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Computing conditional Wiener integrals of functionals of a general form

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A numerical method of second order of accuracy for computing conditional Wiener integrals of smooth functionals of a general form is proposed. The method is based on the simulation of a Brownian bridge via the corresponding stochastic differential equations (SDEs) and on ideas of the weak-sense numerical integration of SDEs. A convergence theorem is proved. Special attention is paid to integral-type functionals. A generalization to the case of pinned diffusions is considered. Results of some numerical experiments are presented.

Keywords: conditional Wiener measure; Feynman path integrals; Brownian bridge; stochastic differential equations; weak approximation; Monte Carlo technique; conditioned diffusions.

1. Introduction

Let $C^d_{0,a;T,b}$ be the set of all d-dimensional continuous vector functions $x(t)$ over $[0, T]$ satisfying the conditions $x(0) = a$ and $x(T) = b$. Consider the conditional Wiener integral

$$\mathcal{J} = \int_{C^d_{0,a;T,b}} F(x(\cdot))\mathrm{d}\mu^{T,b}_{0,a}(x), \tag{1.1}$$

where F is a functional on $C^d_{0,a;T,b}$ and $\mu^{T,b}_{0,a}(x)$ is the conditional Wiener measure, corresponding to the Brownian paths $X^{T,b}_{0,a}(t)$ with fixed initial and final points, i.e., it corresponds to the d-dimensional Brownian bridge from a at the time $t = 0$ to b at the time $t = T$. The integral (1.1) is to be understood in the sense of a Lebesgue integral with respect to the measure $\mu^{T,b}_{0,a}(x)$ and is taken over the set $C^d_{0,a;T,b}$ (see, e.g., Gelfand & Yaglom, 1960; Simon, 2005).

The importance of path integrals (1.1) for computing various quantities in quantum statistical mechanics is well known (Gelfand & Yaglom, 1960; Feynman & Hibbs, 1965; Egorov *et al.*, 1993; Roepstorff, 1994; Kleinert, 1995; Simon, 2005). For instance, the Feynman path integral of the form

$$\begin{aligned}\mathcal{J} &= \langle a|\mathrm{e}^{-TH}|b\rangle \\ &= \int \exp\left(\int_0^T \left[\frac{m\dot{x}^2(t)}{2} - V(x(t))\right]\mathrm{d}t\right)\mathcal{D}x(t), \quad H = -\frac{1}{2}\Delta + V,\end{aligned}$$

is equivalent to the conditional Wiener integral (1.1) with the exponential-type functional

$$F(x(\cdot)) = \exp\left[-\int_0^T V(x(t))\mathrm{d}t\right]. \tag{1.2}$$

Such quantities as the free energy of the system, the ground state energy, the wave function, etc., can be written in terms of the integral given in (1.1) and (1.2) (Gelfand & Yaglom, 1960; Feynman & Hibbs, 1965; Roepstorff, 1994; Kleinert, 1995; Lobanov, 1996; Simon, 2005).

A wider class of functionals than (1.2) is also of interest. For example, correlation functions are expressed via the conditional Wiener integral (1.1) with a more general functional than (1.2) (see, e.g., Roepstorff, 1994; Kleinert, 1995; Lobanov, 1996, and references therein). They are written as the functional averages of products of path positions at different times. For instance, for $d = 1$, a two-point correlation function $\Gamma(\theta)$, where $0 \leqslant \theta \leqslant T$, has the form

$$\begin{aligned}\Gamma(\theta) &= \langle x(0)x(\theta)\rangle \\ &= \frac{1}{\mathcal{Z}(T)}\int_{-\infty}^{\infty}\int_{C_{0,y;T,y}} x(0)\varphi\left(x(\theta), \int_0^T V(t,x(t))\mathrm{d}t\right)\mathrm{d}\mu_{0,y}^{T,y}(x)\mathrm{d}y \\ &= \frac{1}{\mathcal{Z}(T)}\int_{-\infty}^{\infty}\int_{C_{0,y;T,y}} y\varphi\left(x(\theta), \int_0^T V(t,x(t))\mathrm{d}t\right)\mathrm{d}\mu_{0,y}^{T,y}(x)\mathrm{d}y, \qquad (1.3)\end{aligned}$$

where we have

$$\varphi(x,z) = x\exp(-z),$$

the partition function

$$\mathcal{Z}(T) = \mathrm{Tr}\,\mathrm{e}^{-TH} = \int_{-\infty}^{\infty}\int_{C_{0,y;T,y}}\exp\left[-\int_0^T V(x(t))\mathrm{d}t\right]\mathrm{d}\mu_{0,y}^{T,y}(x)\mathrm{d}y$$

and $C_{0,y;T,y}$ means $C^1_{0,y;T,y}$. Correlation functions contain important information about quantum mechanical systems and they are observable in scattering experiments (see, e.g., Kleinert, 1995).

Other important examples of more general functionals than (1.2) are those corresponding to internal and kinetic energies (see, e.g., Feynman, 1972; Takahashi & Imada, 1984; Ceperley, 1995). In Example 6.3 we simulate the kinetic energy of a bosonic system.

We propose a probabilistic numerical method of second order of accuracy for computing conditional Wiener integrals of sufficiently smooth functionals. This method exploits a Markovian representation of the Brownian bridge. Together with the Monte Carlo technique, it gives an effective algorithm for computing the conditional Wiener integral (1.1). A virtue of the approach is that the infinite-dimensional integral is expressed as an expectation with respect to a system of stochastic differential equations (SDEs) before any discretization takes place, rather than beginning by using a finite-dimensional approximation to the integral as is usually done (Creutz & Freedman, 1981; Wagner, 1988; Egorov *et al.*, 1993; Ceperley, 1995; Lobanov, 1996). The proposed algorithm is very simple to realize in practice.

In Gladyshev & Milstein (1984) and Ventzel *et al.* (1984) (see also Milstein & Tretyakov, 2004b) the probabilistic approach was used for computing Wiener integrals with respect to the usual (unconditional) Wiener measure. In Milstein & Tretyakov (2004a) (see also Milstein & Tretyakov, 2004b) this approach was exploited to compute conditional Wiener integrals of exponential-type functionals. Here, on the one hand, we deal with a more complicated system than in Gladyshev & Milstein (1984) and Ventzel *et al.* (1984) since the SDEs involved in the method are singular. This leads to a rather sophisticated proof of the method's convergence, requiring some new ideas. On the other hand, we consider a much wider class of functionals than in Milstein & Tretyakov (2004a). The proposed method is new in comparison with the ones available in Milstein & Tretyakov (2004a) and it is analogous to the one used in the case of the usual Wiener measure (Ventzel *et al.*, 1984). We also note that there are a large number of methods and results (see, e.g., Milstein & Tretyakov, 2004b, and references therein) for approximating simple functionals $f(X(T))$, where f is a function from a sufficiently wide class and $X(t)$, where $t_0 < t < T$, is a solution of SDEs. But not much attention (except, e.g., Ventzel *et al.*, 1984; Mackevicius, 1997; Milstein & Tretyakov, 2004b) has been paid to approximating general functionals depending on trajectories of the SDE solution. Other approaches to computing Wiener integrals can be found, for example, in Creutz & Freedman (1981), Wagner (1988), Egorov *et al.* (1993), Ceperley (1995) and Lobanov (1996) (see also references therein).

In Section 2 we specify the class of functionals considered, together with some examples, propose the numerical methods (analogues of the trapezoidal rule and of an Euler-type scheme) and formulate convergence theorems for them. In Section 3 we prove the convergence theorem for the second-order method, using the Taylor formula for functionals. Section 4 deals with conditional Wiener integrals of integral-type functionals. In Section 5 we consider a generalization to the case of path integrals with respect to nonlinear diffusion bridges (with additive noise). We exploit the results of Clark (1990) and Delyon & Hu (2006) to express path integrals of integral-type functionals over pinned diffusions as expectations with respect to a Markovian process that solves a system of SDEs. In this case we propose an Euler-type method and prove its first-order convergence. See, for example Hairer *et al.* (2009) (and references therein) for other approaches to simulating diffusion bridges. Some results of numerical experiments are presented in Section 6.

2. Functionals of a general form

We start this section by specifying the class of functionals for which the corresponding convergence theorem shall be proved. This is done via the formal assumptions listed below. Then, in Section 2.1, we give some examples from this class of functionals.

Let us consider functionals $F(x)$ defined on the space $A[0,T]$ of right-continuous d-dimensional vector functions $x(t)$ on the interval $[0,T]$ without discontinuities of the second kind, i.e., consider functionals on a larger space than $C^d_{0,a;T,b}$.

ASSUMPTIONS 2.1. We make the following assumptions on F.

(i) Let $0 < \theta_1 < \cdots < \theta_i < \cdots < \theta_n < T$. Introduce the measure ν_r on $[0,T]^r$, which is the sum of the r-dimensional Lebesgue measure on $[0,T]^r$, of the $(r-1)$-dimensional Lebesgue measure on the hyperplanes $\{(s_1,\ldots,s_r) \in [0,T]^r \colon s_j = \theta_i\}$, where $i = 1,\ldots,n$, and $j = 1,\ldots,r$, and on the diagonal hyperplanes $\{(s_1,\ldots,s_r) \in [0,T]^r \colon s_i = s_j\}$, of the $(r-2)$-dimensional Lebesgue measure on the $(r-2)$-dimensional hyperplanes $\{(s_1,\ldots,s_r) \in [0,T]^r \colon s_k = \theta_i$ and $s_l = \theta_j, k \neq l\}$ and $\{(s_1,\ldots,s_r) \in [0,T]^r \colon s_i = s_j$ and $s_k = s_l\}$ and so on, including the one-dimensional Lebesgue measure on the lines $\left\{s_1 = \theta_{i_1},\ldots,s_{r-1} = \theta_{i_{r-1}}\right\}$, where $i_j \in \{1,\ldots,n\}$, and on the diagonal $\{s_1 = s_2 = \cdots = s_r\}$ plus the unit measures concentrated on the points $\left(\theta_{i_1},\ldots,\theta_{i_r}\right)$, where $i_j \in \{1,\ldots,n\}$.

(ii) We assume that the functional $F(x)$ is six times Fréchet differentiable and that its rth derivative has the following form:

$$F^{(r)}(x)(\delta_1,\ldots,\delta_r) = \int_{[0,T]^r} v^{(r)}(x; s_1,\ldots,s_r)\delta_1(s_1)\cdots\delta_r(s_r)\nu_r(\mathrm{d}s_1\cdots\mathrm{d}s_r),$$
$$r = 1,\ldots,6, \tag{2.1}$$

where $\delta_i \in A[0,T]$ and the vector functions $\upsilon^{(r)}(x; s_1, \dots, s_r)$ are symmetric in the arguments $s_1, \dots, s_r$ and uniformly bounded for $x \in A[0,T]$ and $s_i \in [0,T]$.

(iii) For any function $x \in A[0,T]$ that is constant on a semi-interval $[c_0, c^0) \subset [0,T]$, there are the following continuous derivatives:

$$\frac{\mathrm{d}}{\mathrm{d}s}\upsilon^{(1)}(x;s); \quad \frac{\partial}{\partial s_1}\upsilon^{(2)}(x;s_1,s_2),\ \ s_1 \neq s_2,\ s_j \neq \theta_i; \quad \frac{\mathrm{d}}{\mathrm{d}s}\upsilon^{(2)}(x;s,s);$$
$$\frac{\mathrm{d}}{\mathrm{d}s}\upsilon^{(2)}(x;s,\theta_i), \quad i = 1,\dots,n,$$

which are bounded by a constant that is independent of $[c_0, c^0)$ and $x \in A[0,T]$.

We recall (see, e.g., Kolmogorov & Fomin, 1999) that $F^{(r)}(x)(\delta_1, \dots, \delta_r)$ are r-linear functionals. Under Assumptions 2.1, we will prove a convergence theorem (Theorem 2.2) for the method proposed in Section 2.2. We emphasize that the method is applicable much more widely.

Roughly speaking, one might say that we consider functionals of the general form on $A[0,T]$ that satisfy some conditions on smoothness and boundedness. As is usual for any numerical methods, if we weaken the assumptions about the smoothness, then, as a rule, the convergence order of the considered method becomes lower than the optimal one. In physical applications the smoothness part of Assumptions 2.1 is not particularly restrictive since it is usually satisfied. The assumption on the boundedness of derivatives of functionals can be, to some extent, weakened without loss of convergence order, but this would significantly complicate the proof of the convergence theorem. At the same time, the common computational practice in quantum statistical mechanics is to curtail potentials so that they and their derivatives remain bounded, which usually implies the boundedness of derivatives of functionals. Alternatively, the concept of rejecting exploding trajectories from Milstein & Tretyakov (2005) could be exploited here, that is, we might choose not to take into account those trajectories that leave a bounded domain $\mathcal{S}$ during the time T. The domain $\mathcal{S}$ is chosen so that the boundedness condition is satisfied when $x(\cdot) \in \mathcal{S}$.

2.1 *Examples of functionals*

To illustrate the class of functionals satisfying Assumptions 2.1, we give two particular examples here, although many more can be immediately constructed.

