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Weak backward error analysis for SDEs

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Abstract

We consider numerical approximations of stochastic differential equations by the Euler method. In the case where the SDE is elliptic or hypoelliptic, we show a weak backward error analysis result in the sense that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every invariant measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the Euler scheme is exponentially mixing.

Résumé

Nous étudions la discrétisation d'une équation différentielle stochastique (EDS) par le schéma d'Euler. Dans le cas d'une EDS elliptique ou hypoelliptique nous montrons un résultat d'analyse d'erreur 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 obtient ainsi que toute mesure invariante du schéma numérique est proche d'une mesure invariante modifiée obtenue par développement asymptotique. De plus, le schéma est exponentiellement mélangeant à des ordres arbitrairement élevés.

Keywords: backward error analysis, stochastic differential equations, exponential mixing, numerical scheme, Kolmogorov equation, weak error.

MSC number: 65C30, 60H35, 37M25

1 Introduction

In the last decades, *backward error analysis* has become one of the most powerful tool to analyze the long time behavior of numerical schemes applied to evolution equations. 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 $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a smooth vector field, and denote by $\varphi_t^f(y)$ the associated flow. By definition, a numerical method defines for a small time step τ an approximation Φ_τ of the exact flow φ_τ : We have for bounded $y \in \mathbb{R}^n$, $\Phi_\tau(y) = \varphi_\tau^f(y) + \mathcal{O}(\tau^{r+1})$ where r is the order of the method.

The idea of backward error analysis is to show that Φ_τ can be interpreted as the exact flow $\varphi_\tau^{f_\tau}$ or a *modified vector field* defined as a series in powers of τ

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

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

$$\Phi_\tau(y) = \varphi_\tau^{f_\tau^N}(y) + C_N \tau^N,$$

where f_τ^N is the truncated series:

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

Under some analyticity assumptions, the constant $C_N \tau^N$ can be optimized in N , so that the error term in the previous equation can be made exponentially small with respect to τ .

Such a result is very important and has many applications in the case where f has some strong geometric properties, such as Hamiltonian or reversible structure. In this situation, and under some compatibility conditions on the numerical method Φ_τ , the modified vector field f_τ inherits the structure of f . For example if Φ_τ is symplectic and f Hamiltonian, then f_τ remains Hamiltonian. This has major consequences such as the preservation of a modified Hamiltonian over very long time (of order τ^{-N}) for the numerical solution, from which we can deduce long time stability results, existence of numerical invariant tori in the integrable case, etc...

In the Hamiltonian case, this idea goes back to Moser [17], but was applied later to symplectic integrator by Benettin & Giorgilli [3], Hairer & Lubich [7] and Reich [18]. Such results now form the core of the modern *geometric numerical integration theory* for which we refer to the classical textbooks [8] and [14].

More recently, these ideas have been extended in some situations to Hamiltonian PDEs: First in the linear case [4], and then in the semilinear case (nonlinear Schrödinger or wave equations), see [6, 5].

As far as stochastic differential equations (SDEs) are concerned, this approach has not been developed very much so far. Let us recall that given a SDE in \mathbb{R}^d of the form

$$dX = f(X)dt + \sigma(X)dW$$

discretized by a numerical scheme - such as the Euler scheme for instance - with time step τ providing a discrete sequence $(X_p)_{p \in \mathbb{N}}$, then the error can be measured in the strong or weak sense. Strong error means that X_p is a pathwise approximation of $X(p\tau)$, and it is well known that the Euler scheme has strong order 1/2. Under standard assumptions on f and σ , we have

$$\mathbb{E} \left(\sup_{p=0, \dots, [T/\tau]} \|X_p - X(t_p)\|^k \right) \leq c_1(k, T)\tau^{1/2}, \quad k \geq 1, \quad T > 0.$$

In this work, we consider another error which is often more important. We investigate the weak error which concerns the law of the solution. The Euler scheme has weak order 1. Under suitable smoothness assumptions on f , σ and $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$ (see for instance [10, 12, 20]):

$$|\mathbb{E}(\varphi(X_p)) - \mathbb{E}(\varphi(X(t_p)))| \leq c_2(\varphi, T)\tau, \quad p = 0, \dots, [T/\tau], \quad T > 0.$$

An attempt has been made by Shardlow [23] to extend the backward error analysis to this context. He has shown that the construction of a modified SDE associated with the Euler scheme can be performed, but only at the first step, *ie* for $N = 2$, and only for additive noise, *ie* when $\sigma(X)$ does not depend on X . In this case, he is able to write down a modified SDE:

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

such that

$$\left| \mathbb{E}(\varphi(X_p)) - \mathbb{E}(\varphi(\tilde{X}(t_p))) \right| \leq c_3(\varphi, T)\tau^2, \quad p = 0, \dots, [T/\tau], \quad T > 0.$$

He explains that for multiplicative noise or higher order, there are too many conditions to be satisfied by the coefficients of the modified equations.

In this paper we take another approach, and build a modified equation not at the level of the SDE, but at the level of the generator associated with the process solution of the SDE. It is well known that given $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$ and denoting by $X(t, x)$ the solution of the SDE satisfying $X(0) = x$, the function $u(t, x) = \mathbb{E}(\varphi(X(t, x)))$ satisfies the Kolmogorov equation

$$\partial_t u(t, x) = L(x, \partial_x)u(t, x),$$

where L is the order 2 Kolmogorov operator associated with the SDE.

In the case of the Euler method applied to a SDE, we show that with the numerical solution, we can associate *modified Kolmogorov operator* of the form

$$L(\tau, x, \partial_x) = L(x, \partial_x) + \tau L_1(x, \partial_x) + \tau L_2(x, \partial_x) + \dots$$

where L_ℓ , $\ell \geq 1$ are some modified operator of order $2\ell + 2$. Again, the series does not converge but truncated series:

$$L^{(N)}(\tau, x, \partial_x) = L(x, \partial_x) + \tau L_1(x, \partial_x) + \dots + \tau L_N(x, \partial_x)$$

are considered.

