QUASI-MONTE CARLO TIME-SPLITTING METHODS FOR SCHRÖDINGER EQUATION WITH GAUSSIAN RANDOM POTENTIAL

ZHIZHANG WU, ZHIWEN ZHANG*, AND XIAOFEI ZHAO

ABSTRACT. In this work, we consider the Schrödinger equation with a Gaussian random potential (SE-GP), and we aim to efficiently approximate the expectation of physical observables. The unboundedness of Gaussian random variables causes difficulties in sampling and error analysis. Under time-splitting discretizations of SE-GP, we establish the regularity of the semi-discrete solution in the random space. Then by means of a non-standard weighted Sobolev space associated with some properly chosen weight functions, we obtain a randomly shifted lattice-based quasi-Monte Carlo (QMC) quadrature rule for sampling, which forms a QMC time-splitting (QMC-TS) scheme for solving SE-GP. QMC-TS is proved to admit a dimension-independent and almost linear convergence rate with respect to the number of samples. Numerical experiments illustrate the sharpness of the error estimate.

Keywords: Schrödinger equation; Gaussian random potential; quasi-Monte Carlo (QMC) method; time splitting; error estimate; optimal rate.

AMS Subject Classification: 65C30; 65D32; 65M15; 82B44.

1. INTRODUCTION

The Schrödinger equation with a spatial random potential of the following form

$$i\partial_t\psi(t,\omega,x) = -\frac{1}{2}\partial_x^2\psi(t,\omega,x) + V(\omega,x)\psi(t,\omega,x), \tag{1.1}$$

plays an essential role for describing wave propagation in disorder media [10, 17, 40], where t is the time variable, x is the space variable, ω is a random sample, $\psi = \psi(t,\omega,x)$ is the unknown complex-valued wavefunction, and V is an external real-valued spatial random potential. It is also known as the continuous version of the original Anderson model [2] for the localization phenomenon and is mathematically of great interest [12, 13, 16, 22, 65]. In practice, the spatial random potential V could be uniformly distributed in a bounded interval [20] or be a Gaussian noise [10, 19]. In this work, we will be interested in the case that $V(\omega,x) = v_0(x) + V_r(\omega,x)$ with $v_0(x)$ a deterministic function and $V_{\mathrm{r}}(\omega,x)$ a zero-mean Gaussian random field, and we aim to provide an efficient numerical algorithm to solve (1.1) particularly addressing the sampling issue.

Although the standard Monte Carlo (MC) method is handy as used in most of the simulation work, e.g., [10, 20, 65], we get only a half-order convergence rate in the number of samples, and hence a large number of simulations are required for MC to accurately evaluate the statistical quantities. More efficient options for discretizing the random space include the quasi-Monte Carlo (QMC) methods [7, 15, 25, 35, 36, 59], stochastic Galerkin methods [9, 23, 30, 64], stochastic collocation methods [3, 46, 55], etc. Particularly for solving (1.1), [61] and [62] applied the stochastic Galerkin method and the stochastic collocation method, respectively, while due to the curse of dimensionality with respect to the number of samples [46, 51], only one-dimensional cases were considered. Then,

Corresponding author.

a QMC approach for (1.1) under uniformly distributed V has been considered in our previous work [63], where an almost linear convergence rate with dimension-independence is achieved. The analysis and the QMC quadrature rule proposed therein rely on the boundedness of V and would fail for a Gaussian random field. Thus, we continue in this work the development of QMC towards the Schrödinger model but with a Gaussian random potential.