1. We start with the integral-type functionals (see the functional needed to compute the correlation function (1.3))

$$F(x(\cdot)) = \varphi\left(x(\theta), \int_0^T f(t, x(t))\mathrm{d}t\right), \quad 0 \leqslant \theta \leqslant T, \ \ x \in C^d_{0,a;T,b}. \tag{2.2}$$

One can check that, if the functions $f(t,x)$ and $\varphi(x,z)$ have continuous and bounded derivatives up to a sufficiently high order, then Assumptions 2.1 hold. In particular, the Fréchet derivatives (2.1) have the following form:

$$F^{(1)}(x)(\delta_1) = \int_{[0,T]} \upsilon^{(1)}(x; s_1)\delta_1(s_1)\nu_1(\mathrm{d}s_1)$$

with

$$v^{(1)}(x;s_1)\delta_1(s_1)=\frac{\partial\varphi}{\partial z}\nabla_x f(s_1,x(s_1))\cdot\delta_1(s_1),\quad s_1\neq\theta,$$

$$v^{(1)}(x;\theta)\delta_1(\theta)=\nabla_x\varphi\cdot\delta_1(\theta)$$

and the measure ν_1 being the sum of the Lebesgue measure on $[0,T]$ and the unit measure concentrated at the point θ;

$$F^{(2)}(x)(\delta_1,\delta_2)=\int_{[0,T]^2}v^{(2)}(x;s_1,s_2)\delta_1(s_1)\delta_2(s_2)\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2)$$

with

$$v^{(2)}(x;s_1,s_2)\delta_1(s_1)\delta_2(s_2)=\frac{\partial^2\varphi}{\partial z^2}\nabla_x f(s_1,x(s_1))\cdot\delta_1(s_1)\nabla_x f(s_2,x(s_2))\cdot\delta_2(s_2),\qquad s_1\neq s_2,\quad s_i\neq\theta,$$

$$v^{(2)}(x;s,\theta)\delta_1(s)\delta_2(\theta)=\sum_{i=1}^{d}\frac{\partial^2\varphi}{\partial z\partial x^i}\nabla_x f(s,x(s))\cdot\delta_1(s)\delta_2^i(\theta),\quad s\neq\theta,$$

$$v^{(2)}(x;s,s)\delta_1(s)\delta_2(s)=\frac{\partial\varphi}{\partial z}\sum_{i,j=1}^{d}\frac{\partial^2 f}{\partial x^i\partial x^j}(s,x(s))\delta_1^i(s)\delta_2^j(s),\quad s\neq\theta,$$

$$v^{(2)}(x;\theta,\theta)\delta_1(\theta)\delta_2(\theta)=\sum_{i,j=1}^{d}\frac{\partial^2\varphi}{\partial x^i\partial x^j}\delta_1^i(\theta)\delta_2^j(\theta)$$

and the measure ν_2 being the sum of the two-dimensional Lebesgue measure on $[0,T]^2$, the one-dimensional Lebesgue measures on the lines $\{s_1=\theta\}$ and $\{s_2=\theta\}$ and on the diagonal $\{s_1=s_2\}$ and the unit measure concentrated at the point (θ,θ); the other derivatives can be written analogously. In the above formulas the derivatives of the function φ are taken at the point $\left(x(\theta),\int_0^T f(t,x(t))\mathrm{d}t\right)$ and the dot '$\cdot$' means the usual scalar product of vectors.

2. Let the functions $f(t,x)$, $g(t,x)$ and $\varphi(z)$ have continuous and bounded derivatives up to a sufficiently high order. Then the functional

$$F(x(\cdot))=\varphi\left(\int_0^T\int_0^t f(s,x(s))g(t,x(t))\mathrm{d}s\,\mathrm{d}t\right)$$

satisfies Assumptions .

2.2 *Numerical method*

Let $(\Omega,\mathcal{F},\mathcal{F}_t,P)$, where $0\leqslant t\leqslant T$, be a filtered probability space and $w(t)=(w^1(t),\dots,w^d(t))^{\mathrm{T}}$ be a d-dimensional $\{\mathcal{F}_t\}_{t\geqslant 0}$-adapted standard Wiener process. As is known (Ikeda & Watanabe, 1981; Karatzas & Shreve, 1988), the d-dimensional Brownian bridge $X(t)=X_{0,a}^{T,b}(t)$, where $0\leqslant t\leqslant T$, from a to b can be characterized as the pathwise unique solution of the system of SDEs

$$\mathrm{d}X=\frac{b-X}{T-t}\mathrm{d}t+\mathrm{d}w(t),\quad 0\leqslant t<T,\quad X(0)=a,\tag{2.3}$$

with

$$X(T) = b. \tag{2.4}$$

Clearly, the conditional Wiener integral $\mathcal{J}$ from (1.1) is equal to the expectation of the functional taken over all realizations of $X(t)$, where $0 \leqslant t \leqslant T$, that is,

$$\mathcal{J} = EF(X). \tag{2.5}$$

We introduce a discretization of the time interval $[0, T]$ as follows:

$$0 = t_0 < t_1 < \cdots < t_N = T,$$

so that the points θ_i, where $i = 1, \ldots, n$, belong to the set $\{t_0, t_1, \ldots, t_N\}$. Let

$$h := \max_{0 \leqslant k \leqslant N-1} (t_{k+1} - t_k)$$

and $t_{k+1/2} := (t_{k+1} + t_k)/2$, where $k = 0, \ldots, N-1$.

The solution of (2.3) is

$$X(t) = a\frac{T-t}{T} + b\frac{t}{T} + (T-t)\int_0^t \frac{\mathrm{d}w(s)}{T-s}. \tag{2.6}$$

Hence, for any $0 \leqslant \varDelta < T - t$ we have

$$X(t+\varDelta) = X(t) + \varDelta\frac{b - X(t)}{T-t} + (T-t-\varDelta)\int_t^{t+\varDelta} \frac{\mathrm{d}w(s)}{T-s}. \tag{2.7}$$

We also have

$$E\left[(T-t-\varDelta)\int_t^{t+\varDelta}\frac{\mathrm{d}w(s)}{T-s}\,\middle|\, X(t)\right] = 0,$$

$$E\left[\left((T-t-\varDelta)\int_t^{t+\varDelta}\frac{\mathrm{d}w(s)}{T-s}\right)^2 \,\middle|\, X(t)\right] = \left(1 - \frac{\varDelta}{T-t}\right)\varDelta. \tag{2.8}$$

We can exactly simulate the solution of (2.3) by a simple recurrent procedure based on the formula

$$X(t+\varDelta) = X(t) + \varDelta\frac{b - X(t)}{T-t} + \varDelta^{1/2}\sqrt{\frac{T-t-\varDelta}{T-t}}\,\xi, \quad t < T, \tag{2.9}$$

where ξ is a random vector whose components are independent Gaussian random variables with zero mean and unit variance and are also independent of $X(t)$.

We also introduce a piecewise constant function $X^h(t)$, where $t \in [0, T]$, given by

$$\begin{aligned}
&X^h(t) := a, \quad t \in [0, t_{1/2}),\\
&X^h(t) := X(t_k), \quad t \in [t_{k-1/2}, t_{k+1/2}), \quad k = 1, \ldots, N-1,\\
&X^h(t) := b, \quad t \in [t_{N-1/2}, T].
\end{aligned} \tag{2.10}$$

Clearly, the trajectories $X^h(t)$ belong to the space $A[0, T]$.

We define the approximation of the conditional Wiener integral $\mathcal{J}$ as follows:

$$\mathcal{J} = EF(X) \approx \bar{\mathcal{J}} = EF(X^h). \tag{2.11}$$

This method is analogous to the one used in the case of the usual (unconditional) Wiener measure (Ventzel *et al.*, 1984; see also Milstein & Tretyakov, 2004b). We will prove the following convergence theorem.

THEOREM 2.2. Assume that Assumptions 2.1 hold. The method (2.11) and (2.10) applied to the evaluation of the Wiener integral (1.1) is of second order of accuracy, i.e.,

$$|\mathcal{J} - \bar{\mathcal{J}}| = |EF(X) - EF(X^h)| \leqslant Kh^2, \tag{2.12}$$

where the constant K is independent of h.

The proof of the theorem is given in Section 3.

REMARK 2.3. The method (2.11) and (2.10) is exact (i.e., there is no integration error) on the class of functionals that depend only on the value of the function $x(t)$ at a finite number of points θ_i, where $i = 1, \ldots, n$.

The method (2.11) and (2.10) together with the Monte Carlo technique gives an effective algorithm for computing conditional Wiener integrals that is very simple to realize in practice. The method (2.11) and (2.10) can be interpreted as a trapezoidal scheme. This interpretation becomes obvious in the case of integral-type functionals (see (4.4) and (4.5)).

Now consider the Euler method, i.e., introduce the following piecewise constant function $X_E^h(t)$, where $t \in [0, T]$:

$$X_E^h(t) := X(t_k), \quad t \in [t_k, t_{k+1}), \quad k = 0, \ldots, N-1, \qquad X_E^h(T) := b. \tag{2.13}$$

THEOREM 2.4. Assume that Assumptions 2.1(i) and 2.1(iii) hold and 2.1(ii) holds with $r = 1, 2, 3, 4$ in (2.1). Then

$$\tilde{\mathcal{J}} = EF(X_E^h) \tag{2.14}$$

approximates $\mathcal{J}$ with the first order of accuracy.

The proof of this theorem is easier than that of Theorem 2.2 and it is omitted here. In numerical Example 6.3 we compare the method (2.11) and (2.10) and the Euler method (2.14) and (2.13). The experimental results confirm our theoretical predictions.

3. Proof of the convergence theorem

Here we exploit some constructions from Ventzel *et al.* (1984), although the singularity of the drift in (2.3) as t approaches T causes additional difficulties, which are overcome by adopting ideas from Milstein & Tretyakov (2004a). For simplicity and legibility, let us prove the theorem in the one-dimensional case $d = 1$. No additional ideas are required to carry it over to an arbitrary dimension d (see, however, Remark 3.2 at the end of this section). Note that, in this section, we shall use the letter K to denote various constants that are independent of k and h.

In addition to the processes $X(t)$ and $X^h(t)$, we shall also introduce the following two auxiliary processes $X_k(t)$, where $k = 0, \dots, N$, and $\bar{X}_k(t)$, where $k = 0, \dots, N-1$:

$$X_k(t) := X(t)\chi_{[0,t_k)}(t) + X(t_k)\chi_{[t_k,T]}(t) + \sum_{j=k}^{N-1} \Delta_j X \chi_{[t_{j+1/2},T]}(t),$$

$$\Delta_j X := X(t_{j+1}) - X(t_j) \tag{3.1}$$

and

$$\bar{X}_k(t) := X(t)\chi_{[0,t_k)}(t) + X(t_k)\chi_{[t_k,T]}(t) + \sum_{j=k+1}^{N-1} \left(\Delta_j X + (t_{j+1} - t_j) \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T - s'} \right) \chi_{[t_{j+1/2},T]}(t). \tag{3.2}$$

We note that $\bar{X}_k(t) = X(t_k)$ for $t \in [t_k, t_{k+3/2}) \cap [0, T]$, i.e., the random function $\bar{X}_k(t)$ is constant on the interval $[t_k, t_{k+3/2}) \cap [0, T]$.

One can see that $X_N(t) = X(t)$ and $X_0(t) = X^h(t)$. We rewrite the global error in the form

$$EF(X) - EF(X^h) = EF(X_N) - EF(X_0) = \sum_{k=0}^{N-1} [EF(X_{k+1}) - EF(X_k)]. \tag{3.3}$$

Thus we need to analyse the difference

$$\rho_k := EF(X_{k+1}) - EF(X_k). \tag{3.4}$$

Recall the following Taylor formula for functionals (see, e.g., Kolmogorov & Fomin, 1999):

$$F(x + \delta) = F(x) + F^{(1)}(x)(\delta) + \cdots + \frac{1}{5!} F^{(5)}(x)(\delta, \dots, \delta) + \frac{1}{6!} F^{(6)}(x + \lambda\delta)(\delta, \dots, \delta), \quad 0 < \lambda < 1.$$

We expand $F(X_{k+1})$ and $F(X_k)$ at $\bar{X}_k$ as follows:

$$F(X_{k+i}) = F(\bar{X}_k) + \int_{[0,T]} \upsilon^{(1)}(\bar{X}_k; s_1)\delta_{k,i}(s_1)\nu_1(\mathrm{d}s_1) + \cdots + \frac{1}{5!} \int_{[0,T]^5} \upsilon^{(5)}(\bar{X}_k; s_1, \dots, s_5)\delta_{k,i}(s_1) \cdots \delta_{k,i}(s_5)\nu_5(\mathrm{d}s_1 \cdots \mathrm{d}s_5) + \frac{1}{6!} \int_{[0,T]^6} \upsilon^{(6)}(\bar{X}_k + \lambda_i \delta_{k,i}; s_1, \dots, s_6)\delta_{k,i}(s_1) \cdots \delta_{k,i}(s_6)\nu_6(\mathrm{d}s_1 \cdots \mathrm{d}s_6),$$

$$0 < \lambda_i < 1, \quad i = 0, 1, \tag{3.5}$$

where

$$\begin{aligned}\delta_{k,0}(s) &= X_k(s) - \bar{X}_k(s) = \varDelta_k X \chi_{[t_{k+1/2},T]}(s) - \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s)\\ &= \chi_{[t_{k+1/2},T]}(s)\left[(t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k} + (T-t_{k+1})\int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'}\right]\\ &\quad - \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s), \end{aligned} \tag{3.6}$$

$$\begin{aligned}\delta_{k,1}(s) &= X_{k+1}(s) - \bar{X}_k(s) = (X(s)-X(t_k))\chi_{[t_k,t_{k+1})}(s) + \varDelta_k X \chi_{[t_{k+1},T]}(s)\\ &\quad - \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s)\\ &= \chi_{[t_k,t_{k+1})}(s)\left[(s-t_k)\frac{b-X(t_k)}{T-t_k} + (T-s)\int_{t_k}^{s} \frac{\mathrm{d}w(s')}{T-s'}\right]\\ &\quad + \chi_{[t_{k+1},T]}(s)\left[(t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k} + (T-t_{k+1})\int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'}\right]\\ &\quad - \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s).\end{aligned}$$

It is clear that $\delta_{k,0}(s) = \delta_{k,1}(s)$ for $s \notin (t_k, t_{k+1})$. It can also be seen that the measure ν_r, where $r = 1, \ldots, 6$, of the set $S_k^{(r)}$ on which the difference $\prod_{j=1}^r \delta_{k,1}(s_j) - \prod_{j=1}^r \delta_{k,0}(s_j)$ is different from zero has order h. Indeed, $S_k^{(r)} = \bigcup_{j=1}^r \{(s_1, \ldots, s_r)\colon s_j \in (t_k, t_{k+1})\}$ and hence $\nu_r(S_k^{(r)}) < r\nu_r(\{(s_1, \ldots, s_r)\colon s_1 \in (t_k, t_{k+1})\})$, which is of order h. Furthermore, it is not difficult to verify that the integral $\int_{t_k}^{s} \frac{\mathrm{d}w(s')}{T-s'}$, where $t_k \leqslant s \leqslant t_{k+1}$, and $\bar{X}_k$ are independent by showing that $E\left[\bar{X}_k(t)\int_{t_k}^{s} \frac{\mathrm{d}w(s')}{T-s'}\right] = 0$ for any $0 \leqslant t \leqslant T$ and $t_k \leqslant s \leqslant t_{k+1}$. In what follows these properties are used in the analysis of the parts of ρ_k. We shall also exploit the following inequality (see, e.g., Milstein & Tretyakov, 2004a, Lemma A.4) for any $p \geqslant 1$:

$$E|b - X(t_k)|^{2p} \leqslant K(T-t_k)^p. \tag{3.7}$$

We have from (3.4) and (3.5) that

$$\begin{aligned}\rho_k &= E\int_{[0,T]} \upsilon^{(1)}(\bar{X}_k; s_1)[\delta_{k,1}(s_1) - \delta_{k,0}(s_1)]\nu_1(\mathrm{d}s_1)\\ &\quad + \frac{1}{2}E\int_{[0,T]^2} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)[\delta_{k,1}(s_1)\delta_{k,1}(s_2) - \delta_{k,0}(s_1)\delta_{k,0}(s_2)]\nu_2(\mathrm{d}s_1\mathrm{d}s_2) + \cdots\\ &\quad + \frac{1}{5!}E\int_{[0,T]^5} \upsilon^{(5)}(\bar{X}_k; s_1, \ldots, s_5)\left[\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right]\nu_5(\mathrm{d}s_1\cdots\mathrm{d}s_5)\end{aligned}$$

$$+\frac{1}{6!}E\int_{[0,T]^6}\left[v^{(6)}(\bar{X}_k+\lambda_1\delta_{k,1};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,1}(s_j)\right.$$
$$\left.-v^{(6)}(\bar{X}_k+\lambda_0\delta_{k,0};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,0}(s_j)\right]\nu_6(\mathrm{d}s_1\cdots\mathrm{d}s_6). \tag{3.8}$$

Before we start with the analysis of ρ_k, we state the lemma that will be used in estimating the second term of (3.8) and that is proved at the end of this section.