Note that in contrast with the classical case, we do not have a modified SDE and cannot straightforwardly define a solution to the *modified equation*

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

However, in the case where the SDE is elliptic or hypoelliptic, we can build an approximated solution $v^{(N)}$ such that

$$\left| \mathbb{E}(\varphi(X_p)) - v^{(N)}(p\tau, x) \right| \leq c_4(\varphi, T, N) \tau^N, \quad p = 0, \dots, [T/\tau], \quad T > 0.$$

Furthermore, using the exponential convergence to equilibrium, we prove that in fact the constant c_4 does not depend on T so that we have an approximation result valid on very long times. We also show that there exist a modified invariant measure for $L^{(N)}(\tau, x, \partial_x)$.

We can then use this weak backward error analysis to prove that the numerical solution X_p , $p \geq 1$ obtained by the Euler scheme is exponentially mixing up to some very small error, and for all times. This is typically a geometric numerical integration result in the sense that we prove the persistence of a qualitative property of the exact flow (exponential mixing) to the numerical approximation, over long times.

Note that $v^{(N)}$ is in fact constructed as a truncated series: $v^{(N)} = \sum_{n=0}^N \tau^n v_n$ and that $v_0 = u$ is the solution of the Kolmogorov equation. Therefore, our result provides an expansion of the error as in [22] (see also [1, 2]). However, the expansion is different here.

Error estimates on long times for elliptic and hypoelliptic SDEs have already been proved. In [15, 19, 20, 21], it is shown that for a sufficiently small time step the 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 [22], the first term of an expansion of the invariant measure of the Euler scheme with respect to τ is also given. In our work, we provide the expansion at any order.

We emphasize that in our result, there is no particular smallness assumption on the stepsize τ used to define the numerical solution. In particular, the discrete

process is not supposed to have a unique invariant measure, as in [15] or [19, 20, 21].

This is also the case in the recent work [16]. There, it is shown that given an elliptic or hypoelliptic SDE, the ergodic averages provided by the Euler scheme are asymptotically close to the average of the invariant measure of the SDE. Higher order schemes also considered. The main tool in [16] is the ellipticity or hypoellipticity of the Poisson equation, *ie* the equation $L(x, \partial_x)u = g$.

As in [16], we consider the case where the SDE is set on the torus \mathbb{T}^d . This simplifies the presentation and the main ideas are not hidden by technical difficulties. In the same spirit, we only study the Euler scheme. In a forthcoming article, we will present more realistic applications of our method for SDEs set on \mathbb{R}^n with polynomial growth coefficients under suitable assumptions, and for more general schemes. As an example, we will treat the Langevin equation as in [21].

2 Preliminaries

We consider the stochastic differential equation

$$dX(t) = f(X(t))dt + \sigma(X(t))dW,$$

where the unknown $X = (X^i)_{i=1,\dots,d}$ lives in the d -dimensional torus \mathbb{T}^d . Also, $f = (f^i)_{i=1}^d$ and $\sigma = (\sigma_\ell^i(x))_{i=1,\dots,d,\ell=1,\dots,m}$ are smooth vector fields periodic in $x \in \mathbb{T}^d$. The process $(W^1(t), \dots, W^m(t))$ is a m -dimensional standard Wiener process over a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ endowed with a filtration $(\mathcal{F}_t)_{t \geq 0}$. Using these notations, we rewrite the equation as:

$$dX^i(t) = f^i(X(t))dt + \sum_{\ell=1}^m \sigma_\ell^i(X(t))dW^\ell(t), \quad i = 1, \dots, d.$$

In all the paper, smooth functions means \mathcal{C}^∞ functions. Given a smooth function ψ defined on \mathbb{T}^d , we denote by $\|\psi\|_{\mathcal{C}^k}$ its norm in $\mathcal{C}^k(\mathbb{T}^d, \mathbb{R})$. We also denote by $\|\psi\|_\infty = \sup_{x \in \mathbb{T}^d} |\psi(x)|$. For a multiindex $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{N}^d$, we set $|\mathbf{k}| = k_1 + \dots + k_d$ and

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

Therefore

$$\|\psi\|_{\mathcal{C}^k} := \sup_{\substack{\mathbf{j}=(j_1,\dots,j_d) \\ |\mathbf{j}|\leq k}} |\partial_{\mathbf{k}}\psi(x)|.$$

We also define the semi-norm

$$|\psi|_{\mathcal{C}^k} := \sup_{\substack{\mathbf{j}=(j_1,\dots,j_d) \\ 1 \leq |\mathbf{j}| \leq k}} |\partial_{\mathbf{k}} \psi(x)|.$$

In the following, we assume that f and σ are smooth and since we are working with a stochastic differential equation on the torus, standard theorems give existence and uniqueness of a solution for any initial data $X(0) = x \in \mathbb{T}^d$. We denote this solution by $X(t, x)$, $t \geq 0$. Also, since we chose to work on the torus, we do not have any problem of possible unbounded moments and this solution has clearly all moments finite.

We denote by $L(x, \partial_x)$ the Kolmogorov generator associated with the stochastic equation:

$$L(x, \partial_x)v(x) = f^i(x)\partial_i v(x) + a^{ij}(x)\partial_{ij}v(x),$$

where we use the summation convention for repeated indices and $\partial_i = \partial_{x_i}$ and

$$a^{ij}(x) := \frac{1}{2} \sum_{\ell=1}^m \sigma_{\ell}^i(x)\sigma_{\ell}^j(x).$$

It is well known that the Kolmogorov equation:

$$\frac{du}{dt} = L(x, \partial_x)u, \quad x \in \mathbb{T}^d, \quad t > 0, \quad u(0, x) = \varphi(x), \quad x \in \mathbb{T}^d, \quad (2.1)$$

with periodic boundary conditions has a unique solution for a smooth function φ and that for all $x \in \mathbb{T}^d$:

$$u(t, x) = \mathbb{E}(\varphi(X(t, x))).$$

Moreover, this solution is smooth. In the following, we write: $u(t) = P_t\varphi$ so that $(P_t)_{t \geq 0}$ is the transition semigroup associated with the Markov process $(X(t, x))_{t \geq 0, x \in \mathbb{T}^d}$. Note that we use the standard identification $u(t) = u(t, \cdot)$.

