Computing conditional Wiener integrals of functionals of a general form

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Abstract

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 simulation of 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.

AMS 2000 subject classification. 65C30, 28C20, 65C05, 60H35.

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 $x(0)=a$, $x(T)=b$. Consider the conditional Wiener integral

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

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 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. [8, 24]).

The importance of path integrals (1.1) for computing various quantities in quantum statistical mechanics is well known [5, 7, 8, 14, 23, 24]. For instance, the Feynman path integral of the form

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

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

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

Such quantities as the free energy of the system, the ground state energy, wavefunction, etc. can be written in terms of the integral (1.1), (1.2) [7, 8, 14, 16, 23, 24].

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., [14, 16, 23] 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 $\Gamma(\theta)$, $0 \leq \theta \leq T$, has the form

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

where the function

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

the partition function

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

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. [14]).

Other important examples of more general functionals than (1.2) are those corresponding to internal and kinetic energies (see, e.g. [6, 1, 25]). In Example 3 from Section 6 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 discretisation takes place, rather than beginning by using a finite-dimensional approximation to the integral as it is usually done [1, 3, 5, 16, 28]. The proposed algorithm is very simple to realize in practice.

In [10, 27] (see also [20]), the probabilistic approach was used for computing Wiener integrals with respect to the usual (unconditional) Wiener measure. In [19] (see also [20]) 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 [10, 27], 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 [19]. The proposed method is new in comparison with the ones available in [19] and it is analogous to the one used in the case of the usual Wiener measure [27]. We also note that there are a large number of methods and results (see, e.g. [20] and references therein) for approximating simple functionals $f(X(T))$, where f is a function from a sufficiently wide class and $X(t)$, $t_0 < t < T$, is a solution of SDEs. But not much attention (except, e.g. [17, 20, 27]) has been paid to approximating general functionals depending on trajectories of the SDE solution. Other approaches to computing Wiener integrals can be found, e.g. in [1, 3, 5, 16, 28] (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 [2, 4] to express path integrals of integral-type functionals over pinned diffusions as expectations with respect to a Markovian process which solves a system of SDEs. In this case we propose an Euler-type method and prove its first-order convergence. Other approaches to simulating diffusion bridges see, e.g. in [11] and in the references therein. 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 $C^d_{0,a;T,b}$. We impose the following assumptions on F.

(FA) Assumptions.

1. *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 r-dimensional Lebesgue measure on $[0,T]^r$, $(r-1)$-dimensional Lebesgue measure on the hyperplanes $\{(s_1,\dots,s_r) \in [0,T]^r : s_j = \theta_i\}$, $i = 1,\dots,n$, $j = 1,\dots,r$,* and *on the diagonal hyperplanes $\{(s_1,\dots,s_r) \in [0,T]^r : s_i = s_j\}$, $(r-2)$-dimensional Lebesgue measure on $(r-2)$-dimensional hyperplanes $\{(s_1,\dots,s_r) \in [0,T]^r : s_k = \theta_i$ and $s_l = \theta_j,\ k \neq l\}$ and $\{(s_1,\dots,s_r) \in [0,T]^r : s_i = s_j$* and *$s_k = s_l\}$, and so on, including the one-dimensional Lebesgue measure on the lines $\{s_1 = \theta_{i_1},\dots,s_{r-1} = \theta_{i_{r-1}}\}$, $i_j \in \{1,\dots,n\}$, and on the diagonal $\{s_1 = s_2 = \cdots = s_r\}$ plus the unit measures concentrated on the points $(\theta_{i_1},\dots,\theta_{i_r})$, $i_j \in \{1,\dots,n\}$.*

2. *We assume that the functional $F(x)$ is six times Fréchet differentiable and that its*

r-th derivative has the following form:

$$F^{(r)}(x)(\delta_1, \ldots, \delta_r) = \int_{[0,T]^r} v^{(r)}(x; s_1, \ldots, s_r)\delta_1(s_1)\cdots\delta_r(s_r)\nu_r(ds_1\cdots ds_r), \quad (2.1)$$
$$r = 1, \ldots, 6,$$

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

3. *For any function $x \in A[0,T]$ constant on a semi-interval $[c_0, c^0) \subset [0,T]$, there are continuous derivatives*

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

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

We recall (see, e.g. [15]) that $F^{(r)}(x)(\delta_1, \ldots, \delta_r)$ are r-linear functionals. Under Assumptions (FA) we prove a convergence theorem (Theorem 2.1) 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 $A[0,T]$ which 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 (FA) is not particularly restrictive since it is usually satisfied. The assumption on 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 boundedness of derivatives of functionals. Alternatively, the concept of rejecting exploding trajectories from [21] could be exploited here. That is we might choose not to take into account those trajectories which 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 (FA), 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)):

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

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 (FA) hold. In particular, the Fréchet derivatives (2.1) have the form here:

$$F^{(1)}(x)(\delta_1) = \int_{[0,T]} v^{(1)}(x;s_1)\delta_1(s_1)\nu_1(ds_1)$$

with

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

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

$$F^{(2)}(x)(\delta_1,\delta_2) = \int_{[0,T]^2} v^{(2)}(x;s_1,s_2)\delta_1(s_1)\delta_2(s_2)\nu_2(ds_1ds_2)$$

with

$$\begin{aligned} v^{(2)}(x;s_1,s_2)\delta_1(s_1)\delta_2(s_2) &= \frac{\partial^2\varphi}{\partial z^2}\nabla_x f(s_1,x(s_1))\cdot\delta_1(s_1)\ \nabla_x f(s_2,x(s_2))\cdot\delta_2(s_2), \\ &\quad s_1\neq s_2,\ \ s_i\neq\theta; \\ v^{(2)}(x;s,\theta)\delta_1(s)\delta_2(\theta) &= \sum_{i=1}^{d}\frac{\partial^2\varphi}{\partial z\partial x^i}\ \nabla_x f(s,x(s))\cdot\delta_1(s)\delta_2^i(\theta),\ \ s\neq\theta; \\ v^{(2)}(x;s,s)\delta_1(s)\delta_2(s) &= \frac{\partial\varphi}{\partial z}\sum_{i,j=1}^{d}\frac{\partial^2 f}{\partial x^i\partial x^j}(s,x(s))\delta_1^i(s)\delta_2^j(s),\quad s\neq\theta; \\ v^{(2)}(x;\theta,\theta)\delta_1(\theta)\delta_2(\theta) &= \sum_{i,j=1}^{d}\frac{\partial^2\varphi}{\partial x^i\partial x^j}\delta_1^i(\theta)\delta_2^j(\theta); \end{aligned}$$

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 $\left(x(\theta),\int_0^T f(t,x(t))\,dt\right)$ and the dot $\cdot$ means the usual scalar product of vectors.