LEMMA 3.1. Let $U_s(x) := v^{(2)}(x;s,s)$. Then the following estimate holds:

$$\left|EU_{t_k}(\bar{X}_k)\left[\frac{(b-X(t_k))^2}{(T-t_k)^2}-\frac{1}{T-t_k}\right]\right|\leqslant\frac{K}{\sqrt{T-t_k}},$$

where $K>0$ is a constant that is independent of k and h.

Now we analyse the terms forming ρ_k in (3.8). Let us introduce the indicator $I_k=I_{\{\theta_1,\ldots,\theta_n\}}(t_k)$. For the first term in (3.8) we obtain

$$\begin{aligned}
r_k^{(1)} &:= E\int_{[0,T]}v^{(1)}(\bar{X}_k;s_1)[\delta_{k,1}(s_1)-\delta_{k,0}(s_1)]\nu_1(\mathrm{d}s_1)\\
&= E\int_{t_k}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)[\delta_{k,1}(s_1)-\delta_{k,0}(s_1)]\mathrm{d}s_1\\
&\quad+v^{(1)}(\bar{X}_k;t_k)[\delta_{k,1}(t_k)-\delta_{k,0}(t_k)]I_k+v^{(1)}(\bar{X}_k;t_{k+1})[\delta_{k,1}(t_{k+1})-\delta_{k,0}(t_{k+1})]I_{k+1}\\
&= E\int_{t_k}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)\left[(s_1-t_k)\frac{b-X(t_k)}{T-t_k}+(T-s_1)\int_{t_k}^{s_1}\frac{\mathrm{d}w(s')}{T-s'}\right]\mathrm{d}s_1\\
&\quad-E\int_{t_{k+1/2}}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)\left[(t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k}+(T-t_{k+1})\int_{t_k}^{t_{k+1}}\frac{\mathrm{d}w(s')}{T-s'}\right]\mathrm{d}s_1\\
&= E\frac{b-X(t_k)}{T-t_k}\left[\int_{t_k}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)(s_1-t_k)\mathrm{d}s_1-(t_{k+1}-t_k)\int_{t_{k+1/2}}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)\mathrm{d}s_1\right]\\
&= E\frac{b-X(t_k)}{T-t_k}\left[\int_{t_k}^{t_{k+1/2}}v^{(1)}(\bar{X}_k;s_1)(s_1-t_k)\mathrm{d}s_1-\int_{t_{k+1/2}}^{t_{k+1}}v^{(1)}(\bar{X}_k;s_1)(t_{k+1}-s_1)\mathrm{d}s_1\right].
\end{aligned}$$

Integrating by parts, we get

$$\begin{aligned}
r_k^{(1)} = E\frac{b-X(t_k)}{T-t_k}&\left[v^{(1)}(\bar{X}_k;t_{k+1/2})\frac{(t_{k+1}-t_k)^2}{8}-\int_{t_k}^{t_{k+1/2}}\frac{\mathrm{d}}{\mathrm{d}s_1}v^{(1)}(\bar{X}_k;s_1)\frac{(s_1-t_k)^2}{2}\mathrm{d}s_1\right.\\
&\left.-v^{(1)}(\bar{X}_k;t_{k+1/2})\frac{(t_{k+1}-t_k)^2}{8}-\int_{t_{k+1/2}}^{t_{k+1}}\frac{\mathrm{d}}{\mathrm{d}s_1}v^{(1)}(\bar{X}_k;s_1)\frac{(t_{k+1}-s_1)^2}{2}\mathrm{d}s_1\right]
\end{aligned}$$

$$= -E\frac{b-X(t_k)}{T-t_k}\left[\int_{t_k}^{t_{k+1/2}}\frac{\mathrm{d}}{\mathrm{d}s_1}\upsilon^{(1)}(\bar{X}_k;s_1)\frac{(s_1-t_k)^2}{2}\mathrm{d}s_1\right.$$
$$\left.+\int_{t_{k+1/2}}^{t_{k+1}}\frac{\mathrm{d}}{\mathrm{d}s_1}\upsilon^{(1)}(\bar{X}_k;s_1)\frac{(t_{k+1}-s_1)^2}{2}\mathrm{d}s_1\right].$$

It follows from here and the inequality (3.7) that

$$|r_k^{(1)}| \leqslant \frac{Kh^3}{\sqrt{T-t_k}}, \quad k=0,\ldots,N-1. \tag{3.9}$$

Now consider the second term in (3.8). We obtain

$$\begin{aligned}
r_k^{(2)} &:= \frac{1}{2}E\int_{[0,T]^2}\upsilon^{(2)}(\bar{X}_k;s_1,s_2)[\delta_{k,1}(s_1)\delta_{k,1}(s_2)-\delta_{k,0}(s_1)\delta_{k,0}(s_2)]\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2)\\
&= \frac{1}{2}E\int_{[0,T]^2}\upsilon^{(2)}(\bar{X}_k;s_1,s_2)\\
&\quad\times\left\{\left[(s_1-t_k)(s_2-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2}+(s_1\wedge s_2-t_k)\frac{T-s_1\vee s_2}{T-t_k}\right]\right.\\
&\qquad\times\chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_k,t_{k+1})}(s_2)\\
&\qquad+2\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2}+(s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_{k+1},T]}(s_2)\\
&\qquad+\left[(t_{k+1}-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2}+(t_{k+1}-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\\
&\qquad\times\left(\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2)-\chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right)\\
&\qquad-\frac{2}{T-t_k}\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s_2)\\
&\qquad\left.\times\left[(s_1-t_k)\chi_{[t_k,t_{k+1})}(s_1)-(t_{k+1}-t_k)\chi_{[t_{k+1/2},t_{k+1})}(s_1)\right]\right\}\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2).
\end{aligned}\tag{3.10}$$

We decompose the integral from (3.10) and estimate each part separately. We have

$$\begin{aligned}
A_{1k} := E\int_{[0,T]^2}&\upsilon^{(2)}(\bar{X}_k;s_1,s_2)\\
&\times\left[(s_1-t_k)(s_2-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2}+(s_1\wedge s_2-t_k)\frac{T-s_1\vee s_2}{T-t_k}\right]\\
&\times\chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_k,t_{k+1})}(s_2)\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2)
\end{aligned}$$

$$= E\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s, s)\left[(s-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s-t_k)\frac{T-s}{T-t_k}\right]\mathrm{d}s$$

$$+ E\int_{t_k}^{t_{k+1}}\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2)$$

$$\times\left[(s_1-t_k)(s_2-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1\wedge s_2 - t_k)\frac{T-s_1\vee s_2}{T-t_k}\right]\mathrm{d}s_1\,\mathrm{d}s_2, \tag{3.11}$$

where the last integral is estimated by Kh^3 by observing that $\sup|v^{(2)}|$ is bounded (see Assumptions 2.1) and using (3.7) to get

$$E\frac{(b-X(t_k))^2}{(T-t_k)^2} \leqslant \frac{K}{T-t_k} \leqslant \frac{K}{h}.$$

Also note that, in (3.11), we omit the integrals over the measure concentrated on the lines $s = t_k$ and $s = t_{k+1}$ and over the unit measures since it is obvious that they are equal to zero. Furthermore, since $v^{(2)}(\bar{X}_k; s, s) = v^{(2)}(\bar{X}_k; t_k, t_k) + \int_{t_k}^{s}\frac{\mathrm{d}}{\mathrm{d}s'}v^{(2)}(\bar{X}_k; s', s')\mathrm{d}s'$, the first integral on the right-hand side of (3.11) can be written as

$$E\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s, s)\left[(s-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s-t_k)\frac{T-s}{T-t_k}\right]\mathrm{d}s$$

$$= Ev^{(2)}(\bar{X}_k; t_k, t_k)\left[\frac{(b-X(t_k))^2}{(T-t_k)^2}\int_{t_k}^{t_{k+1}}(s-t_k)^2\,\mathrm{d}s + \int_{t_k}^{t_{k+1}}(s-t_k)\frac{T-s}{T-t_k}\mathrm{d}s\right]$$

$$+ E\int_{t_k}^{t_{k+1}}\int_{t_k}^{s}\frac{\mathrm{d}}{\mathrm{d}s'}v^{(2)}(\bar{X}_k; s', s')\left[(s-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s-t_k)\frac{T-s}{T-t_k}\right]\mathrm{d}s'\,\mathrm{d}s,$$

where the second integral is estimated by Kh^3 using the same arguments as in (3.11). So, we have

$$A_{1k} = Ev^{(2)}(\bar{X}_k; t_k, t_k)\left[\frac{(b-X(t_k))^2}{(T-t_k)^2}\frac{(t_{k+1}-t_k)^3}{3} + \frac{(t_{k+1}-t_k)^2}{2}\frac{T-t_{k+1}+(t_{k+1}-t_k)/3}{T-t_k}\right]$$

$$+ \mathcal{O}(h^3)$$

with $|\mathcal{O}(h^3)| \leqslant Kh^3$. The next part of (3.10) can be written as

$$
\begin{aligned}
A_{2k} &:= 2E\int_{[0,T]^2} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right] \\
&\quad \times \chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_{k+1},T]}(s_2)\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2) \\
&= 2E\int_{t_{k+1}}^{T}\int_{t_k}^{t_{k+1}} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\mathrm{d}s_1\,\mathrm{d}s_2 \\
&\quad + \sum_{i=1}^{n} I_{\theta_i>t_k} E\int_{t_k}^{t_{k+1}} \upsilon^{(2)}(\bar{X}_k; s_1, \theta_i)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\mathrm{d}s_1 \\
&= 2E\left[\frac{(t_{k+1}-t_k)^3}{2}\frac{(b-X(t_k))^2}{(T-t_k)^2} + \frac{(t_{k+1}-t_k)^2}{2}\frac{T-t_{k+1}}{T-t_k}\right] \\
&\quad \times \left[\int_{t_{k+1}}^{T} \upsilon^{(2)}(\bar{X}_k; t_k, s_2)\mathrm{d}s_2 + \sum_{i=1}^{n} I_{\theta_i>t_k}\upsilon^{(2)}(\bar{X}_k; t_k, \theta_i)\right] + \mathcal{O}(h^3).
\end{aligned}
$$

The third part of (3.10) is

$$
\begin{aligned}
A_{3k} &:= E\left[(t_{k+1}-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2} + (t_{k+1}-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\int_{[0,T]^2} \upsilon^{(2)}(\bar{X}_k; s_1, s_2) \\
&\quad \times \left[\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2) - \chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right]\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2).
\end{aligned}
$$

For the integral in A_{3k} we have

$$
\begin{aligned}
&\int_{[0,T]^2} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\left[\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2) - \chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right]\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2) \\
&\quad = \int_{t_{k+1}}^{T} \upsilon^{(2)}(\bar{X}_k; s, s)\mathrm{d}s - \int_{t_{k+1/2}}^{T} \upsilon^{(2)}(\bar{X}_k; s, s)\mathrm{d}s \\
&\qquad + 2\sum_{i=1}^{n} I_{\theta_i>t_k}\left[\int_{t_{k+1}}^{T} \upsilon^{(2)}(\bar{X}_k; s, \theta_i)\mathrm{d}s - \int_{t_{k+1/2}}^{T} \upsilon^{(2)}(\bar{X}_k; s, \theta_i)\mathrm{d}s\right] \\
&\qquad + \int_{t_{k+1}}^{T}\int_{t_{k+1}}^{T} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\mathrm{d}s_1\,\mathrm{d}s_2 - \int_{t_{k+1/2}}^{T}\int_{t_{k+1/2}}^{T} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\mathrm{d}s_1\,\mathrm{d}s_2 \\
&\quad = -\frac{(t_{k+1}-t_k)}{2}\upsilon^{(2)}(\bar{X}_k; t_k, t_k) - (t_{k+1}-t_k)\sum_{i=1}^{n} I_{\theta_i>t_k}\upsilon^{(2)}(\bar{X}_k; t_k, \theta_i) + \mathcal{O}(h^2) \\
&\qquad - 2\int_{t_{k+1/2}}^{T}\int_{t_{k+1/2}}^{t_{k+1}} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\mathrm{d}s_1\,\mathrm{d}s_2 + \int_{t_{k+1/2}}^{t_{k+1}}\int_{t_{k+1/2}}^{t_{k+1}} \upsilon^{(2)}(\bar{X}_k; s_1, s_2)\mathrm{d}s_1\,\mathrm{d}s_2
\end{aligned}
$$

$$= -\frac{(t_{k+1}-t_k)}{2}\upsilon^{(2)}(\bar{X}_k; t_k, t_k) - (t_{k+1}-t_k)\sum_{i=1}^{n} I_{\theta_i > t_k}\upsilon^{(2)}(\bar{X}_k; t_k, \theta_i)$$

$$- (t_{k+1}-t_k)\int_{t_{k+1}}^{T}\upsilon^{(2)}(\bar{X}_k; t_k, s_2)\mathrm{d}s_2 + \mathcal{O}(h^2).$$

