\leq C(T) (1 + |x|_{L^\infty}^{8p}) |h|_{-1/2+\varepsilon}^2 |\phi|_0 \int_0^t (1 + (t-s)^{-1/2+2\varepsilon}) ds \\ &\leq C(T) (1 + |x|_{L^\infty}^{8p}) |h|_{-1/2+\varepsilon}^2 |\phi|_0, \end{aligned}$$

by Lemmas 4.1 and 10.2 and Cauchy-Schwarz inequality.

For S_7 , we have, by Lemmas 4.1, 10.2 and 10.5 and Cauchy-Schwarz inequality,

$$\begin{aligned} |S_7|_{L^2} &\leq C(T) \int_0^t \int_0^{t-s} \left(\mathbb{E} \left((1 + |X_x(\tau)|_{L^\infty}^{8p}) |\eta_x^h(\tau)|_{L^2}^2 e^{-K \int_0^\tau g(X_x(v)) dv} \right) \right)^{1/2} d\tau \\ &\quad \times \left(\mathbb{E} \left((1 + |X_x(t-s)|_{L^\infty}^{24p}) |\eta_x^h(t-s)|_{L^2}^2 e^{-K \int_0^{t-s} g(X_x(v)) dv} \right) \right)^{1/2} ds |\phi|_{0,1} \\ &\leq C(T) (1 + |x|_{L^\infty}^{16p}) |\phi|_{0,1} |h|_{-1/2+\varepsilon}^2. \end{aligned}$$

For S_8 , we have, by Lemmas 4.1 and 10.2,

$$\begin{aligned} |S_8|_{L^2} &\leq C \int_0^t \mathbb{E} \left(\int_0^{t-s} (1 + |X_x(\tau)|_{L^\infty}^{4p}) |\eta_x^h(\tau)|_{L^2}^2 e^{-K \int_0^\tau g(X_x(v)) dv} d\tau (1 + |X_x(t-s)|_{L^\infty}^{4p}) \right) ds |\phi|_0 \\ &\leq C(T) (1 + |x|_{L^\infty}^{8p}) |\phi|_0 |h|_{-1/2+\varepsilon}^2. \end{aligned}$$

Using Lemmas 4.1 and 10.7, we have for S_9

$$\begin{aligned} |S_9|_{L^2} &\leq C \int_0^t \mathbb{E} \left(\int_0^{t-s} (1 + |X_x(\tau)|_{L^\infty}^{4p}) |\xi_x^h(\tau)|_{L^2} e^{-K \int_0^\tau g(X_x(v)) dv} d\tau (1 + |X_x(t-s)|_{L^\infty}^{4p}) \right) ds |\phi|_0 \\ &\leq C(T) |\phi|_0 |h|_{-1/2+\varepsilon}^2 (1 + |x|_{L^\infty}^{12p}). \end{aligned}$$

For S_{10} , we have

$$\begin{aligned} |S_{10}|_{L^2} &\leq C \int_0^t \mathbb{E} \left(\int_0^{t-s} (1 + |X_x(\tau)|_{L^\infty}^{8p}) |\eta_x^h(\tau)|_{L^2}^2 e^{-K \int_0^\tau g(X_x(v)) dv} d\tau (1 + |X_x(t-s)|_{L^\infty}^{4p}) \right) ds |\phi|_0 \\ &\leq C(T) (1 + |x|_{L^\infty}^{12p}) |\phi|_0 |h|_{-1/2+\varepsilon}^2, \end{aligned}$$

by Lemmas 4.1 and 10.2. The conclusion follows.

Remark 10.11 *We can easily adapt the proof done in this Appendix to show: For any $0 \leq \alpha < 1/2$, $0 \leq \beta < 1/2$, $0 < t \leq T$ and $x \in H$, we have*

$$|(-A)^\alpha D^2 P_t(x) (-A)^\beta| \leq C(T) (1 + t^{-(\alpha+\beta)}) (1 + |x|_{L^\infty}^{16p}) |\phi|_{0,2}.$$

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