We wish to investigate the approximation properties of the Euler scheme for long times. We need assumptions on the long time behavior of the law of the solutions of (2.1), *ie* of the law of the Markov process. We assume the following mixing properties:

[H1] There exists a $\mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$ function $\rho \geq 0$ such that

$$L(x, \partial_x)^* \rho(x) = 0 \quad \text{and} \quad \int_{\mathbb{T}^d} \rho(x) dx = 1. \quad (2.2)$$

In other words, the measure $\rho(x)dx$ is invariant by $X(t, x)$.

[H2] Let $g \in \mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$, and assume that $\int_{\mathbb{T}^d} g(x) dx = 0$. Then there exists a unique function $\mu(x) \in \mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$ such that

$$L(x, \partial_x)^* \mu(x) = g(x), \quad \text{and} \quad \int_{\mathbb{T}^d} \mu(x) \rho(x) dx = 0. \quad (2.3)$$

[H3] Let $u(t, x)$ be the solution of (2.1). Assume that $\int_{\mathbb{T}^d} \varphi(x) \rho(x) dx = 0$, then there exists a constant λ and, for each $k \in \mathbb{N}$, a polynomial $p_k(t)$, such that if $\varphi(x) \in \mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$ we have the estimates

$$\forall t \geq 0, \quad \|u(t, \cdot)\|_{\mathcal{C}^k} \leq p_k(t) e^{-\lambda t} \|\varphi\|_{\mathcal{C}^k}. \quad (2.4)$$

These hypothesis are usually satisfied under elliptic or hypoelliptic assumptions on the operator $L(x, \partial_x)$. The reader may find in [13] conditions to ensure **[H1]**. We also refer to [1, 16] for a general definition of hypoellipticity and applications to numerical schemes. Combining kernel estimates for hypoelliptic diffusion ([1, 11]) and exponential convergence to equilibrium, **[H3]** can be proved. Note that similar estimates are used in [15, 19, 20, 21], where specific examples are considered. Finally, we mention that these hypothesis can be proved to be fulfilled using partial differential equations techniques (see [9]).

For a smooth function ψ , we set

$$\langle \psi \rangle = \int_{\mathbb{T}^d} \psi(x) \rho(x) dx.$$

Note that by **[H3]**, we have for any solution of (2.1) and $k \in \mathbb{N}$

$$\forall t \geq 0, \quad \|u(t, \cdot) - \langle \varphi \rangle\|_{\mathcal{C}^k} \leq p_k(t) e^{-\lambda t} \|\varphi - \langle \varphi \rangle\|_{\mathcal{C}^k}. \quad (2.5)$$

Now for a small time step $\tau > 0$ and $x \in \mathbb{T}^d$, we consider the Euler method defined, for $i = 1, \dots, d$, by $X_0 = x$ and the formula

$$X_{n+1}^i = X_n^i + \tau f^i(X_n) + \sigma_\ell^i(X_n) (W^\ell((n+1)\tau) - W^\ell(n\tau)), \quad (2.6)$$

for $n \geq 0$. Our main result can be stated as follows:

Theorem 2.1 *Let N and $\tau_0 > 0$ be fixed. Then there exists a modified smooth density*

$$\mu^N(x) = \rho(x) + \tau \mu_1(x) + \dots + \tau^N \mu_N(x)$$

such that $\int_{\mathbb{T}^d} \mu^N(x) dx = 1$, a constant C_N and a polynomial $P_N(t)$ such that the following holds: For all smooth function $\varphi(x)$ on \mathbb{T}^d , we have

$$\forall p \in \mathbb{N}, \quad \|\mathbb{E} \varphi(X_p) - \int_{\mathbb{T}^d} \varphi d\mu^N\|_\infty \leq \left(P_N(t_p) e^{-\lambda t_p} + C_N \tau^N \right) \|\varphi\|_{\mathcal{C}^{8N+2}}, \quad (2.7)$$

where for all p , $t_p = p\tau$ and $d\mu^N(x) = \mu^N(x) dx$.

This result can be viewed as a discrete version of (2.5). Note that it implies that all the invariant measure of the numerical process X_p are close to $d\mu^N$ up to a very small error term $C_N\tau^N$.

Using this result, we can also recover the weak convergence result

$$\forall p \geq 1, \quad \|\mathbb{E}\varphi(X_p) - \int_{\mathbb{T}^d} \varphi d\rho\|_\infty \leq C(\varphi)\tau$$

for some constant $C(\varphi)$ depending on φ , and where we set $d\rho(x) = \rho(x)dx$. This can be compared with [15, 16, 19, 20]. As in [16], the only assumption made on τ is that $\tau \leq \tau_0$ where τ_0 is any fixed number. The influence of τ_0 is only reflected in the constants in the right-hand side - we can for example take $\tau_0 = 1$. In particular, we do not assume that X_p has a unique invariant measure - something that would be guaranteed only if τ is small enough. We also recover an expansion of the invariant measure as in [22].

In the next sections, the constants appearing in the estimate depend in general on bounds on derivatives of f and g defining the SDE. They will also depend in general on τ_0 and N , but not on φ .

3 Asymptotic expansion of the weak error

We have the formal expansion for small t :

$$u(t, x) = \varphi(x) + tL(x, \partial_x)\varphi(x) + \frac{t^2}{2}L(x, \partial_x)^2\varphi(x) + \cdots + \frac{t^n}{n!}L(x, \partial_x)^n\varphi(x) + \cdots$$

This is just obtained by Taylor expansion in time since by (2.1) $\frac{d^n}{dt^n}u(t, x) = L(x, \partial_x)^n u(t, x)$ and in particular $\frac{d^n}{dt^n}u(0, x) = L(x, \partial_x)^n \varphi(x)$.