In view of the Karhunen-Loève expansion [23, 33, 41], the Gaussian random potential in (1.1) admits the following parametric representation:

$$V(\omega,x)=V(\boldsymbol{\xi}(\omega),x)=v_0(x)+V_{\mathrm{r}}(\boldsymbol{\xi}(\omega),x),\ \text{ where } V_{\mathrm{r}}(\boldsymbol{\xi}(\omega),x)=\sum_{j=1}^{\infty}\lambda_j\xi_j(\omega)v_j(x), \tag{1.2}$$

with $\{v_j(x)\}_{j=1}^{\infty}$ the physical components, $\lambda_1\geq\lambda_2\geq\cdots>0$ the corresponding strengths, $\{\xi_j(\omega)\}_{j=1}^{\infty}$ the independent and identically distributed (i.i.d.) standard Gaussian random variables and $\boldsymbol{\xi}(\omega)=(\xi_1(\omega),\xi_2(\omega),\ldots)^{\top}\in\mathbb{R}^{\mathbb{N}}$ (see, e.g., [8, 25] for more details on the parametric representation of a Gaussian random field in the form of Karhunen-Loève expansion). The law of $\boldsymbol{\xi}$ is defined on the product probability space $(\mathbb{R}^{\mathbb{N}},\mathcal{B}(\mathbb{R}^{\mathbb{N}}),\boldsymbol{\mu}_{\infty})$, where $\mathcal{B}(\mathbb{R}^{\mathbb{N}})$ is the sigma-algebra generated by the cylinder sets, and $\boldsymbol{\mu}_{\infty}$ is the product Gaussian measure [6], i.e., $\boldsymbol{\mu}_{\infty}=\bigotimes_{j=1}^{\infty}\mathcal{N}(0,1)$. Then, by the Doob-Dynkin lemma [32], the solution ψ of (1.1) can be represented by a function parameterized by $\boldsymbol{\xi}$. Hence, we can consider the initial value problem of (1.1) in the parametric form as

$$\begin{cases}\mathrm{i}\partial_t\psi(t,\boldsymbol{\xi},x)=-\dfrac{1}{2}\partial_x^2\psi(t,\boldsymbol{\xi},x)+V(\boldsymbol{\xi},x)\psi(t,\boldsymbol{\xi},x), & x\in\mathbb{T},\ \boldsymbol{\xi}\in U:=\mathbb{R}^{\mathbb{N}},\ t>0,\\ \psi(t=0,\boldsymbol{\xi},x)=\psi_{\mathrm{in}}(x), & x\in\mathbb{T},\ \boldsymbol{\xi}\in U,\end{cases} \tag{1.3}$$

where ψ_{in} represents a prescribed (deterministic) initial wave and $\mathbb{T}$ is the one-dimensional torus (periodic boundary). The torus domain serves as a valid approximation of the whole space problem when the initial localized wave is yet to reach the boundary and the one-space-dimensional setup here is mainly for simplicity of illustration.

Our aim is still for a dimension-independent first-order QMC approximation of (1.3), since a random potential from reality can be rough, so the series in (1.2) decays very slowly. To achieve this goal, we choose to work under the framework of QMC with the randomly shifted lattice rule [14, 34, 38, 39, 45, 48, 52, 60], which has been successfully developed for serval random PDEs. In the case of bounded random variables, we find its application to elliptic equations [37], eigenvalue problems [24], optimal control [27, 28], Helmholtz equations [21, 26] and Schrödinger equations [63]. For the case of unbounded random variables, the relevant literature is quite limited: [25] pioneered the work for elliptic equations with Gaussian random coefficients. In fact, due to its unboundedness, the Gaussian random variable in (1.3) poses much greater challenges to approximations and analysis than the uniformly distributed random variable case considered in [63]. Although integration against unbounded random variables can be mapped into an integral over a unit cube using the inverse cumulative distribution function, the transformed integrand may not have square-integrable mixed first derivatives. Therefore, the QMC theory of standard weighted Sobolev spaces [15, 36] cannot be applied. Instead, it is crucial to find the proper decaying weight functions that can counteract the growth of the mixed first derivatives of the integrand and meanwhile lead to the desired convergence rate [38, 45]. In general, slower decay of weight functions (or equivalently slower growth of mixed first derivatives) results in faster convergence of QMC.