Then

$$A_{3k} = -E\left[\left(\upsilon^{(2)}(\bar{X}_k; t_k, t_k) + 2\sum_{i=1}^{n} I_{\theta_i > t_k}\upsilon^{(2)}(\bar{X}_k; t_k, \theta_i)\right)\right.$$
$$\left.\times\left(\frac{(t_{k+1}-t_k)^3}{2}\frac{(b - X(t_k))^2}{(T-t_k)^2} + \frac{(t_{k+1}-t_k)^2}{2}\frac{T-t_{k+1}}{T-t_k}\right)\right]$$
$$- E\left[(t_{k+1}-t_k)^3\frac{(b - X(t_k))^2}{(T-t_k)^2} + (t_{k+1}-t_k)^2\frac{T-t_{k+1}}{T-t_k}\right]\int_{t_{k+1}}^{T}\upsilon^{(2)}(\bar{X}_k; t_k, s_2)\mathrm{d}s_2$$
$$+ \mathcal{O}(h^3).$$

The last part of (3.10) is

$$A_{4k} := -\frac{2}{T-t_k}E\int_{[0,T]^2}\upsilon^{(2)}(\bar{X}_k; s_1, s_2)\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s_2)$$
$$\times\left[(s_1 - t_k)\chi_{[t_k,t_{k+1})}(s_1) - (t_{k+1}-t_k)\chi_{[t_{k+1/2},t_{k+1})}(s_1)\right]\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2)$$
$$= -\frac{2}{T-t_k}E\int_{[0,T]^2}\upsilon^{(2)}(\bar{X}_k; s_1, s_2)\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s_2)$$
$$\times\left[(s_1 - t_k)\chi_{[t_k,t_{k+1/2})}(s_1) - (t_{k+1}-s_1)\chi_{[t_{k+1/2},t_{k+1})}(s_1)\right]\nu_2(\mathrm{d}s_1\,\mathrm{d}s_2)$$
$$= -\frac{2}{T-t_k}E\left[\int_{t_{k+3/2}}^{T}\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s_2)\right.$$
$$\times\left(\int_{t_k}^{t_{k+1/2}}\upsilon^{(2)}(\bar{X}_k; s_1, s_2)(s_1-t_k)\mathrm{d}s_1\right.$$
$$\left.-\int_{t_{k+1/2}}^{t_{k+1}}\upsilon^{(2)}(\bar{X}_k; s_1, s_2)(t_{k+1}-s_1)\mathrm{d}s_1\right)\mathrm{d}s_2 + \sum_{i=1}^{n} I_{\theta_i > t_{k+1}}(\theta_i - t_{k+1})$$
$$\left.\times\left(\int_{t_k}^{t_{k+1/2}}\upsilon^{(2)}(\bar{X}_k; s_1, \theta_i)(s_1-t_k)\mathrm{d}s_1 - \int_{t_{k+1/2}}^{t_{k+1}}\upsilon^{(2)}(\bar{X}_k; s_1, \theta_i)(t_{k+1}-s_1)\mathrm{d}s_1\right)\right].$$

Exploiting arguments similar to the ones used before, it is not difficult to get that $A_{4k} = \mathcal{O}(h^3)$.

As a result, we obtain

$$r_k^{(2)} = \frac{1}{2}(A_{1k} + A_{2k} + A_{3k} + A_{4k})$$
$$= -\frac{(t_{k+1} - t_k)^3}{12} E v^{(2)}(\bar{X}_k; t_k, t_k) \left[\frac{(b - X(t_k))^2}{(T - t_k)^2} - \frac{1}{T - t_k} \right] + \mathcal{O}(h^3). \tag{3.12}$$

Applying Lemma 3.1, we get

$$|r_k^{(2)}| \leqslant \frac{K h^3}{\sqrt{T - t_k}}. \tag{3.13}$$

Now we estimate the remaining terms in (3.8). We obtain from (3.6) that

$$\delta_{k,0}(s) = \chi_{[t_{k+1/2},T]}(s)(t_{k+1} - t_k)\frac{b - X(t_k)}{T - t_k} + \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T - s'} \sum_{j=k+1}^{N-1} (t_{j+1} - t_j)\chi_{[t_{k+1/2},t_{j+1/2})}(s).$$

Then

$$E v^{(3)}(\bar{X}_k; s_1, s_2, s_3) \prod_{i=1}^{3} \delta_{k,0}(s_i)$$
$$= E v^{(3)}(\bar{X}_k; s_1, s_2, s_3)$$
$$\times \prod_{i=1}^{3} \left((t_{k+1} - t_k)\frac{b - X(t_k)}{T - t_k}\chi_{[t_{k+1/2},T]}(s_i) + \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T - s'} \sum_{j=k+1}^{N-1} (t_{j+1} - t_j)\chi_{[t_{k+1/2},t_{j+1/2})}(s_i) \right)$$
$$= E v^{(3)}(\bar{X}_k; s_1, s_2, s_3)(t_{k+1} - t_k)^2 \frac{b - X(t_k)}{(T - t_k)^2} \left((t_{k+1} - t_k)\frac{(b - X(t_k))^2}{T - t_k} \prod_{i=1}^{3} \chi_{[t_{k+1/2},T]}(s_i) \right.$$
$$\left. + \sum_{i=1}^{3} \frac{\chi_{[t_{k+1/2},T]}(s_i)}{T - t_{k+1}} \prod_{l \neq i} \sum_{j=k+1}^{N-1} (t_{j+1} - t_j)\chi_{[t_{k+1/2},t_{j+1/2})}(s_l) \right).$$

From here we get the estimate

$$\left| E \left[v^{(3)}(\bar{X}_k; s_1, s_2, s_3) \prod_{j=1}^{3} \delta_{k,0}(s_j) \right] \right| \leqslant \frac{K h^2}{\sqrt{T - t_k}}.$$

Analogously, we obtain

$$\left| E \left[v^{(3)}(\bar{X}_k; s_1, s_2, s_3) \prod_{j=1}^{3} \delta_{k,1}(s_j) \right] \right| \leqslant \frac{K h^2}{\sqrt{T - t_k}}.$$

Then, also taking into account that the measure ν_3 of the set $S_k^{(3)}$ on which the difference $\prod_{j=1}^{3}\delta_{k,1}(s_j) - \prod_{j=1}^{3}\delta_{k,0}(s_j)$ is different from zero has order $\mathcal{O}(h)$, we arrive at

$$\begin{aligned}
&\left|\frac{1}{6}E\int_{[0,T]^3} v^{(3)}(\bar{X}_k; s_1, s_2, s_3)\left[\prod_{j=1}^{3}\delta_{k,1}(s_j) - \prod_{j=1}^{3}\delta_{k,0}(s_j)\right]\nu_3(\mathrm{d}s_1\,\mathrm{d}s_2\,\mathrm{d}s_3)\right| \\
&\quad = \left|\frac{1}{6}E\int_{[0,T]^3} I_{S_k^{(3)}}(s_1, s_2, s_3)v^{(3)}(\bar{X}_k; s_1, s_2, s_3)\left[\prod_{j=1}^{3}\delta_{k,1}(s_j) - \prod_{j=1}^{3}\delta_{k,0}(s_j)\right]\nu_3(\mathrm{d}s_1\,\mathrm{d}s_2\,\mathrm{d}s_3)\right| \\
&\quad \leqslant \frac{1}{6}\int_{[0,T]^3} I_{S_k^{(3)}}(s_1, s_2, s_3)\left[\left|Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)\prod_{j=1}^{3}\delta_{k,1}(s_j)\right|\right. \\
&\qquad\qquad \left. + \left|Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)\prod_{j=1}^{3}\delta_{k,0}(s_j)\right|\right]\nu_3(\mathrm{d}s_1\,\mathrm{d}s_2\,\mathrm{d}s_3) \\
&\quad \leqslant \frac{Kh^3}{\sqrt{T-t_k}}.
\end{aligned} \tag{3.14}$$

Since we have for the terms in (3.6) that

$$E(\Delta_k X)^4 \leqslant Kh^2, \quad E(X(s) - X(t_k))^4\chi_{[t_k,t_{k+1})}(s) \leqslant Kh^2,$$

$$E\left(\int_{t_k}^{t_{k+1}}\frac{\mathrm{d}w(s')}{T-s'}\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s)\right)^4 \leqslant Kh^2,$$

and the measure ν_4 of the set $S_k^{(4)}$ on which the difference $\prod_{j=1}^{4}\delta_{k,1}(s_j) - \prod_{j=1}^{4}\delta_{k,0}(s_j)$ is different from zero has order $\mathcal{O}(h)$, we obtain

$$\begin{aligned}
&\left|\frac{1}{4!}E\int_{[0,T]^4} v^{(4)}(\bar{X}_k; s_1, \ldots, s_4)\left[\prod_{j=1}^{4}\delta_{k,1}(s_j) - \prod_{j=1}^{4}\delta_{k,0}(s_j)\right]\nu_4(\mathrm{d}s_1\cdots\mathrm{d}s_4)\right| \\
&\quad \leqslant \frac{1}{4!}\sup|v^{(4)}|\int_{[0,T]^4} I_{S_k^{(4)}}(s_1, \ldots, s_4)\left(E\left|\prod_{j=1}^{4}\delta_{k,1}(s_j)\right| + E\left|\prod_{j=1}^{4}\delta_{k,0}(s_j)\right|\right)\nu_4(\mathrm{d}s_1\cdots\mathrm{d}s_4) \\
&\quad \leqslant Kh^3.
\end{aligned} \tag{3.15}$$

By analogous arguments, we get

$$\begin{aligned}
&\left|\frac{1}{5!}E\int_{[0,T]^5} v^{(5)}(\bar{X}_k; s_1, \ldots, s_5)\left[\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right]\nu_5(\mathrm{d}s_1\cdots\mathrm{d}s_5)\right| \\
&\quad \leqslant \frac{1}{5!}\sup|v^{(5)}|\int_{[0,T]^5} E\left|\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right|\nu_5(\mathrm{d}s_1\cdots\mathrm{d}s_5) \\
&\quad \leqslant Kh^{7/2}.
\end{aligned} \tag{3.16}$$

Since $E\prod_{j=1}^{6}|\delta_{k,i}(s_j)| \leqslant Kh^3$, the last term in (3.8) is estimated as

$$\left|\frac{1}{6!}E\int_{[0,T]^6}\left[\upsilon^{(6)}(\bar{X}_k+\lambda_1\delta_{k,i};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,1}(s_j)\right.\right.$$
$$\left.\left.-\upsilon^{(6)}(\bar{X}_k+\lambda_0\delta_{k,i};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,0}(s_j)\right]\nu_6(\mathrm{d}s_1\cdots\mathrm{d}s_6)\right|$$
$$\leqslant \frac{1}{6!}\sup|\upsilon^{(6)}|\left|\int_{[0,T]^6}E\left[\prod_{j=1}^{6}|\delta_{k,1}(s_j)|+\prod_{j=1}^{6}|\delta_{k,0}(s_j)|\right]\nu_6(\mathrm{d}s_1\cdots\mathrm{d}s_6)\right|$$
$$\leqslant Kh^3. \tag{3.17}$$

Substituting (3.9) and (3.13)–(3.17) into (3.8), we get

$$|\rho_k| \leqslant \frac{Kh^3}{\sqrt{T-t_k}}, \quad k=0,\ldots,N-1,$$

which together with (3.3) and (3.4) implies (2.12). Hence Theorem 2.2 is proved.

Proof of Lemma 3.1. Assumptions 2.1 ensure that, for a fixed $\tau \in [0,T]$, the functional $U_\tau(x) = \upsilon^{(2)}(x;\tau,\tau)$ is Fréchet differentiable and its derivative has the form

$$U_\tau^{(1)}(x)(\delta) = \int_0^T u^{(1)}(x;s)\delta(s)\mathrm{d}s + u^{(1)}(x;\tau)\delta(\tau) + \sum_{i=1}^{n}u^{(1)}(x;\theta_i)\delta(\theta_i),$$

where $u^{(1)}(x;s)$ is uniformly bounded for $x \in A[0,T]$ and $s \in [0,T]$.

We also note (Milstein & Tretyakov, 2004a, Corollary A.1) that

$$\psi(t_l) := \frac{(b-X(t_l))^2}{(T-t_l)^2} - \frac{1}{T-t_l}, \quad l=0,\ldots,N-1,$$

is a martingale.

Let us introduce the auxiliary processes $\bar{X}_k^{(0)}(t)$, where $k=0,\ldots,N-1$, as follows:

$$\bar{X}_k^{(0)}(t) := \bar{X}_k(t)\chi_{[0,t_k)}(t) + b\chi_{[t_k,T]}(t).$$

Using the Taylor formula for functionals, we get

$$U_{t_k}(\bar{X}_k) = U_{t_k}(\bar{X}_k^{(0)}) + \int_0^T u^{(1)}(\bar{X}_k^{(0)}+\lambda\delta;s)\delta(s)\mathrm{d}s + u^{(1)}(\bar{X}_k^{(0)}+\lambda\delta;t_k)\delta(t_k)$$
$$+\sum_{i=1}^{n}u^{(1)}(\bar{X}_k^{(0)}+\lambda\delta;\theta_i)\delta(\theta_i),$$

where

$$\delta(s) = \bar{X}_k(s) - \bar{X}_k^{(0)}(s)$$
$$= \left[X(t_k) + \sum_{j=k+1}^{N-1} \left(\varDelta_j X + (t_{j+1} - t_j) \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T - s'} \right) \chi_{[t_{j+1/2},T]}(s) - b \right] \chi_{[t_k,T]}(s)$$

and $0 < \lambda < 1$.