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

$$F(x(\cdot)) = \varphi\left(\int_0^T\int_0^t f(s,x(s))\ g(t,x(t))\,dsdt\right)$$

satisfies Assumptions (FA).

2.2 Numerical method

Let $(\Omega, \mathcal{F}, \mathcal{F}_t, P)$, $0 \le t \le T$, be a filtered probability space and $w(t) = (w^1(t), \dots, w^d(t))^\top$ be a d-dimensional $\{\mathcal{F}_t\}_{t\ge 0}$-adapted standard Wiener process. As it is known [12, 13], the d-dimensional Brownian bridge $X(t) = X_{0,a}^{T,b}(t)$, $0 \le t \le T$, from a to b can be characterized as the pathwise unique solution of the system of SDEs

$$dX = \frac{b - X}{T - t} dt + dw(t),\ 0 \le t < T,\ X(0) = a, \tag{2.3}$$

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 $X(t)$, $0 \le t \le T$:

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

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

$$0 = t_0 < t_1 < \dots < t_N = T$$

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

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

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

The solution of (2.3) is

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

Hence for any $0 \le \Delta < T - t$

$$X(t + \Delta) = X(t) + \Delta\frac{b - X(t)}{T - t} + (T - t - \Delta)\int_t^{t+\Delta} \frac{dw(s)}{T - s}. \tag{2.7}$$

We have

$$E\left[(T - t - \Delta)\int_t^{t+\Delta} \frac{dw(s)}{T - s}\middle| X(t)\right] = 0; \tag{2.8}$$
$$E\left[(T - t - \Delta)\int_t^{t+\Delta} \frac{dw(s)}{T - s}\middle| X(t)\right]^2 = \left(1 - \frac{\Delta}{T - t}\right)\Delta.$$

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

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

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

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

$$X^h(t) := a, \ t \in [0, t_{1/2}); \qquad (2.10)$$
$$X^h(t) := X(t_k), \ t \in [t_{k-1/2}, t_{k+1/2}), \ k = 1, \dots, N-1;$$
$$X^h(t) := b, \ t \in [t_{N-1/2}, T].$$

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

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

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

This method is analogous to the one used in the case of the usual (unconditional) Wiener measure [27] (see also [20]). We prove the following convergence theorem.

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

$$\left|\mathcal{J} - \bar{\mathcal{J}}\right| = \left|EF(X) - EF(X^h)\right| \le Kh^2, \qquad (2.12)$$

where the constant K *is independent of* h.

The proof of the theorem is given in the next section.

Remark 2.1 *The method* (2.11), (2.10) *is exact* (*i.e., there is no integration error*) *on the class of functionals which depend only on the value of the function* $x(t)$ *at a finite number of points* θ_i, $i = 1, \dots, n$.

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

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

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

Theorem 2.2 *Assume that Assumptions* $(FA).1$ *and* $(FA).3$ *hold and* $(FA).2$ *holds with* $r = 1, 2, 3, 4$ *in* (2.1). *Then*

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

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

The proof of this theorem is easier than that of Theorem 2.1 and it is omitted here. In numerical Example 3 from Section 6 we compare the method (2.11), (2.10) and the Euler method (2.14), (2.13). The experimental results confirm our theoretical predictions.

3 Proof of the convergence theorem

Here we exploit some constructions from [27], although the singularity of the drift in (2.3) as t approaches T causes additional difficulties, which are overcome by adopting ideas from [19]. 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 3.1 at the end of this section). Note that in this section we shall use the letter K to denote various constants which are independent of k and h.

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

$$X_k(t) := X(t)\chi_{[0,t_k)}(t) + X(t_k)\chi_{[t_k,T]}(t) + \sum_{j=k}^{N-1} \Delta_j X \chi_{[t_{j+1/2},T]}(t), \tag{3.1}$$

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

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

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:

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

Thus, we need to analyze the difference

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

Recall the Taylor formula for functionals (see, e.g. [15]):

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

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

$$\begin{aligned} F(X_{k+i}) &= F(\bar{X}_k) + \int_{[0,T]} v^{(1)}(\bar{X}_k; s_1)\delta_{k,i}(s_1)\nu_1(ds_1) + \cdots \\ &+ \frac{1}{5!} \int_{[0,T]^5} v^{(5)}(\bar{X}_k; s_1, \dots, s_5)\delta_{k,i}(s_1) \cdots \delta_{k,i}(s_5)\nu_5(ds_1 \cdots ds_5) \\ &+ \frac{1}{6!} \int_{[0,T]^6} v^{(6)}(\bar{X}_k + \lambda_i \delta_{k,i}; s_1, \dots, s_6)\delta_{k,i}(s_1) \cdots \delta_{k,i}(s_6)\nu_6(ds_1 \cdots ds_6), \\ & 0 < \lambda_i < 1, \quad i = 0, 1, \end{aligned} \tag{3.5}$$

where

$$\delta_{k,0}(s) = X_k(s) - \bar{X}_k(s) = \Delta_k X \chi_{[t_{k+1/2},T]}(s) - \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s) \tag{3.6}$$

$$= \chi_{[t_{k+1/2},T]}(s) \left[(t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k} + (T-t_{k+1}) \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \right]$$
$$- \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s),$$

$$\delta_{k,1}(s) = X_{k+1}(s) - \bar{X}_k(s) = (X(s)-X(t_k))\,\chi_{[t_k,t_{k+1})}(s) + \Delta_k X \chi_{[t_{k+1},T]}(s)$$
$$- \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s)$$
$$= \chi_{[t_k,t_{k+1})}(s) \left[(s-t_k)\frac{b-X(t_k)}{T-t_k} + (T-s) \int_{t_k}^{s} \frac{dw(s')}{T-s'} \right]$$
$$+\chi_{[t_{k+1},T]}(s) \left[(t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k} + (T-t_{k+1}) \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \right]$$
$$- \int_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j)\chi_{[t_{j+1/2},T]}(s).$$