Since the solution u of the Kolmogorov equation is smooth and has its derivatives bounded in terms of the initial data φ , the above formal expansion can be justified and we have the following proposition whose proof is easy and left to the reader:

Proposition 3.1 *Assume that $\varphi \in C^\infty(\mathbb{T}^d, \mathbb{R})$, and let $\tau_0 > 0$. Then for all N , there exist a constant C_N such that for all $\tau < \tau_0$,*

$$\|u(\tau, x) - \sum_{n=0}^N \frac{\tau^n}{n!} L(x, \partial_x)^n \varphi(x)\|_\infty \leq C_N \tau^{N+1} |\varphi|_{C^{2N+2}}. \quad (3.1)$$

With the Euler scheme defined in (2.6), we associate the continuous process

$$\tilde{X}_x^i(t) = X_n^i + (t - n\tau)f^i(X_n) + \sigma_\ell^i(X_n)(W^\ell(t) - W^\ell(n\tau)), \quad t \in [n\tau, (n+1)\tau], \quad (3.2)$$

and $\tilde{X}(n\tau) = X_n$. We thus have $X_{n+1} = \tilde{X}_x(t_{n+1})$. The process (3.2) satisfies the equation

$$d\tilde{X}_x^i(t) = f^i(X_n)dt + \sigma_\ell^i(X_n)dW^\ell(t), \quad t \in [n\tau, (n+1)\tau]. \quad (3.3)$$

Clearly, (X_n) defines a discrete in time homogeneous Markov process but \tilde{X}_x is not Markov.

In this work, we are only interested in the distributions of the solutions and of their approximation. We now examine in detail the first time step and its approximation properties in terms of the law. By Markov property, it is sufficient to then obtain information at all steps. Next result gives an expansion similar to Proposition 3.1 for the Euler process.

Theorem 3.2 *Then for all $n \geq 1$, there exist operators $A_n(x, \partial_x)$ of order $2n$, such that for all $N \geq 1$, there exist a constant C_N satisfying*

$$\|\mathbb{E} \varphi(\tilde{X}_x(\tau)) - \sum_{n=0}^N \tau^n A_n(x, \partial_x) \varphi(x)\|_\infty \leq C_N \tau^{N+1} |\varphi|_{\mathcal{C}^{2N+2}}, \quad (3.4)$$

for all $\varphi \in \mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$ and $x \in \mathbb{T}^d$.

Proof. Using (3.3) and the Itô formula, we get for $t \leq \tau$,

$$d\varphi(\tilde{X}_x(t)) = L(x, \partial_x) \varphi(\tilde{X}_x(t)) + \sigma_\ell^i(x) \partial_i \varphi(\tilde{X}_x(t)) dW^\ell(t),$$

or equivalently,

$$\varphi(\tilde{X}_x(t)) = \varphi(x) + \int_0^t L(x, \partial_x) \varphi(\tilde{X}_x(s)) ds + \int_0^t \sigma_\ell^i(x) \partial_i \varphi(\tilde{X}_x(s)) dW^\ell(s). \quad (3.5)$$

Note that the last term is a martingale. We define the operator

$$R_{0,\ell}(x, \partial_x) = \sigma_\ell^i(x) \partial_i.$$

We have for all s and all x ,

$$L(x, \partial_x) \varphi(\tilde{X}_x(s)) = (f^i(x) \partial_i \varphi)(\tilde{X}_x(s)) + (a^{ij}(x) \partial_{ij} \varphi)(\tilde{X}_x(s)).$$

Hence applying (3.5) to $\partial_i\varphi$ and $\partial_{ij}\varphi$, we obtain

$$\begin{aligned}
L(x, \partial_x)\varphi(\tilde{X}_x(s)) &= L(x, \partial_x)\varphi(x) \\
&+ \int_0^s f^i(x)f^j(x)\partial_{ij}\varphi(\tilde{X}_x(\sigma)) + f^i(x)a^{n\ell}(x)\partial_{n\ell i}\varphi(\tilde{X}_x(\sigma))d\sigma \\
&+ \int_0^s a^{ij}(x)f^n(x)\partial_{ijn}\varphi(\tilde{X}_x(\sigma)) + a^{ij}(x)a^{n\ell}(x)\partial_{ijn\ell}\varphi(\tilde{X}_x(\sigma))d\sigma \\
&+ \int_0^s f^i(x)\sigma_\ell^j(x)\partial_{ij}\varphi(\tilde{X}_x(\sigma))dW^\ell(\sigma) \\
&+ \int_0^s a^{in}(x)\sigma_\ell^j(x)\partial_{inj}\varphi(\tilde{X}_x(\sigma))dW^\ell(\sigma).
\end{aligned}$$

We set $A_0 = I$, $A_1 = L$ and plugg this in (3.5) to obtain

$$\begin{aligned}
\varphi(\tilde{X}_x(t)) &= \varphi(x) + tA_1(x, \partial_x)\varphi(x) + \int_0^t \int_0^s A_2(x, \partial_x)\varphi(\tilde{X}_x(\sigma))d\sigma ds \\
&+ \int_0^t \int_0^s R_{1,\ell}(x, \partial_x)\varphi(\tilde{X}_x(\sigma))dW^\ell(\sigma)ds + \int_0^t R_{0,\ell}(x, \partial_x)\varphi(\tilde{X}_x(\sigma))dW^\ell(\sigma).
\end{aligned}$$

where

$$A_2(x, \partial_x) = f^i(x)f^j(x)\partial_{ij} + f^i(x)a^{n\ell}(x)\partial_{n\ell i} + a^{ij}(x)f^n(x)\partial_{ijn} + a^{ij}(x)a^{n\ell}(x)\partial_{ijn\ell}$$

is an operator of order 4, and

$$R_{1,\ell}(x, \partial_x) = f^i(x)\sigma_\ell^j(x)\partial_{ij} + a^{in}(x)\sigma_\ell^j(x)\partial_{inj}$$

are operators of order 3. Taking the expectation so that the last two term disappear, we easily deduce the result for $N = 1$.