We have

$$\left| EU_{t_k}(\bar{X}_k)\psi(t_k) \right| \leqslant \left| EU_{t_k}(\bar{X}_k^{(0)})\psi(t_k) \right| + \Bigg| E\psi(t_k) \int_{t_k}^{T} u^{(1)}(\bar{X}_k^{(0)} + \lambda\delta; s)$$
$$\times \left[X(t_k) + \sum_{j=k+1}^{N-1} \left(\varDelta_j X + (t_{j+1} - t_j) \int_{t_k}^{t_{k+1}} \frac{\mathrm{d}w(s')}{T - s'} \right) \chi_{[t_{j+1/2},T]}(s) - b \right] \mathrm{d}s \Bigg|$$
$$+ \left| E\psi(t_k) u^{(1)}(\bar{X}_k^{(0)} + \lambda\delta; t_k)(X(t_k) - b) \right|$$
$$+ \sum_{i=1}^{n} I_{\theta_i > t_k} \left| E\psi(t_k) u^{(1)}(\bar{X}_k^{(0)} + \lambda\delta; \theta_i)\delta(\theta_i) \right|. \tag{3.18}$$

It is not difficult to see that the second term on the right-hand side of (3.18) is bounded by a constant and the third and fourth terms are bounded by $K/\sqrt{T - t_k}$. Thus, we have

$$\left| EU_{t_k}(\bar{X}_k)\psi(t_k) \right| \leqslant \left| EU_{t_k}(\bar{X}_k^{(0)})\psi(t_k) \right| + \frac{K}{\sqrt{T - t_k}}. \tag{3.19}$$

Now introduce the auxiliary processes $\bar{X}_k^{(j)}(t)$, where $j = 1, \ldots, k$ and $k = 0, \ldots, N-1$, as follows:

$$\bar{X}_k^{(j)}(t) := \bar{X}_k^{(j-1)}(t)\chi_{[0,t_{k-j})}(t) + b\chi_{[t_{k-j},T]}(t).$$

We have

$$U_{t_k}(\bar{X}_k^{(j-1)}) = U_{t_k}(\bar{X}_k^{(j)}) + \int_0^T u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; s)\delta(s)\mathrm{d}s + \sum_{i=1}^{n} u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; \theta_i)\delta(\theta_i),$$

where

$$\delta(s) = \bar{X}_k^{(j-1)}(s) - \bar{X}_k^{(j)}(s) = (X(s) - b)\chi_{[t_{k-j},t_{k-j+1})}(s).$$

Then (as before, $I_k = I_{\{\theta_1,\ldots,\theta_n\}}(t_k)$)

$$U_{t_k}(\bar{X}_k^{(j-1)}) = U_{t_k}(\bar{X}_k^{(j)}) + \int_{t_{k-j}}^{t_{k-j+1}} u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; s)[X(s) - b]\mathrm{d}s$$
$$+ I_{k-j} u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; t_{k-j})[X(t_{k-j}) - b]. \tag{3.20}$$

Recalling that $\psi(t_l)$, where $l = 0, \ldots, N-1$, is a martingale and observing that $U_{t_k}(\bar{X}_k^{(j)})$ is $\mathcal{F}_{t_{k-j}}$-measurable, we get that

$$\left|EU_{t_k}(\bar{X}_k^{(j)})\psi(t_{k-j+1})\right| = \left|EU_{t_k}(\bar{X}_k^{(j)})\psi(t_{k-j})\right|. \tag{3.21}$$

It follows from (3.20) and (3.21) that

$$\begin{aligned}\left|EU_{t_k}(\bar{X}_k^{(j-1)})\psi(t_{k-j+1})\right| \leqslant \left|EU_{t_k}(\bar{X}_k^{(j)})\psi(t_{k-j})\right| \\ + \left|E\psi(t_{k-j+1})\int_{t_{k-j}}^{t_{k-j+1}} u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; s)[X(s) - b]\mathrm{d}s\right| \\ + I_{k-j}\left|E\psi(t_{k-j+1})u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; t_{k-j})[X(t_{k-j}) - b]\right|.\end{aligned} \tag{3.22}$$

The second term on the right-hand side of (3.22) is estimated as

$$\begin{aligned}&\left|E\psi(t_{k-j+1})\int_{t_{k-j}}^{t_{k-j+1}} u^{(1)}(\bar{X}_k^{(j)} + \lambda\delta; s)[X(s) - b]\mathrm{d}s\right| \\ &\leqslant \sup|u^{(1)}|\int_{t_{k-j}}^{t_{k-j+1}} \sqrt{E\psi^2(t_{k-j+1})}\sqrt{E[X(s) - b]^2}\,\mathrm{d}s \\ &\leqslant \frac{K}{T - t_{k-j+1}}\int_{t_{k-j}}^{t_{k-j+1}} \sqrt{T-s}\,\mathrm{d}s \\ &\leqslant \frac{K}{\sqrt{T - t_{k-j+1}}}(t_{k-j+1} - t_{k-j}).\end{aligned}$$

The third term on the right-hand side of (3.22) is estimated as $KI_{k-j}/\sqrt{T - t_{k-j+1}}$. Then

$$\begin{aligned}\left|EU_{t_k}(\bar{X}_k^{(j-1)})\psi(t_{k-j+1})\right| \leqslant \left|EU_{t_k}(\bar{X}_k^{(j)})\psi(t_{k-j})\right| + \frac{K}{\sqrt{T - t_{k-j+1}}}(t_{k-j+1} - t_{k-j}) \\ + \frac{KI_{k-j}}{\sqrt{T - t_{k-j+1}}}, \quad j = 1, \ldots, k.\end{aligned} \tag{3.23}$$

It follows from (3.19), (3.23) and the evident inequality $\left|EU_{t_k}(\bar{X}_k^{(k)})\psi(0)\right| \leqslant K$ that

$$\left|EU_{t_k}(\bar{X}_k)\psi(t_k)\right| \leqslant \frac{K}{\sqrt{T - t_k}} + K\sum_{j=1}^{k}\frac{(t_{k-j+1} - t_{k-j})}{\sqrt{T - t_{k-j+1}}} + K\sum_{j=1}^{k}\frac{I_{k-j}}{\sqrt{T - t_{k-j+1}}}.$$

Recalling that the number of points θ_i is equal to the fixed n, we get $\sum_{j=1}^{k} I_{k-j} \leqslant n$. Finally, we obtain

$$\begin{aligned}\left|EU_{t_k}(\bar{X}_k)\psi(t_k)\right| &\leqslant \frac{K}{\sqrt{T - t_k}} + \frac{K}{\sqrt{T - t_k}}\sum_{j=1}^{k}(t_{k-j+1} - t_{k-j}) + \frac{K}{\sqrt{T - t_k}}\sum_{j=1}^{k} I_{k-j} \\ &\leqslant \frac{K}{\sqrt{T - t_k}}.\end{aligned}$$

Hence Lemma 3.1 is proved. □

REMARK 3.2. It is notable that, in the multidimensional case ($d > 1$), the integrand of (3.10) contains cross-terms in all coordinate pairs i and j, namely, $\delta^i_{k,1}(s_1)\delta^j_{k,1}(s_2) - \delta^i_{k,0}(s_1)\delta^j_{k,0}(s_2)$. The terms corresponding to $i = j$ are estimated in the same way as in the considered one-dimensional case. For $i \neq j$ the contribution from all stochastic integral terms is zero and the right-hand side of (3.10) has terms with $(b^i - X^i(t_k))(b^j - X^j(t_k))/(T - t_k)^2$, which are martingales (Milstein & Tretyakov, 2004a, Corollary A.1), and their further estimation yields $\mathcal{O}(h^3/\sqrt{T - t_k})$ again. In (3.12) it should be understood that the term $1/(T - t_k)$ only appears for $i = j$.

4. Integral-type functionals

In this section we consider conditional Wiener integrals of integral-type functionals as follows:

$$F(x(\cdot)) = \varphi\left(x(\theta), \int_0^T f(t, x(t))\mathrm{d}t\right), \quad 0 < \theta < T, \quad x \in C^d_{0,a;T,b}. \tag{4.1}$$

Let us introduce the scalar process $Z(t)$ satisfying the equation

$$\mathrm{d}Z = f(t, X(t))\mathrm{d}t, \quad Z(0) = 0, \tag{4.2}$$

where $X(t)$ is the solution of (2.3) and (2.4). Clearly, the conditional Wiener integral $\mathcal{J}$ from (1.1) of the functional (4.1) is equal to the expectation, that is,

$$\mathcal{J} = E\varphi(X(\theta), Z(T)). \tag{4.3}$$

The approximation (2.11) and (2.10) applied to (1.1) and (4.1) results in the following trapezoidal method for Z:

$$\mathcal{J} \approx \bar{\mathcal{J}} = E\varphi(X(\theta), Z_N), \tag{4.4}$$

where

$$\begin{aligned} &Z_0 = 0, \\ &Z_{k+1} = Z_k + \frac{t_{k+1} - t_k}{2}[f(t_k, X(t_k)) + f(t_{k+1}, X(t_{k+1}))], \quad k = 0, \ldots, N-1. \end{aligned} \tag{4.5}$$

Recall that the time discretization used here is so that $\theta \in \{t_0, t_1, \ldots, t_N\}$.

If we assume that $\varphi(x, z)$ and $f(t, x)$ have bounded derivatives up to a sufficiently high order, then it follows from the general Theorem 2.2 that the method (4.4) and (4.5) for (1.1) and (4.1) has the second order of accuracy, i.e., the estimate (2.12) is valid for it. The other assumptions under which Theorem 2.2 is valid are that $f(t, x)$ and its derivatives up to a sufficiently high order are bounded and $\varphi(x, z)$ is sufficiently smooth. We note that, in the case of integral-type functionals, the convergence theorem can be proved more simply, exploiting a more standard technique used in the weak-sense approximation of SDEs (Milstein & Tretyakov, 2004b) (see its application in the case of conditional Wiener integrals of exponential-type functionals in Milstein & Tretyakov (2004a) and in the case of usual Wiener integrals in Ventzel *et al.* (1984)). It is interesting that no method of the form

$$Z_{k+1} = Z_k + (t_{k+1} - t_k)\sum_{i=1}^{3} \alpha_i f(t_k + \beta_i, X(t_k + \beta_i)), \quad \alpha_i \in \mathbf{R}, \quad \beta_i \in [0, t_{k+1} - t_k],$$

has order of accuracy higher than two (in the case of usual Wiener integrals, see a similar comment in Ventzel *et al.*, 1984). At the same time, in the case of integral-type functionals of a particular form, namely, the exponential-type functionals $F(x(\cdot)) = \exp\left[\int_0^T f(t, x(t))\mathrm{d}t\right]$, a fourth-order Runge–Kutta method was constructed in Milstein & Tretyakov (2004a).

We made a computational comparison between (4.5) and the fourth-order Runge–Kutta method in computing the ground state energy of one particle in a one-dimensional harmonic oscillator. Despite being of lower order, the method (4.5) turns out to be preferable due to its stability properties. These follow from preservation by (4.5) of such structural properties of exponential-type functionals as positivity and monotonicity, which can be broken down in the case of the fourth-order Runge–Kutta method from Milstein & Tretyakov (2004a) (see similar observations, although in a different context, in Milstein and Tretyakov, 2009). Furthermore, instead of the trapezoidal rule (4.5), we can use the Simpson rule to give:

$$\begin{aligned} Z_0 &= 0, \\ Z_{k+1} &= Z_k + \frac{t_{k+1} - t_k}{6}[f(t_k, X(t_k)) + 4f(t_{k+1/2}, X(t_{k+1/2})) + f(t_{k+1}, X(t_{k+1}))], \\ k &= 0, \ldots, N-1. \end{aligned} \tag{4.6}$$

Although both methods (4.5) and (4.6) are of order two, the method (4.6) has a much smaller bias in our experiments than the method (4.5) and thus is computationally more effective. The method (4.4) and (4.5) and the method (4.4) and (4.6) extend the arsenal of numerical tools considered in Milstein & Tretyakov (2004a,b) for computing exponential-type functionals (1.2).

5. Extension to the case of pinned diffusions

In this section we extend the Euler method (2.14) and (2.13) to the case of paths of R^d-diffusions

$$\mathrm{d}\mathbb{X} = \alpha(t, \mathbb{X})\mathrm{d}t + \mathrm{d}w(t), \quad \mathbb{X}(t_0) = a, \tag{5.1}$$

that are conditioned to pass through a point $b \in R^d$ at time T, where $t_0 \leqslant t \leqslant T$. Conditioned diffusions are used, for example, in parameter estimation problems (see, e.g., Delyon & Hu, 2006). We note that the Brownian bridge case considered in the previous sections 2–4 corresponds to (5.1) with $\alpha = 0$.

Analogously to Section 4, we will be interested here in simulating the expectations of integral-type functionals

$$F(x(\cdot)) = \varphi\left(\int_{t_0}^T f(t, x(t))\mathrm{d}t\right), \quad x \in C^d_{t_0,a;T,b}, \tag{5.2}$$

but now with respect to the measure on paths corresponding to the conditioned diffusion (5.1). It is clear that this expectation is equal to

$$\mathcal{J} = E\varphi(\mathbb{Z}(T)), \tag{5.3}$$

where the scalar process $\mathbb{Z}(t)$ satisfies the equation

$$\mathrm{d}\mathbb{Z} = f(t, \mathbb{X}(t))\mathrm{d}t, \quad \mathbb{Z}(t_0) = 0, \tag{5.4}$$

and $\mathbb{X}(t)$ is the solution of (5.1). In what follows we assume that the functions $\alpha(t, x)$ and $f(t, x)$ are bounded and have bounded derivatives up to a sufficiently high order and that $\varphi(z)$ is sufficiently smooth.