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 $\nu_r,\ r = 1, \ldots, 6$, 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 $O(h)$. Indeed, $S_k^{(r)} = \bigcup_{j=1}^{r} \{(s_1, \ldots, s_r) : s_j \in (t_k, t_{k+1})\}$ and hence $\nu_r\left(S_k^{(r)}\right) < r\nu_r\left(\{(s_1, \ldots, s_r) : s_1 \in (t_k, t_{k+1})\}\right)$, which is of order $O(h)$. Further, it is not difficult to verify that the integral $\int_{t_k}^{s} \frac{dw(s')}{T-s'}$, $t_k \le s \le t_{k+1}$, and $\bar{X}_k$ are independent by showing that $E\left[\bar{X}_k(t)\int_{t_k}^{s} \frac{dw(s')}{T-s'}\right] = 0$ for any $0 \le t \le T$ and $t_k \le s \le t_{k+1}$. In what follows these properties are used in analysis of the parts of ρ_k. We shall also exploit the inequality (see, e.g. [19, Lemma A.4]) for any $p \ge 1$

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

We have from (3.4) and (3.5):

$$\rho_k = E\int_{[0,T]} v^{(1)}(\bar{X}_k; s_1)\,[\delta_{k,1}(s_1) - \delta_{k,0}(s_1)]\,\nu_1(ds_1) \tag{3.8}$$
$$+ \frac{1}{2}E\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)\,[\delta_{k,1}(s_1)\delta_{k,1}(s_2) - \delta_{k,0}(s_1)\delta_{k,0}(s_2)]\,\nu_2(ds_1 ds_2) + \cdots$$
$$+ \frac{1}{5!}E\int_{[0,T]^5} v^{(5)}(\bar{X}_k; s_1, \dots, s_5)\left[\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right]\nu_5(ds_1\cdots ds_5)$$
$$+ \frac{1}{6!}E\int_{[0,T]^6}[v^{(6)}(\bar{X}_k + \lambda_1\delta_{k,1}; s_1, \dots, s_6)\prod_{j=1}^{6}\delta_{k,1}(s_j)$$
$$- v^{(6)}(\bar{X}_k + \lambda_0\delta_{k,0}; s_1, \dots, s_6)\prod_{j=1}^{6}\delta_{k,0}(s_j)]\nu_6(ds_1\cdots ds_6).$$

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

Lemma 3.1 *Let $U_s(x) := v^{(2)}(x; s, s)$. The following estimate holds*

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

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

Now we analyze the terms forming ρ_k in (3.8). Introduce the indicator $I_k = I_{\{\theta_1,\dots,\theta_n\}}(t_k)$. We obtain for the first term in (3.8):

$$r_k^{(1)} := E\int_{[0,T]} v^{(1)}(\bar{X}_k; s_1)\,[\delta_{k,1}(s_1) - \delta_{k,0}(s_1)]\,\nu_1(ds_1)$$
$$= E\int_{t_k}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)\,[\delta_{k,1}(s_1) - \delta_{k,0}(s_1)]\,ds_1$$
$$+ v^{(1)}(\bar{X}_k; t_k)\,[\delta_{k,1}(t_k) - \delta_{k,0}(t_k)]\,I_k + v^{(1)}(\bar{X}_k; t_{k+1})\,[\delta_{k,1}(t_{k+1}) - \delta_{k,0}(t_{k+1})]\,I_{k+1}$$
$$= E\int_{t_k}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)\left[(s_1 - t_k)\frac{b - X(t_k)}{T - t_k} + (T - s_1)\int_{t_k}^{s_1}\frac{dw(s')}{T - s'}\right]ds_1$$
$$- E\int_{t_{k+1/2}}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)\left[(t_{k+1} - t_k)\frac{b - X(t_k)}{T - t_k} + (T - t_{k+1})\int_{t_k}^{t_{k+1}}\frac{dw(s')}{T - s'}\right]ds_1$$

$$= E\frac{b - X(t_k)}{T - t_k}\left[\int_{t_k}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)(s_1 - t_k)ds_1 - (t_{k+1} - t_k)\int_{t_{k+1/2}}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)ds_1\right]$$
$$= E\frac{b - X(t_k)}{T - t_k}\left[\int_{t_k}^{t_{k+1/2}} v^{(1)}(\bar{X}_k; s_1)(s_1 - t_k)ds_1 - \int_{t_{k+1/2}}^{t_{k+1}} v^{(1)}(\bar{X}_k; s_1)(t_{k+1} - s_1)ds_1\right].$$

Integrating by parts, we get

$$r_k^{(1)} = E\frac{b - X(t_k)}{T - t_k}\left[v^{(1)}(\bar{X}_k; t_{k+1/2})\frac{(t_{k+1} - t_k)^2}{8} - \int_{t_k}^{t_{k+1/2}} \frac{d}{ds_1}v^{(1)}(\bar{X}_k; s_1)\frac{(s_1 - t_k)^2}{2}ds_1\right.$$
$$\left. - v^{(1)}(\bar{X}_k; t_{k+1/2})\frac{(t_{k+1} - t_k)^2}{8} - \int_{t_{k+1/2}}^{t_{k+1}} \frac{d}{ds_1}v^{(1)}(\bar{X}_k; s_1)\frac{(t_{k+1} - s_1)^2}{2}ds_1\right]$$
$$= -E\frac{b - X(t_k)}{T - t_k}\left[\int_{t_k}^{t_{k+1/2}} \frac{d}{ds_1}v^{(1)}(\bar{X}_k; s_1)\frac{(s_1 - t_k)^2}{2}ds_1\right.$$
$$\left. + \int_{t_{k+1/2}}^{t_{k+1}} \frac{d}{ds_1}v^{(1)}(\bar{X}_k; s_1)\frac{(t_{k+1} - s_1)^2}{2}ds_1\right].$$