Let us now prove recursively that there exist operators $A_n(x, \partial_x)$ of order $2n$ and $R_{n,\ell}(x, \partial_x)$ of order $2n + 1$, such that

$$\begin{aligned}
\varphi(\tilde{X}_x(t)) &= \varphi(x) + tL(x, \partial_x)\varphi(x) + \sum_{n=2}^N t^n A_n(x, \partial_x)\varphi(x) \\
&+ \int_0^t \cdots \int_0^{s_N} A_{N+1}(x, \partial_x)\varphi(\tilde{X}_x(s_{N+1}))ds_1 \cdots ds_{N+1} \\
&+ \sum_{n=1}^N \int_0^t \cdots \int_0^{s_n} R_{n,\ell}(x, \partial_x)\varphi(\tilde{X}_x(s_{n+1}))ds_1 \cdots ds_n dW^\ell(s_{n+1}).
\end{aligned} \tag{3.6}$$

Note the expectation of the last term vanishes so that (3.6) easily implies (3.4). To prove (3.6), assume that A_{N+1} and $R_{N,\ell}$ are known, and let us decompose A_{N+1} as $A_{N+1}(x, \partial_x) = A_{N+1}^{\mathbf{j}}(x)\partial_{\mathbf{j}}$, where $\mathbf{j} = (j_1, \dots, j_m)$ are multiindices

(with the summation convention) and $A_{N+1}^{\mathbf{j}}$ smooth functions of x . Such decomposition is easy to write for $N = 1$ or 2 . We apply (3.5) to $\partial_{\mathbf{j}}\varphi(\tilde{X}_x(s_{N+1}))$ for a given multi-index \mathbf{j} , and obtain

$$\begin{aligned} A_{N+1}^{\mathbf{j}}(x)\partial_{\mathbf{j}}\varphi(\tilde{X}_x(s_{N+1})) &= A_{N+1}^{\mathbf{j}}(x)\partial_{\mathbf{j}}\varphi(x) \\ &+ \int_0^{s_{N+1}} A_{N+1}^{\mathbf{j}}(x)f^n(x)\partial_n\partial_{\mathbf{j}}\varphi(\tilde{X}_x(s_{N+2}))ds_{N+2} \\ &+ \int_0^{s_{N+1}} A_{N+1}^{\mathbf{j}}(x)a^{n\ell}(x)\partial_{n\ell}\partial_{\mathbf{j}}\varphi(\tilde{X}_x(s_{N+2}))ds_{N+2} \\ &+ \int_0^{s_{N+1}} A_{N+1}^{\mathbf{j}}(x)\sigma_{\ell}^n(x)\partial_n\partial_{\mathbf{j}}\varphi(\tilde{X}_x(s_{N+2}))dW^{\ell}(s_{N+2}). \end{aligned}$$

We thus choose

$$A_{N+2}(x) = A_{N+1}^{\mathbf{j}}(x)f^n(x)\partial_n\partial_{\mathbf{j}} + A_{N+1}^{\mathbf{j}}(x)a^{ij}(x)\partial_{ij}\partial_{\mathbf{j}}$$

and

$$R_{N+1,\ell}(x) = A_{N+1}^{\mathbf{j}}(x)\sigma_{\ell}^n(x)\partial_n\partial_{\mathbf{j}},$$

and obtain (3.6) with $N + 1$ replaced by $N + 2$. ■

4 Modified generator

4.1 Formal series analysis

Let us now consider τ as fixed. We want to construct a formal series

$$L(\tau; x, \partial_x) = L(x, \partial_x) + \tau L_1(x, \partial_x) + \cdots + \tau^n L_n(x, \partial_x) + \cdots \quad (4.1)$$

with operator coefficients $L_n(x, \partial_x)$ smooth on \mathbb{T}^d , and such that formally the solution $v(t, x)$ at time $t = \tau$ of the equation

$$\partial_t v(t, x) = L(\tau; x, \partial_x)v(t, x), \quad v(0, x) = \varphi(x)$$

coincides in the sense of asymptotic expansion with the approximation of the transition semigroup $\mathbb{E}(\varphi(\tilde{X}_x(\tau)))$ studied in the previous section. In other words, we want to have the equality in the sense of asymptotic expansion in powers of τ

$$\exp(\tau L(\tau; x, \partial_x))\varphi(x) = \varphi(x) + \sum_{n \geq 1} \tau^n A_n(x, \partial_x)\varphi(x),$$

where the operators $A_n(x, \partial_x)$ are defined in Theorem 3.2.

Formally, this equation can be written

$$\exp(\tau L(\tau; x, \partial_x)) - \text{Id} = \tau \tilde{A}(\tau) \quad (4.2)$$

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

We have

$$\exp(\tau L(\tau; x, \partial_x)) - \text{Id} = \tau L(\tau; x, \partial_x) \left(\sum_{n \geq 0} \frac{\tau^n}{(n+1)!} L(\tau; x, \partial_x)^n \right).$$

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

$$\left(\sum_{n \geq 0} \frac{\tau^n}{(n+1)!} L(\tau; x, \partial_x)^n \right)^{-1} = \sum_{n \geq 0} \frac{B_n}{n!} \tau^n L(\tau; x, \partial_x)^n.$$

where the B_n are the Bernoulli numbers: see for instance [8, 5] and [4] for a similar analysis involving operators. Hence equations (4.1), (4.2) are equivalent in the sense of formal series to

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

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

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

Each of the terms of the above sum is an operator of order $2n + 2$ with smooth coefficients and therefore L_n is also an operator of order $2n + 2$ with smooth coefficients.

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

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

Moreover, we have clearly

$$L_n(x, \partial_x) \mathbb{1} = 0,$$

where $\mathbb{1}$ denote the constant function equal to 1.

4.2 Approximate solution of the modified flow

For a given N , we have constructed in the previous section an operator

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

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 $v^N(t, x)$ of the modified flow

$$\partial_t v^N(t, x) = L^{(N)}(\tau; x, \partial_x) v^N(t, x), \quad v^N(0, x) = \varphi(x). \quad (4.7)$$

However, in our situation we do not know whether this equation has a solution. This is in contrast with standard backward error analysis where the modified flow can always be defined.

The goal of the next proposition is to give a proper definition of the modified flow (4.7).