The expectation (5.3) can be rewritten as (Clark, 1990; Delyon & Hu, 2006)

$$\mathcal{J} = \frac{E\varphi(Z(T))Y(T)}{EY(T)}, \tag{5.5}$$

where $Z_{t_0,a,z}(t)$ and $Y_{t_0,a,y}(t)$, with $t \geqslant t_0$, satisfy the equations

$$\mathrm{d}Z = f(t, X(t))\mathrm{d}t, \quad Z(t_0) = 0, \tag{5.6}$$

$$\mathrm{d}Y = \alpha^{\mathrm{T}}(t, X)\frac{b - X}{T - t}Y\mathrm{d}t + \alpha^{\mathrm{T}}(t, X)Y\mathrm{d}w(t), \quad Y(t_0) = 1, \tag{5.7}$$

with $X(t) = X_{t_0,a}(t)$ being the Brownian bridge from a at the time $t = t_0$ to b at the time $t = T$ (cf. (2.3) and (2.4)), that is,

$$\mathrm{d}X = \frac{b - X}{T - t}\mathrm{d}t + \mathrm{d}w(t), \quad X(t_0) = a. \tag{5.8}$$

We note that

$$Y(T) = \exp(Q(T)), \tag{5.9}$$

where

$$\mathrm{d}Q = \left[\alpha^{\mathrm{T}}(t, X)\frac{b - X}{T - t} - \frac{1}{2}\alpha^2(t, X)\right]\mathrm{d}t + \alpha^{\mathrm{T}}(t, X)\mathrm{d}w(t), \quad Q(t_0) = 0. \tag{5.10}$$

We remark that, for $\alpha = 0$ (the Brownian bridge case), $\mathcal{J}$ from (5.5) coincides with $\mathcal{J}$ from (4.3).

We introduce a discretization of the time interval $[t_0, T]$ given by $t_0 < t_1 < \cdots < t_N = T$, which, for simplicity is equidistant with the time step $h = t_{k+1} - t_k$. To construct the numerical method we simulate the Brownian bridge $X(t)$ at the nodes t_k exactly (see (2.9)), that is,

$$X_{k+1} = X_k + h\frac{b - X_k}{T - t_k} + \sqrt{h}\sqrt{\frac{T - t_{k+1}}{T - t_k}}\xi_{k+1}, \quad X_0 = a, \tag{5.11}$$

and we approximate (5.6) and (5.10) as follows:

$$Z_{k+1} = Z_k + hf(t_k, X_k), \quad Z_0 = 0 \tag{5.12}$$

and

$$\begin{aligned} Q_{k+1} &= Q_k + h\left[\alpha^{\mathrm{T}}(t_k, X_k)\frac{b - X_k}{T - t_k} - \frac{\alpha^2(t_k, X_k)}{2}\right] + \sqrt{h}\sqrt{\frac{T - t_{k+1}}{T - t_k}}\alpha^{\mathrm{T}}(t_k, X_k)\xi_{k+1}, \\ Q_0 &= 0, \end{aligned} \tag{5.13}$$

where ξ_{k+1}, for $k = 0, \ldots, N - 1$, are d-dimensional random vectors whose components are mutually independent random variables with standard normal distribution $\mathcal{N}(0, 1)$.

We remark that we choose to approximate (5.9) and (5.10) rather than (5.7) since it has been observed (see, e.g., Milstein and Tretyakov, 2009, and also Section 4 here) that positivity preservation automatically guaranteed by (5.13) has computational advantages, while an explicit scheme applied directly to (5.13) does not possess this property. We also emphasize that $X(t_k) = X_k$, i.e., there is no numerical error introduced in (5.11).

Now we define the approximation of the path integral $\mathcal{J}$ from (5.3) as follows:

$$\mathcal{J} = E\varphi(\mathbb{Z}(T)) = \frac{E\varphi(Z(T))Y(T)}{EY(T)} \approx \bar{\mathcal{J}} = \frac{E\varphi(Z_N)\exp(Q_N)}{E\exp(Q_N)}. \tag{5.14}$$

Let us introduce the function

$$u(t,x,z)y = E[\varphi(Z_{t,x,z}(T))Y_{t,x,y}(T)] \tag{5.15}$$

and let

$$Y_k = \exp(Q_k). \tag{5.16}$$

Under the assumptions we imposed on the coefficients at the beginning of this section, the function $u(t,x,z)$ is smooth in x and z, and sufficiently high moments of $u(t_0, X_{t_0,a}(t), Z_{t_0,a,0}(t))Y_{t_0,a,1}(t)$ and $u(t_k, X_k, Z_k)Y_k$ and their derivatives with respect to x and z are bounded (Gikhman & Skorokhod, 1972). The method itself is applicable more widely and the assumptions can be relaxed in the spirit of the comment after Assumptions 2.1.

THEOREM 5.1. The method (5.11)–(5.13) is of first order of accuracy, i.e.,

$$|E\varphi(Z(T))Y(T) - E\varphi(Z_N)\exp(Q_N)| \leqslant Kh, \tag{5.17}$$

where the constant K is independent of h.

This theorem has the following evident corollary.

COROLLARY 5.2. The method (5.14) and (5.11)–(5.13) for evaluating the path integral (5.3) is of first order of accuracy, i.e.,

$$|\mathcal{J} - \bar{\mathcal{J}}| \leqslant Kh, \tag{5.18}$$

where the constant K is independent of h.

REMARK 5.3. We note that, if in (5.14) we substitute Q_N simulated by the standard Euler scheme for (5.10), that is,

$$Q_{k+1} = Q_k + h\left[\alpha^{\mathrm{T}}(t_k, X_k)\frac{b - X_k}{T - t_k} - \frac{\alpha^2(t_k, X_k)}{2}\right] + \sqrt{h}\alpha^{\mathrm{T}}(t_k, X_k)\xi_{k+1}, \tag{5.19}$$
$$Q_0 = 0,$$

then the method (5.14), (5.11), (5.12) and (5.19) is of order $h \ln h$ instead of $\mathcal{O}(h)$ for (5.14) and (5.11)–(5.13) (also see footnote 1 at the end of this section).

Proof of Theorem 5.1. Using the standard technique (see Milstein & Tretyakov, 2004b, p. 100), we can write the global error in the form

$$R := \left|E\left[\varphi\left(Z_{t_0,a,0}(T)\right)Y_{t_0,a,1}(T)\right] - E[\varphi(Z_N)Y_N]\right|$$
$$= \left|\sum_{k=0}^{N-1}\left(Eu\left(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1})\right)Y_{t_k,X_k,Y_k}(t_{k+1}) - Eu(t_{k+1}, X_{k+1}, Z_{k+1})Y_{k+1}\right)\right|$$

$$= \left| \sum_{k=0}^{N-1} EY_k \left[u\left(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1})\right) Y_{t_k,X_k,1}(t_{k+1}) - u(t_{k+1}, X_{k+1}, Z_{k+1}) Y_{t_k,X_k,1}(t_{k+1}) \right] \right|$$

$$\leqslant \sum_{k=0}^{N-1} R_k, \tag{5.20}$$

where

$$R_k = \left| EY_k \left[u\left(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1})\right) Y_{t_k,X_k,1}(t_{k+1}) - u(t_{k+1}, X_{k+1}, Z_{k+1}) Y_{t_k,X_k,1}(t_{k+1}) \right] \right|$$
$$= \left| EY_k E \left[u\left(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1})\right) Y_{t_k,X_k,1}(t_{k+1}) \right.\right.$$
$$\left.\left. - u(t_{k+1}, X_{k+1}, Z_{k+1}) Y_{t_k,X_k,1}(t_{k+1}) | \mathcal{F}_{t_k} \right] \right|. \tag{5.21}$$

Above we have exploited the fact that we simulate X_{k+1} exactly.

We first analyse the errors R_k for $k = 0, \ldots, N-2$ and introduce the function

$$v(x, z) := u(t+h, x, z),$$

the operators

$$L = L_1 + L_2 + L_3,$$

$$L_1 = \frac{\partial}{\partial t} + \frac{b-x}{T-t}\nabla + \frac{1}{2}\sum_{i=1}^{d} \frac{\partial^2}{(\partial x^i)^2}, \quad L_2 = f(t,x)\frac{\partial}{\partial z},$$

$$L_3 = \alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t} y \frac{\partial}{\partial y} + \sum_{i=1}^{d} \alpha^i(t,x) y \frac{\partial^2}{\partial x^i \partial y} + \frac{1}{2}\alpha^2(t,x) y^2 \frac{\partial^2}{\partial y^2}, \quad 0 \leqslant t < T,$$

and the one-step error for $t \leqslant T - 2h$ given by

$$r(t,x,z) := Ev(X_{t,x}(t+h), Z_{t,x,z}(t+h)) Y_{t,x,1}(t+h)$$
$$- Ev(X_{t,x}(t+h), \bar{Z}_{t,x,z}(t+h)) \bar{Y}_{t,x,1}(t+h), \tag{5.22}$$

where $\bar{Z}_{t,x,z}(t+h)$ and $\bar{Y}_{t,x,1}(t+h)$ are the one-step approximations of $Z_{t,x,z}(t+h)$ and $Y_{t,x,1}(t+h)$, respectively, that correspond to the method (5.11)–(5.13) and (5.16).

The second term in (5.22) can be rewritten as

$$r_2 := Ev(X_{t,x}(t+h), \bar{Z}_{t,x,z}(t+h)) \bar{Y}_{t,x,1}(t+h)$$
$$= Ev(X_{t,x}(t+h), z) \bar{Y}_{t,x,1}(t+h)$$
$$+ hf(t,x) E \frac{\partial}{\partial z} v(X_{t,x}(t+h), z) \bar{Y}_{t,x,1}(t+h) + \rho_1(t,x,z),$$

where $\rho_1(t,x,z)$ is such that $E|\rho_1(t_k, X_k, Z_k)| \leqslant Kh^2$ with a constant K that is independent of h and t.

Furthermore, expanding the nonsingular part of $\bar{Y}_{t,x,1}(t+h)$, that is,

$$\exp\left(-\frac{h}{2}\frac{T-t-h}{T-t}\alpha^2(t,x) + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\alpha^{\mathrm{T}}(t,x)\xi \right)$$

and

$$v(X_{t,x}(t+h),z) = v\left(x + h\frac{b-x}{T-t} + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\xi, z\right),$$

and also $\frac{\partial}{\partial z}v(X_{t,x}(t+h),z)$ in powers of h, we obtain

$$\begin{aligned} r_2(t,x,z) = \exp&\left(h\alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t} - \frac{\alpha^2(t,x)}{2}\frac{h^2}{T-t}\right) \\ &\times E\left\{\left[1 - \frac{h}{2}\frac{T-t-h}{T-t}\alpha^2(t,x) + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\alpha^{\mathrm{T}}(t,x)\xi\right.\right. \\ &\qquad\left. + \frac{h}{2}\frac{T-t-h}{T-t}[\alpha^{\mathrm{T}}(t,x)\xi]^2 + \frac{h^{3/2}}{6}\left[\sqrt{\frac{T-t-h}{T-t}}\alpha^{\mathrm{T}}(t,x)\xi\right]^3\right] \\ &\times\left[v(x,z) + h\frac{(b-x)^{\mathrm{T}}}{T-t}\nabla v(x,z) + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\xi^{\mathrm{T}}\nabla v(x,z)\right. \\ &\quad + h^{3/2}\sqrt{\frac{T-t-h}{T-t}}\sum_{i,j=1}^{d}\frac{b^i-x^i}{T-t}\xi^j\frac{\partial^2 v}{\partial x^i\partial x^j}(x,z) \\ &\quad + \frac{1}{2}\sum_{i,j=1}^{d}\left[h^2\frac{(b^i-x^i)(b^j-x^j)}{(T-t)^2} + h\frac{T-t-h}{T-t}\xi^i\xi^j\right]\frac{\partial^2 v}{\partial x^i\partial x^j}(x,z) \\ &\quad\left.\left. + hf(t,x)\left[\frac{\partial}{\partial z}v(x,z) + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\xi^{\mathrm{T}}\nabla\frac{\partial}{\partial z}v(x,z)\right]\right]\right\} + h^2\rho_2(t,x,z), \end{aligned} \tag{5.23}$$

where the remainder $\rho_2(t,x,z)$ is such that, due to the inequality (3.7) and that $1/(T-t-h) \leqslant 1/h$ for $t \leqslant T-2h$, we can estimate it as

$$|E\rho_2(t_k,X_k,Z_k)| \leqslant \frac{K}{\sqrt{T-t_{k+1}}}. \tag{5.24}$$

After taking the expectation in (5.23), we get the following simplified expression:

$$\begin{aligned} r_2(t,x,z) = \exp&\left(h\alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t} - \frac{\alpha^2(t,x)}{2}\frac{h^2}{T-t}\right)\times\left\{v(x,z) + h(L_1+L_2)v(x,z)\right. \\ &+ h\alpha^{\mathrm{T}}(t,x)\nabla v(x,z) + \frac{h^2}{2}\sum_{i,j=1}^{d}\frac{(b^i-x^i)(b^j-x^j)}{(T-t)^2}\frac{\partial^2 v}{\partial x^i\partial x^j}(x,z) \\ &\left. - \frac{h^2}{2}\frac{1}{T-t}\sum_{i=1}^{d}\frac{\partial^2 v}{(\partial x^i)^2}(x,z) - \frac{h^2}{T-t}\alpha^{\mathrm{T}}(t,x)\nabla v(x,z)\right\} + h^2\rho_3(t,x,z), \end{aligned}$$

where ρ_3 satisfies an inequality of the form (5.24). Furthermore, expanding the exponent in powers of h, we have

$$
\begin{aligned}
r_2(t,x,z) = {} & v(x,z) + h(L_1+L_2)v(x,z) + h\alpha^{\mathrm{T}}(t,x)\left[\frac{b-x}{T-t}v(x,z) + \nabla v(x,z)\right] \\
& + \frac{h^2}{2}\left(\left[\alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t}\right]^2 - \frac{\alpha^2(t,x)}{T-t}\right)v(x,z) \\
& + h^2\left(\alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t}\right)\left(\frac{b-x}{T-t}\nabla v(x,z)\right) - \frac{h^2}{T-t}\alpha^{\mathrm{T}}(t,x)\nabla v(x,z) \\
& + \frac{h^2}{2}\sum_{i,j=1}^{d}\frac{(b^i-x^i)(b^j-x^j)}{(T-t)^2}\frac{\partial^2 v}{\partial x^i \partial x^j}(x,z) - \frac{h^2}{2}\frac{1}{T-t}\sum_{i=1}^{d}\frac{\partial^2 v}{(\partial x^i)^2}(x,z) \\
& + h^2\rho_4(t,x,z),
\end{aligned}
$$

where ρ_4 satisfies an inequality of the form (5.24).