It follows from here and the inequality (3.7) that

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

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

$$r_k^{(2)} := \frac{1}{2}E\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)\left[\delta_{k,1}(s_1)\delta_{k,1}(s_2) - \delta_{k,0}(s_1)\delta_{k,0}(s_2)\right]\nu_2(ds_1 ds_2) \tag{3.10}$$
$$= \frac{1}{2}E\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)$$
$$\times\left\{\left[(s_1 - t_k)(s_2 - t_k)\frac{(b - X(t_k))^2}{(T - t_k)^2} + (s_1 \wedge s_2 - t_k)\frac{T - s_1 \vee s_2}{T - t_k}\right]\right.$$
$$\times\, \chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_k,t_{k+1})}(s_2)$$

$$+ 2\left[(t_{k+1} - t_k)(s_1 - t_k)\frac{(b - X(t_k))^2}{(T - t_k)^2} + (s_1 - t_k)\frac{T - t_{k+1}}{T - t_k}\right]\chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_{k+1},T]}(s_2)$$
$$+ \left[(t_{k+1} - t_k)^2\frac{(b - X(t_k))^2}{(T - t_k)^2} + (t_{k+1} - t_k)\frac{T - t_{k+1}}{T - t_k}\right]$$
$$\times\left(\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2) - \chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right)$$

$$- \frac{2}{T - t_k}\sum_{j=k+1}^{N-1}(t_{j+1} - t_j)\chi_{[t_{j+1/2},T]}(s_2)$$
$$\times\left.\left[(s_1 - t_k)\chi_{[t_k,t_{k+1})}(s_1) - (t_{k+1} - t_k)\chi_{[t_{k+1/2},t_{k+1})}(s_1)\right]\right\}\nu_2(ds_1 ds_2).$$

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

$$A_{1k} := E\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2) \tag{3.11}$$
$$\times \left[(s_1 - t_k)(s_2 - t_k)\frac{(b - X(t_k))^2}{(T - t_k)^2} + (s_1 \wedge s_2 - t_k)\frac{T - s_1 \vee s_2}{T - t_k}\right]$$
$$\times \chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_k,t_{k+1})}(s_2)\nu_2(ds_1 ds_2)$$
$$= E\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s, s)\left[(s - t_k)^2\frac{(b - X(t_k))^2}{(T - t_k)^2} + (s - t_k)\frac{T - s}{T - t_k}\right] ds$$
$$+ E\int_{t_k}^{t_{k+1}}\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2)$$
$$\times \left[(s_1 - t_k)(s_2 - t_k)\frac{(b - X(t_k))^2}{(T - t_k)^2} + (s_1 \wedge s_2 - t_k)\frac{T - s_1 \vee s_2}{T - t_k}\right] ds_1 ds_2,$$

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

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

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. Further, since $v^{(2)}(\bar{X}_k; s, s) = v^{(2)}(\bar{X}_k; t_k, t_k) + \int_{t_k}^{s} \frac{d}{ds'} v^{(2)}(\bar{X}_k; s', s')ds'$, the first integral in the right-hand side of (3.11) can be written as

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

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

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

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

$$A_{2k} := 2E\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right]$$
$$\times \chi_{[t_k,t_{k+1})}(s_1)\chi_{[t_{k+1},T]}(s_2)\nu_2(ds_1ds_2)$$
$$= 2E\int_{t_{k+1}}^{T}\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2}\right.$$
$$\left.+(s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right] ds_1 ds_2$$

$$+\sum_{i=1}^{n} I_{\theta_i>t_k} E\int_{t_k}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, \theta_i)\left[(t_{k+1}-t_k)(s_1-t_k)\frac{(b-X(t_k))^2}{(T-t_k)^2} + (s_1-t_k)\frac{T-t_{k+1}}{T-t_k}\right] ds_1$$
$$= 2E\left[\frac{(t_{k+1}-t_k)^3}{2}\frac{(b-X(t_k))^2}{(T-t_k)^2} + \frac{(t_{k+1}-t_k)^2}{2}\frac{T-t_{k+1}}{T-t_k}\right]$$
$$\times\left[\int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; t_k, s_2)ds_2 + \sum_{i=1}^{n} I_{\theta_i>t_k} v^{(2)}(\bar{X}_k; t_k, \theta_i)\right] + O(h^3).$$

The third part of (3.10) is

$$A_{3k} := E\left[(t_{k+1}-t_k)^2\frac{(b-X(t_k))^2}{(T-t_k)^2} + (t_{k+1}-t_k)\frac{T-t_{k+1}}{T-t_k}\right]\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)$$
$$\times\left[\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2) - \chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right]\nu_2(ds_1ds_2).$$

We have for the integral in A_{3k} :

$$\int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2)\left[\chi_{[t_{k+1},T]}(s_1)\chi_{[t_{k+1},T]}(s_2) - \chi_{[t_{k+1/2},T]}(s_1)\chi_{[t_{k+1/2},T]}(s_2)\right]\nu_2(ds_1ds_2)$$
$$= \int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; s, s)ds - \int_{t_{k+1/2}}^{T} v^{(2)}(\bar{X}_k; s, s)ds$$
$$+ 2\sum_{i=1}^{n} I_{\theta_i>t_k}\left[\int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; s, \theta_i)ds - \int_{t_{k+1/2}}^{T} v^{(2)}(\bar{X}_k; s, \theta_i)ds\right]$$
$$+ \int_{t_{k+1}}^{T}\int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; s_1, s_2)ds_1ds_2 - \int_{t_{k+1/2}}^{T}\int_{t_{k+1/2}}^{T} v^{(2)}(\bar{X}_k; s_1, s_2)ds_1ds_2$$

$$
\begin{aligned}
&= -\frac{(t_{k+1}-t_k)}{2} v^{(2)}(\bar{X}_k; t_k, t_k) - (t_{k+1}-t_k) \sum_{i=1}^{n} I_{\theta_i > t_k} v^{(2)}(\bar{X}_k; t_k, \theta_i) + O(h^2) \\
&- 2 \int_{t_{k+1/2}}^{T} \int_{t_{k+1/2}}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2) ds_1 ds_2 + \int_{t_{k+1/2}}^{t_{k+1}} \int_{t_{k+1/2}}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2) ds_1 ds_2 \\
&= -\frac{(t_{k+1}-t_k)}{2} v^{(2)}(\bar{X}_k; t_k, t_k) - (t_{k+1}-t_k) \sum_{i=1}^{n} I_{\theta_i > t_k} v^{(2)}(\bar{X}_k; t_k, \theta_i) \\
&- (t_{k+1}-t_k) \int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; t_k, s_2) ds_2 + O(h^2).
\end{aligned}
$$