Theorem 4.1 *Let φ be a smooth functions on \mathbb{T}^d . For all $n \in \mathbb{N}$, there exist smooth functions $v_\ell(t, x)$, defined for all times $t \geq 0$, and such that for all $t \geq 0$ and $n \in \mathbb{N}$,*

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

with initial conditions $v_0(0, x) = \varphi(x)$ and $v_n(0, x) = 0$ for $n \geq 1$. For all $N \geq 0$, setting

$$v^{(N)}(t, x) = \sum_{k=0}^N \tau^k v_k(t, x), \quad (4.9)$$

then the following holds:

(i) *There exists a constant C_N such that for all time $t \geq 0$, and all $\tau \geq 0$,*

$$\|\mathbb{E} v^{(N)}(t, \tilde{X}_x(\tau)) - v^{(N)}(t + \tau, x)\|_\infty \leq C_N \tau^{N+1} \sup_{\substack{s \in (0, \tau) \\ n=0, \dots, N}} |v_n(t + s)|_{\mathcal{C}^{4N+2}}. \quad (4.10)$$

(ii) *For fixed $\tau_0 > 0$, there exists a constant C_N such that for all $\tau \leq \tau_0$,*

$$\|\mathbb{E} \varphi(\tilde{X}_x(\tau)) - v^{(N)}(\tau, x)\|_\infty \leq C_N \tau^{N+1} \|\varphi\|_{\mathcal{C}^{4N+2}}.$$

Proof. For $n = 0$, the equation (4.8) implies $v_0(t, x) = u(t, x)$, the solution of (2.1). Let $n \in \mathbb{N}$ and assume that $v_j(t, x)$ are constructed for $j = 1 \dots, n - 1$. Let

$$F_n(t, x) := \sum_{\ell=1}^n L_\ell v_{n-\ell}(t, x) \quad (4.11)$$

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

$$v_n(t) = \int_0^t P_{t-s} F_n(s) ds, \quad t \geq 0. \quad (4.12)$$

By [H3], it is not difficult to check that v_n , $n \in \mathbb{N}$ are smooth and that for all $t \geq 0$,

$$\|v_n(t)\|_{C^k} \leq C(t) \|\varphi\|_{C^{k+4n}}, \quad k \in \mathbb{N}, \quad (4.13)$$

where the constant $C(t)$ depends on t , k , n and on the coefficient of the equation. Clearly, this type of estimate can be improved in the elliptic case. This proves the first part of the Theorem.

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

$$\partial_s w_n(s, x) - L w_n(s, x) = \sum_{\ell=1}^n L_\ell w_{n-\ell}(s, x), \quad w_n(0, x) = v_n(t, x).$$

Let us consider the successive time derivatives of the functions $w_n(s, x)$. We have using the definition of w_n , for all $s \geq 0$,

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

and we see by induction that for all $m \geq 1$ and $s \geq 0$

$$\partial_s^m w_n(s, x) = \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1} \cdots L_{\ell_m} w_{\ell_{m+1}}(s, x). \quad (4.14)$$

Using the fact that the operators L_ℓ are of order $\ell + 2$ with no terms of order zero, we see that there exists a constant C depending on n and m , such that

$$\|\partial_s^m w_n(s, x)\|_\infty \leq C \sup_{k=0, \dots, n} |w_k(s)|_{C^{2k+2m}}.$$

Now let us consider the Taylor expansion of $w_n(\tau)$, for $\tau \leq \tau_0$ and $n = 0, \dots, N$,

$$\begin{aligned} w_n(\tau, x) &= \sum_{m=0}^{N-n} \frac{\tau^m}{m!} \partial_t^m w_n(0, x) + \int_0^\tau \frac{s^{N-m}}{(N-m)!} \partial_t^{N-m+1} w_n(s, x) ds \\ &= \sum_{m=0}^{N-n} \frac{\tau^m}{m!} \sum_{\ell_1+\dots+\ell_{m+1}=n} L_{\ell_1} \cdots L_{\ell_m} w_{\ell_{m+1}}(0, x) + R_{N,n}(\tau, x). \end{aligned}$$

Using the bounds on the time derivatives of $w_n(s, x)$, we obtain that for all $\tau \geq 0$ and all $n = 0, \dots, N$,

$$\|R_{N,n}(\tau, x)\|_\infty \leq C \tau^{N-m+1} \sup_{\substack{s \in (0, \tau) \\ n=0, \dots, N}} |w_n(s, x)|_{C^{4N+2}},$$

for some constant depending on N, m . After summation in n , and using the expression (4.5) of the operators A_n and the definition of w_n , we get

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

where

$$\|R_N(t, \tau, x)\|_\infty \leq C_N \tau^{N+1} \sup_{\substack{s \in (0, \tau) \\ n=0, \dots, N}} |v_n(t + s, x)|_{C^{4N+2}}.$$

To conclude, we use (3.4) applied to $\varphi = v^{(N)}(t, x)$, and we easily verify that $\mathbb{E}v^{(N)}(\tau, \tilde{X}_x(\tau))$ satisfy the same asymptotic expansion.

The second estimate (ii) is then a consequence of (i) with $t = 0$ and (4.13). ■

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

$$\partial_t v^{(N)}(t, x) = L^{(N)}(\tau; x, \partial_x) v^{(N)}(t, x) + R^{(N)}(t, x), \quad v^{(N)}(0, x) = \varphi(x),$$

where

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

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

5 Asymptotic expansion of the invariant measure and long time behavior

We now analyze the long time behavior of the solution of the modified equation (4.7). In the following, for a given operator $B(x, \partial_x)$, we denote by $B(x, \partial_x)^*$ its adjoint with respect to the L^2 product. We start by an asymptotic expansion of a formal invariant measure for the numerical scheme.

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

$$L_0^* \mu_n = - \sum_{\ell=1}^n (L_\ell)^* \mu_{n-\ell}. \quad (5.1)$$

Let $N \geq 0$ be fixed and $L^{(N)}(\tau; x, \partial_x)$ the operator defined by (4.6). Then the function

$$\mu^{(N)}(\tau; x) = \rho(x) + \sum_{n=1}^N \tau^n \mu_n(x) \in \mathcal{C}^\infty(\mathbb{T}^d, \mathbb{R})$$

satisfies

$$\int_{\mathbb{T}^d} \mu^{(N)}(\tau; x) dx = 1,$$

and

$$L^{(N)}(\tau; x, \partial_x)^* \mu^{(N)}(\tau; x) = G^{(N)}(\tau; x),$$

with for all k and all $\tau \in [0, \tau_0]$,

$$\|G^{(N)}(\tau; x)\|_{\mathcal{C}^k} \leq C_{N,k} \tau^{N+1} \quad \text{and} \quad \int_{\mathbb{T}^d} G^{(N)}(\tau; x) dx = 0,$$

where $C_{N,k}$ depends on N and k .