Now consider the first term in (5.22). Using the Taylor expansion of the expectations of SDE solutions (Milstein & Tretyakov, 2004b, Lemma 2.1.9, p. 99), we obtain

$$
\begin{aligned}
r_1(t,x,z) := {} & Ev(X_{t,x}(t+h), Z_{t,x,z}(t+h))Y_{t,x,1}(t+h) \\
= {} & v(x,z) + h(L_1+L_2)v(x,z) + h\alpha^{\mathrm{T}}(t,x)\frac{b-x}{T-t}v(x,z) + h\alpha^{\mathrm{T}}(t,x)\nabla v(x,z) \\
& + \frac{h^2}{2}L^2[v(x,z)y]_{y=1} + \int_t^{t+h}\frac{(t+h-s)^2}{2}EL^3[v(X_{t,x}(s), Z_{t,x,z}(s))Y_{t,x,1}(s)]\mathrm{d}s. \quad (5.25)
\end{aligned}
$$

Denote the last term in (5.25) as $h^2\rho_5(t,x,z)$. Using the inequality (3.7) and that $1/(T-t-h) \leqslant 1/h$ for $t \leqslant T-2h$, one can show that ρ_5 satisfies an inequality of the form (5.24). Furthermore, we have

$$
\begin{aligned}
L^2[v(x,z)y]_{y=1} = {} & 2\left(\alpha^{\mathrm{T}}\frac{b-x}{T-t}\right)\left(\frac{b-x}{T-t}\nabla v\right) - \frac{2\alpha^{\mathrm{T}}}{T-t}\nabla v + \left(\alpha^{\mathrm{T}}\frac{b-x}{T-t}\right)^2 v - \frac{\alpha^2}{T-t}v \\
& + \sum_{i,j=1}^{d}\frac{(b^i-x^i)(b^j-x^j)}{(T-t)^2}\frac{\partial^2 v}{\partial x^i \partial x^j} - \frac{1}{T-t}\sum_{i=1}^{d}\frac{\partial^2 v}{(\partial x^i)^2} \\
& + \sum_{i=1}^{d}\left[\frac{(b^i-x^i)^2}{(T-t)^2} - \frac{1}{T-t}\right]\frac{\partial \alpha^i}{\partial x^i}v + \sum_{i\neq j}\frac{(b^i-x^i)(b^j-x^j)}{(T-t)^2}\frac{\partial \alpha^i}{\partial x^j}v \\
& + \rho_6(t,x,z),
\end{aligned}
$$

where ρ_6 satisfies an inequality of the form (5.24).

Hence

$$r(t,x,z) = r_1(t,x,z) - r_2(t,x,z)$$
$$= \frac{h^2}{2}\sum_{i=1}^{d}\left[\frac{(b^i - x^i)^2}{(T-t)^2} - \frac{1}{T-t}\right]\frac{\partial\alpha^i}{\partial x^i}(t,x)v(x,z)$$
$$+ \frac{h^2}{2}\sum_{i\neq j}\frac{(b^i - x^i)(b^j - x^j)}{(T-t)^2}\frac{\partial\alpha^i}{\partial x^j}(t,x)v(x,z) + h^2\rho_7(t,x,z), \tag{5.26}$$

where ρ_7 satisfies an inequality of the form (5.24).

We recall (Milstein & Tretyakov, 2004a, Corollary A.1) that

$$\psi^i(t_k) := \frac{(b^i - X^i(t_k))^2}{(T-t_k)^2} - \frac{1}{T-t_k} \quad \text{and} \quad \psi^{i,j}(t_k) := \frac{(b^i - X^i(t_k))(b^j - X^j(t_k))}{(T-t_k)^2}, \quad i \neq j,$$
$$k = 0, \ldots, N-1,$$

are martingales.

It follows from (5.21) and (5.26) that, for $k = 0, \ldots, N-2$, we have[1]

$$R_k \leqslant h^2\left|EY_k\left[\sum_{i=1}^{d}\psi^i(t_k)g^i(t_k, X_k, Z_k) + \sum_{i\neq j}\psi^{i,j}(t_k)g^{i,j}(t_k, X_k, Z_k)\right]\right| + \frac{Kh^2}{\sqrt{T-t_{k+1}}},$$

where g^i and $g^{i,j}$ are the corresponding functions appearing in (5.26). Using arguments similar to those in Milstein & Tretyakov (2004a, Lemma B.1), one can show that, for $k = 0, \ldots, N-2$, we have

$$\left|EY_k\left[\sum_{i=1}^{d}\psi^i(t_k)g^i(t_k, X_k, Z_k) + \sum_{i\neq j}\psi^{i,j}(t_k)g^{i,j}(t_k, X_k, Z_k)\right]\right| \leqslant \frac{Kh^2}{\sqrt{T-t_{k+1}}}.$$

Finally, we note that it is not difficult to obtain that

$$R_{N-1} \leqslant Kh.$$

Thus $R \leqslant Kh + Kh\sum_{k=0}^{N-2} h/\sqrt{T-t_{k+1}} \leqslant Kh$, as required. □

The Monte Carlo estimator for the path integral (5.3) based on the method (5.14) and (5.11)–(5.13) has the form

$$\mathcal{J} \approx \bar{\mathcal{J}} = \frac{E\varphi(Z_N)\exp(Q_N)}{E\exp(Q_N)} \approx \widehat{\mathcal{J}} = \frac{\sum_{m=1}^{M}\varphi({}_mZ_N)\exp({}_mQ_N)}{\sum_{m=1}^{M}\exp({}_mQ_N)}, \tag{5.27}$$

where ${}_mZ_N$ and ${}_mQ_N$, for $m = 1, \ldots, M$, are independent realizations of the corresponding random variables. Note that the second approximate equality in (5.27) is related to the statistical error.

[1] If one were to use (5.19) instead of (5.13), then $R_k \leqslant Kh^2/(T - t_{k+1})$ (cf. Remark 5.3).

TABLE 1 *Square integral of the Brownian bridge. Errors in evaluating the conditional Wiener integral* (1.1) *and* (6.1) *with* $p = 1$ *and* $p = 4$ *and for various time steps* h. *Here* M *is the number of Monte Carlo runs*

h	M	$p = 1$	$p = 4$
0.20	1×10^9	$6.66 \times 10^{-3} \pm 0.01 \times 10^{-3}$	$-1.3 \times 10^{-3} \pm 0.012 \times 10^{-3}$
0.10	1×10^9	$1.67 \times 10^{-3} \pm 0.009 \times 10^{-3}$	$-0.32 \times 10^{-3} \pm 0.011 \times 10^{-3}$
0.05	5×10^{10}	$0.417 \times 10^{-3} \pm 0.001 \times 10^{-3}$	$-0.080 \times 10^{-3} \pm 0.002 \times 10^{-3}$
0.02	5×10^{10}	$0.067 \times 10^{-3} \pm 0.001 \times 10^{-3}$	$-0.015 \times 10^{-3} \pm 0.002 \times 10^{-3}$

REMARK 5.4. It is possible to consider further generalizations. One may look at the possibility of higher-order methods for pinned diffusions (5.1) as we did in the previous sections 2 and 4 in the case of a Brownian bridge. Furthermore, the method (5.11)–(5.13) and Theorem 5.1 are not difficult to adapt to a slightly more general additive noise situation than (5.1), in that we could consider conditioned diffusions with any constant diffusion matrix, rather than particularly a unit diffusion matrix. At the same time, we note that the case of pinned diffusions with multiplicative noise (i.e., when the diffusion coefficients are state dependent) requires further development, and, in connection with this topic, we also refer to the related works Milstein *et al.* (2004), Hairer *et al.* (2009) and the references therein.

6. Numerical examples

EXAMPLE 6.1. We consider the square integral of the Brownian bridge that has applications in statistics. To test the proposed method we compute moments of this integral, i.e., we deal with the functionals

$$F(x(\cdot)) = \left(\int_0^1 x^2(t)\mathrm{d}t\right)^p, \quad p \geqslant 0, \quad x \in C_{0,0;1,0}. \tag{6.1}$$

The results of our simulation are presented in Table 1. The values before '$\pm$' are the differences between the exact value of the Wiener integral $\mathcal{J}$ (see (1.1)) with $F(x(\cdot))$ from (6.1) and its sampled approximations. The reference values for $\mathcal{J}$ are $1/6$ for $p = 1$ and 0.0166799 for $p = 4$ (Tolmatz, 2002). The values after '$\pm$' reflect the Monte Carlo error only. They correspond to the confidence interval for the corresponding estimator with probability 0.95. One can observe convergence with order two that is in good agreement with our theoretical results.

EXAMPLE 6.2. Consider the following correlation function $\Gamma(\theta)$, where $0 \leqslant \theta \leqslant T$ (see (1.3)):

$$\begin{aligned}\Gamma(\theta) &= \langle x(0)x(\theta)\rangle \\ &= \frac{1}{\mathcal{Z}(T)}\int_{-\infty}^{\infty}\int_{C_{0,y;T,y}} x(0)x(\theta)\exp\left(-\int_0^T V(t,x(t))\mathrm{d}t\right)\mathrm{d}\mu_{0,y}^{T,y}(x)\mathrm{d}y = \frac{\int_{-\infty}^{\infty} y\mathcal{J}_1(y)\mathrm{d}y}{\int_{-\infty}^{\infty}\mathcal{J}_2(y)\mathrm{d}y},\end{aligned} \tag{6.2}$$

where

$$\mathcal{J}_1(y) = \int_{C_{0,y;T,y}} x(\theta) \exp\left(-\int_0^T V(t, x(t))\mathrm{d}t\right) \mathrm{d}\mu_{0,y}^{T,y}(x), \tag{6.3}$$

$$\mathcal{J}_2(y) = \int_{C_{0,y;T,y}} \exp\left[-\int_0^T V(x(t))\mathrm{d}t\right] \mathrm{d}\mu_{0,y}^{T,y}(x). \tag{6.4}$$

We evaluate (6.2)–(6.4) for the harmonic potential

$$V(x) = \frac{\omega^2}{2}x^2 \tag{6.5}$$

and for the anharmonic potential

$$V(x) = \frac{\omega^2}{2}x^4. \tag{6.6}$$

We recall (see, e.g., Kleinert, 1995; Lobanov, 1996) that T has the meaning of inverse temperature here. In the case of the harmonic potential (6.5) the correlation function is equal to (Kleinert, 1995, Chapter 3)

$$\Gamma(\theta) = \frac{1}{2\omega}\frac{\cosh \omega(\theta - T/2)}{\sinh(\omega T/2)}, \quad 0 \leqslant \theta \leqslant T. \tag{6.7}$$

We rewrite the integrals in (6.2) as

$$\mathcal{G} = \int_{-\infty}^{\infty} y\mathcal{J}_1(y)\mathrm{d}y = \sqrt{2\pi\sigma_1^2}E\left[\eta_1\mathcal{J}_1(\eta_1)\exp\left(\frac{\eta_1}{2\sigma_1^2}\right)\right],$$

$$\mathcal{Z} = \int_{-\infty}^{\infty} \mathcal{J}_2(y)\mathrm{d}y = \sqrt{2\pi\sigma_2^2}E\left[\mathcal{J}_2(\eta_2)\exp\left(\frac{\eta_2}{2\sigma_2^2}\right)\right], \tag{6.8}$$

where η_1 and η_2 are Gaussian random variables, that is, $\mathcal{N}(0, \sigma_1^2)$ and $\mathcal{N}(0, \sigma_2^2)$, with zero mean and variances σ_1^2 and σ_2^2, respectively. The parameters σ_1^2 and σ_2^2 are chosen so that the variances of the random variables under the expectations in (6.8) are small.

The following estimators for $\mathcal{G}$ and $\mathcal{Z}$ are used in our simulation:

$$\widehat{\mathcal{G}} = \frac{\sqrt{2\pi\sigma_1^2}}{M}\sum_{m=1}^{M}\left[{}_m\eta_1{}_m\bar{\mathcal{J}}_1(\eta_1)\exp\left(\frac{{}_m\eta_1}{2\sigma_1^2}\right)\right],$$

$$\widehat{\mathcal{Z}} = \frac{\sqrt{2\pi\sigma_2^2}}{M}\sum_{m=1}^{M}\left[{}_m\bar{\mathcal{J}}_2({}_m\eta_2)\exp\left(\frac{{}_m\eta_2}{2\sigma_2^2}\right)\right], \tag{6.9}$$

where ${}_m\eta_1$ and ${}_m\eta_2$ are sampled from $\mathcal{N}(0, \sigma_1^2)$ and $\mathcal{N}(0, \sigma_2^2)$, respectively, so that the pairs $({}_m\eta_1, {}_m\eta_2)$ are independent, while ${}_m\eta_1$ and ${}_m\eta_2$ in the same pair are dependent, that is, ${}_m\eta_2 = \sigma_{2m}\eta_1/\sigma_1$. Here

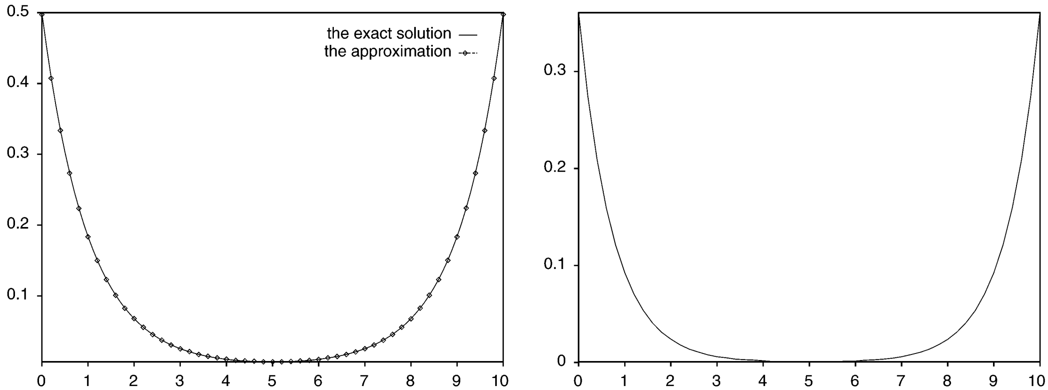

FIG. 1. The dependence of the correlation function $\Gamma(\theta)$ from (6.2) on θ simulated with $h = 0.2$ and $M = 10^8$ for $T = 10$. Part (a) corresponds to the harmonic potential (6.5) and part (b) to the anharmonic potential (6.6), both with $\omega = 1$.