Then

$$
\begin{aligned}
A_{3k} = &-E\left[\left(v^{(2)}(\bar{X}_k; t_k, t_k) + 2\sum_{i=1}^{n} I_{\theta_i > t_k} v^{(2)}(\bar{X}_k; t_k, \theta_i)\right)\right. \\
&\left.\times \left(\frac{(t_{k+1}-t_k)^3}{2} \frac{(b - X(t_k))^2}{(T-t_k)^2} + \frac{(t_{k+1}-t_k)^2}{2} \frac{T - t_{k+1}}{T - t_k} \right)\right] \\
&- E\left[(t_{k+1}-t_k)^3 \frac{(b - X(t_k))^2}{(T-t_k)^2} + (t_{k+1}-t_k)^2 \frac{T - t_{k+1}}{T - t_k} \right] \int_{t_{k+1}}^{T} v^{(2)}(\bar{X}_k; t_k, s_2) ds_2 \\
&+ O(h^3).
\end{aligned}
$$

The last part of (3.10) is

$$
\begin{aligned}
A_{4k} := &-\frac{2}{T-t_k} E \int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2) \sum_{j=k+1}^{N-1} (t_{j+1}-t_j) \chi_{[t_{j+1/2}, T]}(s_2) \\
&\times \left[(s_1 - t_k) \chi_{[t_k, t_{k+1})}(s_1) - (t_{k+1} - t_k) \chi_{[t_{k+1/2}, t_{k+1})}(s_1) \right] \nu_2(ds_1 ds_2) \\
&= -\frac{2}{T-t_k} E \int_{[0,T]^2} v^{(2)}(\bar{X}_k; s_1, s_2) \sum_{j=k+1}^{N-1} (t_{j+1}-t_j) \chi_{[t_{j+1/2}, T]}(s_2) \\
&\times \left[(s_1 - t_k) \chi_{[t_k, t_{k+1/2})}(s_1) - (t_{k+1} - s_1) \chi_{[t_{k+1/2}, t_{k+1})}(s_1) \right] \nu_2(ds_1 ds_2)
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{2}{T-t_k} E\left[\int_{t_{k+3/2}}^{T} \sum_{j=k+1}^{N-1} (t_{j+1}-t_j) \chi_{[t_{j+1/2}, T]}(s_2) \right. \\
&\times \left(\int_{t_k}^{t_{k+1/2}} v^{(2)}(\bar{X}_k; s_1, s_2)(s_1 - t_k) ds_1 - \int_{t_{k+1/2}}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, s_2)(t_{k+1} - s_1) ds_1 \right) ds_2
\end{aligned}
$$

$$
\begin{aligned}
&+ \sum_{i=1}^{n} I_{\theta_i > t_{k+1}} (\theta_i - t_{k+1}) \\
&\left.\times \left(\int_{t_k}^{t_{k+1/2}} v^{(2)}(\bar{X}_k; s_1, \theta_i)(s_1 - t_k) ds_1 - \int_{t_{k+1/2}}^{t_{k+1}} v^{(2)}(\bar{X}_k; s_1, \theta_i)(t_{k+1} - s_1) ds_1 \right)\right].
\end{aligned}
$$

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

As a result, we obtain

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

Applying Lemma 3.1, we get

$$|r_k^{(2)}| \le \frac{Kh^3}{\sqrt{T-t_k}}. \tag{3.13}$$

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

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

Then

$$Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)\prod_{i=1}^{3}\delta_{k,0}(s_i)$$
$$= Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)$$
$$\times \prod_{i=1}^{3}\left((t_{k+1}-t_k)\frac{b-X(t_k)}{T-t_k}\chi_{[t_{k+1/2},T]}(s_i) + \int\limits_{t_k}^{t_{k+1}} \frac{dw(s')}{T-s'} \sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{k+1/2},t_{j+1/2})}(s_i)\right)$$

$$= Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)(t_{k+1}-t_k)^2\frac{b-X(t_k)}{(T-t_k)^2}\left((t_{k+1}-t_k)\frac{(b-X(t_k))^2}{T-t_k}\prod_{i=1}^{3}\chi_{[t_{k+1/2},T]}(s_i)\right.$$
$$\left. + \sum_{i=1}^{3}\frac{\chi_{[t_{k+1/2},T]}(s_i)}{T-t_{k+1}}\prod_{l\neq i}\sum_{j=k+1}^{N-1}(t_{j+1}-t_j)\chi_{[t_{k+1/2},t_{j+1/2})}(s_l)\right).$$

From here, we get the estimate

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

Analogously, we obtain

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

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 $O(h)$, we arrive at

$$\left|\frac{1}{6}E\int_{[0,T]^3} v^{(3)}(\bar{X}_k; s_1, s_2, s_3)\left[\prod_{j=1}^{3}\delta_{k,1}(s_j) - \prod_{j=1}^{3}\delta_{k,0}(s_j)\right]\nu_3(ds_1ds_2ds_3)\right| \tag{3.14}$$

$$= \left|\frac{1}{6}E\int_{[0,T]^3} I_{S_k^{(3)}}(s_1, s_2, s_3)v^{(3)}(\bar{X}_k; s_1, s_2, s_3)\left[\prod_{j=1}^{3}\delta_{k,1}(s_j) - \prod_{j=1}^{3}\delta_{k,0}(s_j)\right]\nu_3(ds_1ds_2ds_3)\right|$$

$$\leq \frac{1}{6}\int_{[0,T]^3} I_{S_k^{(3)}}(s_1, s_2, s_3)\left[|Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)\prod_{j=1}^{3}\delta_{k,1}(s_j)|\right.$$

$$\left. + |Ev^{(3)}(\bar{X}_k; s_1, s_2, s_3)\prod_{j=1}^{3}\delta_{k,0}(s_j)|\right]\nu_3(ds_1ds_2ds_3) \leq \frac{Kh^3}{\sqrt{T-t_k}}.$$