Proof. Assume that $\mu_0 = \rho$ and $\mu_j(x)$ are known, for $j = 0, \dots, n-1$ with $n \geq 1$. Consider the equation (5.1) given by

$$L_0^* \mu_n = - \sum_{\ell=1}^n (L_\ell)^* \mu_{n-\ell} = G_n.$$

Note that the right-hand side $G_n(x)$ is a smooth function satisfying

$$\int_{\mathbb{T}^d} G_n(x) dx = - \sum_{\ell=1}^n \int_{\mathbb{T}^d} (L_\ell)^* \mu_{n-\ell} dx = - \sum_{\ell=1}^n \int_{\mathbb{T}^d} \mu_{n-\ell} L_\ell \mathbb{1} dx = 0,$$

where $\mathbb{1}$ denotes the constant function equal to 1, which as already seen is in the Kernel of all the L_ℓ .

Using Hypothesis **[H2]**, we easily obtain the existence of a \mathcal{C}^∞ function μ_n satisfying (5.1) and $\int_{\mathbb{T}^d} \mu_n(x) dx = 0$. This shows the first part of the Proposition.

We then write

$$\begin{aligned} L^{(N)}(\tau; x, \partial_x)^* \mu^{(N)}(\tau; x) &= \sum_{n=0}^{2N} \tau^n \sum_{\substack{\ell_1 + \ell_2 = n \\ \ell_i \leq N}} (L_{\ell_1})^* \mu_{\ell_2} \\ &= \sum_{n=N+1}^{2N} \tau^n \sum_{\substack{\ell_1 + \ell_2 = n \\ \ell_i \leq N}} (L_{\ell_1})^* \mu_{\ell_2} \\ &=: G^{(N)}(\tau; x), \end{aligned}$$

and we easily verify that $G^{(N)}$ satisfies the hypothesis of the Proposition, owing to the fact that $L_\ell \mathbb{1} = 0$ for all $\ell \geq 0$. \blacksquare

Proposition 5.2 For all n and k there exists a polynomial $P_{k,n}(t)$ such that for all $t \geq 0$,

$$\|v_n(t, x) - \int_{\mathbb{T}^d} \varphi d\mu_n\|_{C^k} \leq P_{k,n}(t)e^{-\lambda t} \|\varphi - \langle \varphi \rangle\|_{C^{k+4n}}. \quad (5.2)$$

Proof. Using the fact that $\mu_0 = \rho$ and $v_0 = u$, we see that estimate (5.2) is satisfied for $n = 0$ (see Equation (2.5)). Let $n \geq 1$ and assume that v_j , $j = 0, \dots, n-1$ satisfy for $k \in \mathbb{N}$, $t \geq 0$:

$$\|v_j(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_j(x) dx\|_{C^k} \leq P_{k,j}(t)e^{-t\lambda} \|\varphi(x) - \langle \varphi \rangle\|_{C^k},$$

for some polynomial $P_{k,j}$.

Let us set

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

We claim that $c_n(t)$ does not depend on time. Indeed:

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

by definition of the coefficients μ_n , see (5.1). Note that, thanks to the smoothness properties of all the functions, the computation above is easily justified.

We deduce:

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

Next, we compute the average of F_n . By (4.8), (4.11) and (5.3), we have

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

We rewrite (4.12) as follows

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

Using the previous expression obtained for $\langle F_n(s) \rangle$ and recalling the initial data for v_n , we deduce that

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

Then, using $\int_{\mathbb{T}^d} \mu_m(x) dx = 0$, $m \in \mathbb{N}$, we get

$$\begin{aligned} v_n(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_n(x) dx = & \sum_{m=1}^n \int_{\mathbb{T}^d} (v_{n-m}(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_{n-m}(x) dx) \mu_m(x) dx \\ & + \int_0^t P_{t-s}(F_n(s, x) - \langle F_n(s) \rangle) ds. \end{aligned}$$

Note that, since L_ℓ , $\ell \in \mathbb{N}$ is a differential operator of order $2\ell + 2$ with smooth coefficients and containing no zero order terms, we have

$$\|F_n(s) - \langle F_n(s) \rangle\|_{C^k} \leq c_{k,\ell} \sum_{\ell=0}^{n-1} \|v_\ell(s) - \int_{\mathbb{T}^d} v_\ell(s, x) \mu_\ell(x) dx\|_{C^{k+2(n-\ell)+2}}.$$

Then by [H3]

$$\begin{aligned} \|v_n(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_n(x) dx\|_{C^k} \leq & \sum_{m=1}^n \|v_{n-m}(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_{n-m}(x) dx\|_\infty \int_{\mathbb{T}^d} |\mu_m(x)| dx \\ & + \int_0^t p_k(t-s) e^{-\lambda(t-s)} \|F_n(s, x) - \langle F_n(s) \rangle\|_{C^k} ds, \end{aligned}$$

and using the recursion assumption

$$\begin{aligned} \|v_n(t, x) - \int_{\mathbb{T}^d} \varphi(x) \mu_n(x) dx\|_{C^k} \leq & \sum_{m=1}^n c_{n,m} P_{0,n-m}(t) e^{-t\lambda} \|\varphi(x) - \langle \varphi \rangle\|_\infty \\ & + \sum_{\ell=0}^{n-1} \int_0^t p_k(t-s) P_{k+2(n-\ell)+2,\ell}(s) e^{-\lambda t} ds \|\varphi(x) - \langle \varphi \rangle\|_{k+4n}. \end{aligned}$$

The conclusion follows. ■

We give now our main result concerning the long time behavior of the numerical solution:

Theorem 5.3 *Let τ_0 and N be fixed. Then there exists C_N and a polynomial $P_N(t)$ such that the following holds: Let X_p be the discrete process defined by (2.6), then we have for $p \geq 0$, $\tau \geq 0$ and smooth function $\varphi(x)$*

$$\forall p \in \mathbb{N}, \quad \|\mathbb{E} \varphi(X_p) - v^{(N)}(t_p, x)\|_\infty \leq C_N \tau^N \|\varphi\|_{\mathcal{C}^{8N+2}}, \quad (5.4)$$

where for all p , $t_p = p\tau$. Moreover, we have

$$\forall p \in \mathbb{N}, \quad \|\mathbb{E} \varphi(X_p) - \int_{\mathbb{T}^d} \varphi d\mu^{(N)}\|_\infty \leq \left(P_N(t_p) e^{-\lambda t_p} + C_N \tau^N \right) \|\varphi\|_{\mathcal{C}^{8N+2}}, \quad (5.5)$$

where $d\mu^{(N)}(x) = \mu^{(N)}(x) dx$.