TABLE 2 *Correlation function. The error in evaluating the correlation function $\Gamma(\theta)$ from (6.2) in the case of the harmonic potential (6.5) with $\omega = 1$, $T = 10$ and $\theta = 1$*

h	M	Error
0.250	10^9	$9.78 \times 10^{-4} \pm 0.72 \times 10^{-4}$
0.200	10^9	$6.18 \times 10^{-4} \pm 0.72 \times 10^{-4}$
0.125	10^{10}	$2.45 \times 10^{-4} \pm 0.23 \times 10^{-4}$
0.100	5×10^{10}	$1.46 \times 10^{-4} \pm 0.10 \times 10^{-4}$

${}_m\bar{\mathcal{J}}_1({}_m\eta_1)$ and ${}_m\bar{\mathcal{J}}_2({}_m\eta_2)$ are values of the corresponding functionals evaluated along a path according to the method (2.10). The pairs $({}_m\bar{\mathcal{J}}_1({}_m\eta_1), {}_m\bar{\mathcal{J}}_2({}_m\eta_2))$ are simulated along independent paths, while ${}_m\bar{\mathcal{J}}_1({}_m\eta_1)$ and ${}_m\bar{\mathcal{J}}_2({}_m\eta_2)$ in the same pair are evaluated along the same path. Recall (see Section 2.2) that a discretization of the time interval $[0, T]$ should be so that the point θ belongs to the set of discretization points $\{t_0, t_1, \ldots, t_N\}$.

The results of the experiment are presented in Tables 2 and 3 and in Fig. 1. The parameters σ_1 and σ_2 are taken as 1.2 and 0.8, respectively. As before, in these tables the values before '$\pm$' are estimates of the bias, computed as the difference between the exact $\Gamma(\theta)$ and its sampled approximations, while the values after '$\pm$' give half of the size of the confidence interval for the corresponding estimator with probability 0.95. To compute the bias the exact values $\Gamma(1) \doteq 0.1840098$ and $\Gamma(8) \doteq 0.0678385$ obtained from (6.7) are used. The number of Monte Carlo runs M is chosen here so that the Monte Carlo error is small in comparison with the bias. It is not difficult to see that the experiment illustrates second-order convergence of the method. We note that fitting Ch^2 to, for example, the data of Table 2 yields $C \doteq 0.015$, with the maximum absolute value of the residuals being equal to 3×10^{-5}.

In Fig. 1(a) the results of the simulation of $\Gamma(\theta)$ with $h = 0.2$ are compared with the exact curve from (6.7). Due to the second order of accuracy of the proposed numerical method, these curves visually coincide even for this relatively large time step. Figure 1(b) demonstrates the behaviour of the correlation

TABLE 3 *Correlation function. The error in evaluating the correlation function $\Gamma(\theta)$ from (6.2) in the case of the harmonic potential (6.5) with $\omega = 1$, $T = 10$, $\theta = 8$ and when the number of Monte Carlo runs is $M = 10^{11}$*

h	Error
0.250	$1.688 \times 10^{-4} \pm 0.079 \times 10^{-4}$
0.200	$1.134 \times 10^{-4} \pm 0.079 \times 10^{-4}$
0.125	$0.331 \times 10^{-4} \pm 0.080 \times 10^{-4}$
0.100	$0.231 \times 10^{-4} \pm 0.080 \times 10^{-4}$

function in the case of the anharmonic potential (6.6). The presented curve is obtained with the time step $h = 0.2$ and it visually coincides with the one simulated with $h = 0.05$. These experiments give further confirmation of our theoretical results.

We note that, in Examples 6.1 and 6.2, the second-order method (2.11) and (2.10) and the Euler method (2.14) and (2.13) coincide since in these examples the starting and ending points of Brownian bridge paths coincide. In the next example we deal with a system of bosons and the advantage of the method (2.11) and (2.10) in comparison with the Euler method (which is, in general, of order one—see Theorem 2.4) is clearly seen.

EXAMPLE 6.3. Consider a system of r identical n-dimensional boson particles of mass m. The partition function for this system has the form (Feynman, 1972)

$$\mathcal{Z} = \int_{\mathbf{R}^{rn}} \sum_{\boldsymbol{\pi} \in \Pi_r} (2\pi T/m)^{-rn/2} \exp\left(-\frac{|x - \boldsymbol{\pi} x|^2}{2T/m}\right) u_T(x, \boldsymbol{\pi} x)\mathrm{d}x, \tag{6.10}$$

where T is the inverse temperature, $\boldsymbol{\pi} x$ means a permutation of the r-tuple $x = (x_1, \ldots, x_r)$, Π_r is the set of all such permutations and

$$u_T(x, \boldsymbol{\pi} x) = E \exp\left(-\int_0^T V(X_{0,x}^{T,\boldsymbol{\pi} x}(t))\mathrm{d}t\right) \tag{6.11}$$

with $X_{0,x}^{T,\boldsymbol{\pi} x}(t)$ solving the rn-dimensional system of SDEs

$$\mathrm{d}X = \frac{\boldsymbol{\pi} x - X}{T - t}\mathrm{d}t + \frac{1}{\sqrt{m}}\mathrm{d}w(t), \quad 0 \leqslant t < T, \quad X(0) = x. \tag{6.12}$$

The kinetic energy of the system of particles can be found as (see, e.g., Feynman, 1972; Takahashi & Imada, 1984; Ceperley, 1995)

$$E_K = \frac{m}{T\mathcal{Z}} \frac{\partial \mathcal{Z}}{\partial m}.$$

Differentiating $\mathcal{Z}$ from (6.10), one can obtain

$$E_K = \frac{m}{T} \frac{\mathcal{K}}{\mathcal{Z}}, \tag{6.13}$$

where

$$\mathcal{K} = \int_{\mathbf{R}^{rn}} \left\{ \sum_{\boldsymbol{\pi} \in \Pi_r} (2\pi T/m)^{-rn/2} \exp\left(-\frac{|x - \boldsymbol{\pi} x|^2}{2T/m} \right) E \left[\exp\left(-\int_0^T V(X_{0,x}^{T,\boldsymbol{\pi} x}(t)) \mathrm{d}t \right) \right. \right.$$
$$\left. \left. \times \left[\frac{rn}{2m} - \frac{|x - \boldsymbol{\pi} x|^2}{2T} + \frac{1}{2m} \int_0^T \nabla V(X_{0,x}^{T,\boldsymbol{\pi} x}(t)) \cdot \left(X_{0,x}^{T,\boldsymbol{\pi} x}(t) - \frac{x}{T}(T-t) - \frac{\boldsymbol{\pi} x}{T} t \right) \mathrm{d}t \right] \right] \right\} \mathrm{d}x. \tag{6.14}$$

Here ∇V is an rn-dimensional vector. We note that this expression for the kinetic energy is different from the ones exploited in Takahashi & Imada (1984) and Ceperley (1995). As was pointed out in Ceperley (1995), it is desirable for computational purposes to have various representations of the kinetic energy.

For our numerical example here, we consider one-dimensional ($n = 1$) bosons with mass $m = 1$ in the harmonic potential

$$V(x_1, \ldots, x_r) = \frac{x_1^2}{2} + \cdots + \frac{x_r^2}{2}. \tag{6.15}$$

It is known (see, e.g., Takahashi & Imada, 1984) that, in this case, the kinetic energy is equal to

$$E_{\mathrm{kin}} = \frac{1}{4} \sum_{l=1}^{r} l \coth\left(\frac{lT}{2} \right) - \frac{r(r-1)}{8}.$$

In the experiment we use a system of four bosons ($r = 4$) with inverse temperature $T = 1.2$. The exact value of the kinetic energy is $E_{\mathrm{kin}} \doteq 1.3740081$.

As with Example 6.2, correlated estimates of both the integral $\mathcal{K}$ and the partition function $\mathcal{Z}$ in (6.13) are produced simultaneously, and the ratio is then taken. Specifically, as before, we may write the integrals $\mathcal{K}$ and $\mathcal{Z}$ with $n = 1$ in the form

$$\mathcal{K} = \int_{\mathbf{R}^r} \mathcal{I}_1(x) \mathrm{d}x = \sqrt{2\pi\sigma^2} E \left[\mathcal{I}_1(\eta) \exp\left(\frac{\eta}{2\sigma^2} \right) \right],$$
$$\mathcal{Z} = \int_{\mathbf{R}^r} \mathcal{I}_2(x) \mathrm{d}x = \sqrt{2\pi\sigma^2} E \left[\mathcal{I}_2(\eta) \exp\left(\frac{\eta}{2\sigma^2} \right) \right],$$

where η is an r-dimensional Gaussian random variable whose components are mutually independent with zero mean and variance σ^2, i.e., $\eta \sim \mathcal{N}(0, \sigma^2 \mathrm{I}_{r\times r})$ with $\mathrm{I}_{r\times r}$ being the $r \times r$ unit matrix, and $\mathcal{I}_1$ and $\mathcal{I}_2$ are the corresponding integrands in (6.10) and (6.14), respectively. Furthermore, since the particles are noninteracting, we can decompose $\mathcal{I}_1$ and $\mathcal{I}_2$ to permanents as follows (see a similar idea

TABLE 4 *Kinetic energy of bosons. The errors in evaluating the kinetic energy* E_{kin} *of the system of four bosons* (6.13) *in the case of the harmonic potential* (6.15) *with* $T = 1.2$, $r = 4$ *and* $m = 1$*. The number of Monte Carlo runs is* $M = 10^9$

h	Euler method	Method (2.11) and (2.10)
0.20	$0.236 \pm 0.55 \times 10^{-4}$	$0.533 \times 10^{-2} \pm 0.75 \times 10^{-4}$
0.15	$0.175 \pm 0.61 \times 10^{-4}$	$0.300 \times 10^{-2} \pm 0.75 \times 10^{-4}$
0.10	$0.116 \pm 0.66 \times 10^{-4}$	$0.128 \times 10^{-2} \pm 0.76 \times 10^{-4}$
0.05	$0.057 \pm 0.71 \times 10^{-4}$	$0.035 \times 10^{-2} \pm 0.75 \times 10^{-4}$

in Takahashi & Imada, 1984). Let $U\colon \mathbb{R} \to \mathbb{R}$ be such that $V(x) = \sum_{i=1}^{r} U(x_i)$ and let

$$\mathcal{J}_1(x_i, x_j) = (2\pi T/m)^{-1/2} \exp\left(-\frac{(x_i - x_j)^2}{2T/m}\right) E\left[\exp\left(-\int_0^T U(X_{0,x_i}^{T,x_j}(t))\mathrm{d}t\right)\right.$$
$$\left.\times\left(\frac{1}{2m} - \frac{(x_i - x_j)^2}{2T} + \frac{1}{2m}\int_0^T U'(X_{0,x_i}^{T,x_j}(t))\left(X_{0,x_i}^{T,x_j}(t) - \frac{x_i}{T}(T-t) - \frac{x_j}{T}t\right)\mathrm{d}t\right)\right],$$
$$\mathcal{J}_2(x_i, x_j) = (2\pi T/m)^{-1/2} \exp\left(-\frac{(x_i - x_j)^2}{2T/m}\right) E \exp\left(-\int_0^T U(X_{0,x_i}^{T,x_j}(t))\mathrm{d}t\right).$$

It is not difficult to show that

$$\mathcal{I}_1(\eta) = \sum_{\boldsymbol{\pi} \in \Pi_r} \sum_{l=1}^{r} \mathcal{J}_1(\eta_l, (\boldsymbol{\pi}\eta)_l) \prod_{k \in \{1,\dots,r\}\setminus\{l\}} \mathcal{J}_2(\eta_k, (\boldsymbol{\pi}\eta)_k), \quad \mathcal{I}_2(\eta) = \sum_{\boldsymbol{\pi} \in \Pi_r} \prod_{k=1}^{r} \mathcal{J}_2(\eta_k, (\boldsymbol{\pi}\eta)_k). \tag{6.16}$$

Consequently, the following estimators for $\mathcal{K}$ and $\mathcal{Z}$ are used in the simulation:

$$\widehat{\mathcal{K}} = \frac{\sqrt{2\pi\sigma^2}}{M} \sum_{m=1}^{M} \left[{}_m\bar{\mathcal{I}}_1({}_m\eta) \exp\left(\frac{{}_m\eta}{2\sigma^2}\right)\right], \quad \widehat{\mathcal{Z}} = \frac{\sqrt{2\pi\sigma^2}}{M} \sum_{m=1}^{M} \left[{}_m\bar{\mathcal{I}}_2({}_m\eta) \exp\left(\frac{{}_m\eta}{2\sigma^2}\right)\right],$$

where ${}_m\eta$ are sampled independently from $\mathcal{N}(0, \sigma^2 \mathrm{I}_{r\times r})$ and ${}_m\bar{\mathcal{I}}_1$ and ${}_m\bar{\mathcal{I}}_2$ are approximate sample values of $\mathcal{I}_1$ and $\mathcal{I}_2$, calculated as per (6.16) from the approximate sample values of functionals $\mathcal{J}_1$ and $\mathcal{J}_2$ evaluated along the same Brownian bridge paths using the method (2.11) and (2.10) or the Euler method (2.14) and (2.13).

We note that the value of σ^2 may be chosen to make the variances of $\widehat{\mathcal{K}}$ and $\widehat{\mathcal{Z}}$ small. In the presented experiments, σ is taken equal to 2. We remark that, although we illustrate the above decomposition into permanents in order to compute $\mathcal{K}$ and $\mathcal{Z}$ for the case of one-dimensional particles, its generalization for n-dimensional noninteracting particles is straightforward.

We analyse two methods, namely, the method (2.11) and (2.10) and the Euler method (2.14) and (2.13). The results are presented in Table 4, which gives the errors of the two methods. As in the previous examples, the Monte Carlo error is made relatively small in order to be able to analyse the bias. It is clearly seen from the data that the method (2.11) and (2.10) converges with order two, while the Euler method exhibits the first-order convergence as expected (see Theorems 2.2 and 2.4).

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