Since we have for the terms in (3.6)

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

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

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 $O(h)$, we obtain

$$\left|\frac{1}{4!}E\int_{[0,T]^4} v^{(4)}(\bar{X}_k; s_1, \dots, s_4)\left[\prod_{j=1}^{4}\delta_{k,1}(s_j) - \prod_{j=1}^{4}\delta_{k,0}(s_j)\right]\nu_4(ds_1\cdots ds_4)\right| \tag{3.15}$$

$$\leq \frac{1}{4!}\sup|v^{(4)}|\int_{[0,T]^4} I_{S_k^{(4)}}(s_1, \dots, s_4)\left(E|\prod_{j=1}^{4}\delta_{k,1}(s_j)| + E|\prod_{j=1}^{4}\delta_{k,0}(s_j)|\right)\nu_4(ds_1\cdots ds_4)$$

$$\leq Kh^3.$$

By analogous arguments, we get

$$\left|\frac{1}{5!}E\int_{[0,T]^5} v^{(5)}(\bar{X}_k; s_1, \dots, s_5)\left[\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right]\nu_5(ds_1\cdots ds_5)\right| \tag{3.16}$$

$$\leq \frac{1}{5!}\sup|v^{(5)}|\int_{[0,T]^5} E\left|\prod_{j=1}^{5}\delta_{k,1}(s_j) - \prod_{j=1}^{5}\delta_{k,0}(s_j)\right|\nu_5(ds_1\cdots ds_5)$$

$$\leq Kh^{7/2}.$$

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

$$\left|\frac{1}{6!}E\int_{[0,T]^6}[v^{(6)}(\bar{X}_k+\lambda_1\delta_{k,i};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,1}(s_j)\right. \tag{3.17}$$

$$\left.-v^{(6)}(\bar{X}_k+\lambda_0\delta_{k,i};s_1,\ldots,s_6)\prod_{j=1}^{6}\delta_{k,0}(s_j)]\nu_6(ds_1\cdots ds_6)\right|$$

$$\leq \frac{1}{6!}\sup|v^{(6)}|\left|\int_{[0,T]^6}E\left[\prod_{j=1}^{6}|\delta_{k,1}(s_j)|+\prod_{j=1}^{6}|\delta_{k,0}(s_j)|\right]\nu_6(ds_1\cdots ds_6)\right|$$

$$\leq Kh^3.$$

Substituting (3.9), (3.13)-(3.17) in (3.8), we get

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

which together with (3.3)-(3.4) implies (2.12). Theorem 2.1 is proved. □

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

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

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

We also note [19, 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.

Introduce the auxiliary processes $\bar{X}_k^{(0)}(t)$, $k=0,\ldots,N-1$:

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

Using the Taylor formula for functionals, we get

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

where

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

and $0<\lambda<1$.

We have

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

It is not difficult to see that the second term in 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,

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

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

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

We have

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

where

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

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

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

Recalling that $\psi(t_l)$, $l=0,\ldots,N-1$, 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)-(3.21) that

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

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

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

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

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

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

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

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

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

Lemma 3.1 is proved. □

Remark 3.1 *It is notable that in the multidimensional case* ($d > 1$)*, the integrand of* (3.10) *contains cross-terms in all coordinate pairs* i, j*, viz* $\delta^i_{k,1}(s_1)\delta^j_{k,1}(s_2) - \delta^i_{k,0}(s_1)\delta^j_{k,0}(s_2)$*. The terms corresponding to* $i = j$ *are estimated in the same way as in the considered one-dimensional case. For* $i \ne j$*, 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 [19, Corollary A.1] and their further estimation yields* $O(h^3/\sqrt{T - t_k})$ *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:

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

Introduce the scalar process $Z(t)$ satisfying the equation

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

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

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

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

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

where

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

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, it follows from the general Theorem 2.1 that the method (4.4), (4.5) for (1.1), (4.1) has the second order of accuracy; i.e., the estimate (2.12) is valid for it. The other set of assumptions under which the theorem 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 [20] (see its application in the case of conditional Wiener integrals of exponential-type functionals in [19] and in the case of usual Wiener integrals in [27]). It is interesting that no method of the form

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

has order of accuracy higher than two (in the case of usual Wiener integrals, see a similar comment in [27]). At the same time, in the case of integral-type functionals of a particular form – the exponential-type functionals $F(x(\cdot)) = \exp[\int_0^T f(t, x(t))\, dt]$, a fourth-order Runge-Kutta method was constructed in [19].

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 1D 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 [19] (see similar observations although in a different context in [22]). Further, instead of the trapezoidal rule (4.5), we can use the Simpson rule:

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

Although both methods (4.5) and (4.6) are of order two, the method (4.6) had much smaller bias in our experiments than the method (4.5) and thus was computationally more effective. The methods (4.4), (4.5) and (4.4), (4.6) extend the arsenal of numerical tools considered in [19, 20] for computing exponential-type functionals (1.2).

5 Extension to the case of pinned diffusions[1]

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

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

that are conditioned to pass through a point $b \in R^d$ at time T, $t_0 \leq t \leq T$. Conditioned diffusions are used, e.g. in parameter estimation problems (see e.g. [4]). We note that the Brownian bridge case considered in the previous sections corresponds to (5.1) with $\alpha = 0$.

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

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

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

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

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

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

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 re-written as [2, 4]:

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

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

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

$$dY = \alpha^\top(t, X)\frac{b - X}{T - t}Y dt + \alpha^\top(t, X)Y dw(t), \quad Y(t_0) = 1, \tag{5.7}$$

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)-(2.4)):

$$dX = \frac{b - X}{T - t}dt + dw(t), \quad X(t_0) = a. \tag{5.8}$$

[1] The authors thank the anonymous Associate Editor for providing them with the reference [2], and G.N. Milstein for the reference [4], which are the basis for this section.