Proof. For all p , with $t_j = j\tau$, we have

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

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} . By the Markov property of the Euler process at times t_j :

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

Using (4.10) with $t = t_j$, and Proposition 5.2, we deduce that

$$\begin{aligned} \|\mathbb{E} \varphi(X_p) - v^{(N)}(t_p, x)\|_\infty &\leq C_N \tau^{N+1} \sum_{j=0}^{p-1} \sup_{\substack{s \in (0, \tau) \\ n=0, \dots, N}} |v_n(t_j + s, x)|_{4N+2} \\ &\leq C_N \tau^{N+1} \|\varphi\|_{\mathcal{C}^{8N+2}} \sum_{j=0}^{p-1} Q_N(t_j) e^{-\lambda t_j} \end{aligned}$$

for some constant C_N and polynomial $Q_N(t)$. We have used: $|v_n(t_j + s, x)|_{4N+2} = |v_n(t_j + s, x) - \int_{\mathbb{T}^d} \varphi d\mu_n|_{4N+2}$. We conclude by using the fact that for a fixed constant $\gamma > 0$, we have

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

where the constant C depends on γ and τ_0 . This shows (5.4). The second estimate is a consequence of Proposition 5.2. ■

References

- [1] V. Bally and D. Talay *The law of the Euler scheme for stochastic differential equations (I): convergence rate of the distribution function*, Prob. Theory and Rel. Fields, (1995), 104:43-60.
- [2] V. Bally and D. Talay *The law of the Euler scheme for stochastic differential equations (II): convergence rate of the density*, Monte Carlo Methods and Applications, (1996), 2:93-128.
- [3] G. Benettin and A. Giorgilli, *On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms*, J. Statist. Phys. 74 (1994), 1117–1143.
- [4] A. Debussche and E. Faou, *Modified energy for split-step methods applied to the linear Schrödinger equation* SIAM J. Numer. Anal. 47 (2009) 3705–3719.
- [5] E. Faou, *Geometric numerical integration of Hamiltonian PDEs and applications to computational quantum mechanics*. European. Math. Soc, to appear.
- [6] E. Faou and B. Grébert *Hamiltonian interpolation of splitting approximations for nonlinear PDEs*. Found. Comput. Math. to appear.
- [7] E. Hairer and C. Lubich, *The life-span of backward error analysis for numerical integrators*, Numer. Math. 76 (1997) 441–462
- [8] E. Hairer, C. Lubich and G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Second Edition. Springer 2006.
- [9] L. Hörmander, *The analysis of linear partial differential operators. III*, Classics in Mathematics, Springer, Berlin, 2007.
- [10] P. Kloeden and E. Platen, *Numerical Solution of Stochastic Differential Equations*, Applications of Mathematics (New York) 23, Springer-Verlag, Berlin, 1992.
- [11] S. Kusuoka and D. Stroock, *Applications of the Malliavin Calculus, part II*, J. Fac. Sci. Univ. Tokyo, 32:1–76, 1985.
- [12] G. Milstein and M. Tretyakov, *Stochastic Numerics for Mathematical Physics*, Springer, Berlin, Heidelberg, New York, 2004.
- [13] D. Nualart, *Malliavin Calculus and Related Topics*, Second Edition, Springer-Verlag, 2006.

- [14] B. Leimkuhler, S. Reich, *Simulating Hamiltonian dynamics*. Cambridge Monographs on Applied and Computational Mathematics, 14. Cambridge University Press, Cambridge, 2004.
- [15] J. C. Mattingly, A.M. Stuart and D.J. Higham, *Ergodicity for SDEs and approximations: locally Lipschitz vector fields and degenerate noise*. Stochastic Processes and their Applications 101(2) (2002) 185–232
- [16] J. C. Mattingly, A.M. Stuart and M.V. Tretyakov, *Convergence of numerical time-averaging and stationary measures via Poisson equations*, SIAM Journal on Numerical Analysis, vol. 48 no. 2 (2010), pp. 552–577.
- [17] J. Moser, *Lectures on Hamiltonian systems*, Mem. Am. Math. Soc. 81 (1968) 1–60.
- [18] S. Reich, *Backward error analysis for numerical integrators*, SIAM J. Numer. Anal. 36 (1999) 1549–1570.
- [19] D. Talay, *Second order discretization schemes of stochastic differential systems for the computation of the invariant law*. Stochastics and Stochastic Reports, 29(1) (1990) 13–36.
- [20] D. Talay. *Probabilistic numerical methods for partial differential equations: elements of analysis*. In D. Talay and L. Tubaro (Eds.), Probabilistic Models for Nonlinear Partial Differential Equations, Lecture Notes in Mathematics 1627 (1996) 48–196.
- [21] D. Talay, *Stochastic Hamiltonian dissipative systems: exponential convergence to the invariant measure, and discretization by the implicit Euler scheme*. Markov Processes and Related Fields 8(2) (2002) 163–198.
- [22] D. Talay and L. Tubaro, *Expansion of the global error for numerical schemes solving stochastic differential equations*. Stochastic Analysis and Applications, 8(4) (1990) 94–120.
- [23] T. Shardlow, *Modified equations for stochastic differential equations*. BIT Numerical Mathematics, 46 (2006) 111–125.