We note that

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

where

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

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 $[t_0, T] : t_0 < t_1 < \cdots < t_N = T$, for simplicity 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)):

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

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

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

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

$$Q_0 = 0,$$

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

We remark that we choose to approximate (5.9), (5.10) rather than (5.7) since it was observed (see, e.g. [22] 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):

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

Introduce the function

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

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 [9]. The method itself is applicable more widely and the assumptions can be relaxed in the spirit of the comment after Assumptions (FA) in Section 2.

Theorem 5.1 *The method* (5.11)-(5.13) *is of first order of accuracy, i.e.,*

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

where the constant K is independent of h.

This theorem has the evident corollary.

Corollary 5.1 *The method* (5.14), (5.11)-(5.13) *for evaluating the path integral* (5.3) *is of first order of accuracy, i.e.,*

$$\left|\mathcal{J} - \bar{\mathcal{J}}\right| \leq Kh, \tag{5.18}$$

where the constant K is independent of h.

Remark 5.1 *We note that if in* (5.14) *we substitute Q_N simulated by the standard Euler scheme for* (5.10)*:*

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

then the method (5.14), (5.11), (5.12), (5.19) *is of order $O(h\ln h)$ instead of $O(h)$ for* (5.14), (5.11)-(5.13) (*also see footnote* 2)*.*

Proof of Theorem 5.1. Using the standard technique (see [20, p. 100]), we can write the global error in the form:

$$\begin{aligned} R &:= |E\left[\varphi(Z_{t_0,a,0}(T))Y_{t_0,a,1}(T)\right] - E\left[\varphi(Z_N)Y_N\right]| \qquad (5.20)\\ &= \left|\sum_{k=0}^{N-1}(Eu(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1}))Y_{t_k,X_k,Y_k}(t_{k+1}) - Eu(t_{k+1}, X_{k+1}, Z_{k+1})Y_{k+1})\right| \\ &= \left|\sum_{k=0}^{N-1} EY_k\left[u(t_{k+1}, X_{k+1}, Z_{t_k,X_k,Z_k}(t_{k+1}))Y_{t_k,X_k,1}(t_{k+1}) - u(t_{k+1}, X_{k+1}, Z_{k+1})Y_{t_k,X_k,1}(t_{k+1})\right]\right| \\ &\leq \sum_{k=0}^{N-1} R_k, \end{aligned}$$

where

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

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

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

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

the operators

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

$$L_1 = \frac{\partial}{\partial t} + \frac{b-x}{T-t}\nabla + \frac{1}{2}\sum_{i=1}^{d}\frac{\partial^2}{(\partial x^i)^2}, \quad L_2 = f(t,x)\frac{\partial}{\partial z},$$
$$L_3 = \alpha^\top(t,x)\frac{b-x}{T-t}y\frac{\partial}{\partial y} + \sum_{i=1}^{d}\alpha^i(t,x)y\frac{\partial^2}{\partial x^i \partial y} + \frac{1}{2}\alpha^2(t,x)y^2\frac{\partial^2}{\partial y^2}, \quad 0 \le t < T,$$

and the one-step error for $t \le T - 2h$:

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

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 $Y_{t,x,1}(t+h)$, which correspond to the method (5.11)-(5.13), (5.16).

The second term in (5.22) can be re-written 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 $E|\rho_1(t_k, X_k, Z_k)| \le Kh^2$ with a constant K independent of h and t.

Further, expanding the non-singular part of $\bar{Y}_{t,x,1}(t+h)$ (i.e. $\exp(-\frac{h}{2}\frac{T-t-h}{T-t}\alpha^2(t,x) + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\alpha^\top(t,x)\,\xi)$ and $v(X_{t,x}(t+h), z) = v(x + h\frac{b-x}{T-t} + \sqrt{h}\sqrt{\frac{T-t-h}{T-t}}\,\xi, z)$ and also $\frac{\partial}{\partial z}v(X_{t,x}(t+h), z)$ in powers of h, we obtain :

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

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

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

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

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

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

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

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 [20, Lemma 2.1.9, p. 99], we obtain

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

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

(5.24). Further, we have

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

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

Hence,

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

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

We recall [19, 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 $k = 0,\ldots,N-2$:[2]

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

where g^i and $g^{i,j}$ are the corresponding functions appearing in (5.26). Using arguments similar to those in [19, Lemma B.1], one can show that for $k = 0,\ldots,N-2$:

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

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

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

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

[2]If one were to use (5.19) instead of (5.13) then $R_k \leq Kh^2/(T-t_{k+1})$ (cf. Remark 5.1).

The Monte Carlo estimator for the path integral (5.3) based on the method (5.14), (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 ${}_mZ_N$, ${}_mQ_N$, $m = 1, \ldots, M$, are independent realizations of the corresponding random variables. Note that the second approximate equality in (5.27) is related to the statistical error.

Remark 5.2 *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 in the case of Brownian bridge. Further, the method* (5.11)-(5.13) *and Theorem 5.1 are easy to adapt to a slightly more general additive noise situation than* (5.1) *with the unit diffusion matrix – to conditioned diffusions with a constant 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 [11, 18] (and the references therein).*

6 Numerical examples

Example 1. We consider the square integral of the Brownian bridge which has applications in statistics. To test the proposed method, we compute moments of this integral; i.e., we deal with the functionals

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

The results of our simulation are presented in Table 1. The values before "±" 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 $p = 4$ [26]. The values after "±" 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.

Table 1: *Square integral of the Brownian bridge.* Errors in evaluating the conditional Wiener integral (1.1), (6.1) with $p = 1$ and $p = 4$ and various time steps h. 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}	$0.067 \times 10^{-3} \pm 0.001 \times 10^{-3}$	$-0.015 \times 10^{-3} \pm 0.002 \times 10^{-3}$

Example 2. Consider the correlation function $\Gamma(\theta)$, $0 \le \theta \le T$ (see (1.3)):

$$\Gamma(\theta) = < x(0)x(\theta) > \tag{6.2}$$
$$= \frac{1}{\mathcal{Z}(T)} \int_{-\infty}^{\infty} \int_{C_{0,y;T,y}} x(0)\ x(\theta) \exp\left(- \int_0^T V(t, x(t))\, dt \right) d\mu_{0,y}^{T,y}(x) dy = \frac{\int_{-\infty}^{\infty} y \mathcal{J}_1(y) dy}{\int_{-\infty}^{\infty} \mathcal{J}_2(y) dy},$$

where

$$\mathcal{J}_1(y) = \int_{C_{0,y;T,y}} x(\theta) \exp\left(- \int_0^T V(t, x(t))\, dt \right) d\mu_{0,y}^{T,y}(x), \tag{6.3}$$
$$\mathcal{J}_2(y) = \int_{C_{0,y;T,y}} \exp\left[- \int_0^T V(x(t))\, dt \right] d\mu_{0,y}^{T,y}(x). \tag{6.4}$$

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. [14, 16]) that T has the meaning of inverse temperature here. In the case of the harmonic potential (6.5), the correlation function is equal to [14, Chapter 3]:

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

We rewrite the integrals in (6.2) as

$$\mathcal{G} = \int_{-\infty}^{\infty} y \mathcal{J}_1(y) dy = \sqrt{2\pi\sigma_1^2} E\left[\eta_1 \mathcal{J}_1(\eta_1) \exp\left(\frac{\eta_1}{2\sigma_1^2} \right) \right], \tag{6.8}$$
$$\mathcal{Z} = \int_{-\infty}^{\infty} \mathcal{J}_2(y) dy = \sqrt{2\pi\sigma_2^2} E\left[\mathcal{J}_2(\eta_2) \exp\left(\frac{\eta_2}{2\sigma_2^2} \right) \right],$$

where η_1 and η_2 are Gaussian random variables, $\mathcal{N}(0, \sigma_1^2)$ 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

$$\hat{\mathcal{G}} = \frac{\sqrt{2\pi\sigma_1^2}}{M} \sum_{m=1}^{M} \left[{}_m\eta_1\ {}_m\bar{\mathcal{J}}_1(\eta_1) \exp\left(\frac{{}_m\eta_1}{2\sigma_1^2} \right) \right], \tag{6.9}$$
$$\hat{\mathcal{Z}} = \frac{\sqrt{2\pi\sigma_2^2}}{M} \sum_{m=1}^{M} \left[{}_m\bar{\mathcal{J}}_2({}_m\eta_2) \exp\left(\frac{{}_m\eta_2}{2\sigma_2^2} \right) \right],$$

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:

Figure 1: *Correlation function.* The dependence of the correlation function $\Gamma(\theta)$ from (6.2) on θ simulated with $h = 0.2$ and $M = 10^8$ for $T = 10$. The left figure corresponds to the harmonic potential (6.5) and the right figure to the anharmonic potential (6.6), both with $\omega = 1$.

${}_m\eta_2 = \sigma_2 \; {}_m\eta_1/\sigma_1$; ${}_m\bar{\mathcal{J}}_1({}_m\eta_1)$ 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 ${}_m\bar{\mathcal{J}}_1({}_m\eta_1)$, ${}_m\bar{\mathcal{J}}_2({}_m\eta_2)$ 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 on Fig. 1. The parameters σ_1 and σ_2 are taken 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) were 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, e.g., the data of Table 2 yields $C \doteq 0.015$, with the maximum absolute value of the residuals being equal to 3×10^{-5}.

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}	$1.46 \times 10^{-4} \pm 0.10 \times 10^{-4}$

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 the number of Monte Carlo runs $M = 10^{11}$.

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	$0.231 \times 10^{-4} \pm 0.080 \times 10^{-4}$

In Fig. 1 (left) the results of simulation of $\Gamma(\theta)$ with $h = 0.2$ are compared with the exact curve from (6.7). Thanks to the second-order of accuracy of the proposed numerical method, these curves visually coincide even for this relatively large time step. Figure 1 (right) demonstrates behavior of the correlation 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 1 and 2 the second-order method (2.11), (2.10) and the Euler method (2.14), (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), (2.10) in comparison with the Euler method (which is in general of order one – see Theorem 2.2) is clearly seen.

Example 3. Consider a system of r identical n-dimensional boson particles of mass m. The partition function for this system has the form [6]:

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

where T is 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

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

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

$$dX = \frac{\boldsymbol{\pi}x - X}{T-t}dt + \frac{1}{\sqrt{m}}dw(t),\ 0 \le t < T,\ X(0) = x. \tag{6.12}$$

The kinetic energy of the system of particles can be found as (see, e.g. [6, 1, 25]):

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

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

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

where

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

Here ∇V is an rn-dimensional vector. We note that this expression for the kinetic energy is different to the ones exploited in [1, 25]. As was pointed out in [1], 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

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

It is known (see, e.g. [25]) that in this case the kinetic energy is equal to

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

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

As with Example 2, correlated estimates of both the integral $\mathcal{K}$ and 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:

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

where η is an r-dimensional Gaussian random variable, of which the 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 in [25]). Let $U : \mathbb{R} \longrightarrow \mathbb{R}$ be such that $V(x) = \sum_{i=1}^{r} U(x_i)$ and let

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

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 $\mathcal{Z}$ were used in the simulation:

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

where ${}_m\eta$ are sampled independently from $\mathcal{N}(0, \sigma^2 \mathrm{I}_{r\times r})$,and ${}_m\overline{\mathcal{I}}_1$ and ${}_m\overline{\mathcal{I}}_2$ 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), (2.10), or the Euler method (2.14), (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 was 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.

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 $M = 10^9$.

h	Euler method	Method (2.11), (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	$0.057 \pm 0.71 \times 10^{-4}$	$0.035 \times 10^{-2} \pm 0.75 \times 10^{-4}$

We analyze two methods: the method (2.11), (2.10) and the Euler method (2.14), (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 was made relatively small in order to be able to analyze the bias. It is clearly seen from the data that the method (2.11), (2.10) converges with order two while the Euler method exhibits the first order convergence as expected (see Theorems 2.1 and 2.2).

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