To this end, we first adopt the time-splitting scheme which is one of the most popular classes of methods [4, 31, 42] for time discretization of Schrödinger models. The resulting subflows are self-adjoint, which yields a polynomially-growing bound on the mixed first derivatives of the semi-discrete solution with respect to $\boldsymbol{\xi}$. Such bound leads to the favorable choice of weight functions. Then, by means of a non-standard weighted Sobolev space associated with the chosen weight functions, we derive the QMC quadrature rule that ends up as a class of QMC time-splitting schemes. Rigorous error estimates established the desired dimension-independent and almost first-order convergence rate of QMC with the optimal temporal error bound. The theoretical results are validated by numerical experiments.

The rest of the paper is organized as follows. In Section 2, we present the QMC time splitting (QMC-TS) scheme and the main result on its convergence. The derivation of the main result (i.e., the convergence analysis) is given in detail in Section 3. Finally, we show numerical results to verify the convergence rates of our numerical method in Section 4.

Notation. We will usually omit the variables $t, \boldsymbol{\xi}, x$ in the functions for notational brevity when there is no confusion caused. We denote by C a generic constant whose value may vary at each occurrence but is always independent of the truncation dimension m, the time step size τ, and the number of samples N. For any $1 \le q < \infty$ and any temporal-spatial function space W, we define the space $L^q_{\boldsymbol{\mu}_\infty}(U, W)$ equipped with the norm $\|\cdot\|_{L^q_{\boldsymbol{\mu}_\infty}(U,W)}$ such that for any $f(t, \boldsymbol{\xi}, x) \in L^q_{\boldsymbol{\mu}_\infty}(U, W)$, $f(\cdot, \boldsymbol{\xi}, \cdot) \in W$ for almost surely (a.s.) $\boldsymbol{\xi} \in U$ and $\|f\|_{L^q_{\boldsymbol{\mu}_\infty}(U,W)} := \left(\int_U (\|f(\boldsymbol{\xi})\|_W)^q \,\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi})\right)^{1/q} < \infty$.

2. Numerical method and main result

We present the QMC-TS scheme to evaluate the expectation of physical observable, which is typically in the form of $G(|\psi(t)|^2)$, where G is a linear functional and $|\psi|^2$ is the so-called position density (or probability density function).

2.1. Numerical method.

2.1.1. *Dimension truncation.* From the perspective of numerical computations, we will in practice work with the following truncated Schrödinger equation:

$$\begin{cases} \mathrm{i}\partial_t \psi_m(t, \boldsymbol{\xi}_m, x) = -\dfrac{1}{2}\partial_x^2 \psi_m(t, \boldsymbol{\xi}_m, x) + V_m(\boldsymbol{\xi}_m, x)\psi_m(t, \boldsymbol{\xi}_m, x), \quad x \in \mathbb{T}, \boldsymbol{\xi}_m \in \mathbb{R}^m, t > 0, \\ \psi_m(t = 0, \boldsymbol{\xi}_m, x) = \psi_{\mathrm{in}}(x), \quad x \in \mathbb{T}, \boldsymbol{\xi}_m \in \mathbb{R}^m, \end{cases} \tag{2.1}$$

where

$$V_m(\boldsymbol{\xi}_m, x) = v_0(x) + V_{\mathrm{r},m}(\boldsymbol{\xi}_m, x), \text{ with } V_{\mathrm{r},m}(\boldsymbol{\xi}_m, x) = \sum_{j=1}^{m} \lambda_j \xi_j(\omega) v_j(x), \tag{2.2}$$

and $\boldsymbol{\xi}_m = (\xi_1, \dots, \xi_m)^\top \in \mathbb{R}^m$. Note that any function of $\boldsymbol{\xi}_m \in \mathbb{R}^m$ can also be seen as a function of $\boldsymbol{\xi} \in U$. The first step of QMC-TS is to approximate $\mathbb{E}[G(|\psi(t)|^2)]$ by

$$\mathbb{E}[G(|\psi_m(t)|^2)] = \int_U G(|\psi_m(t, \boldsymbol{\xi})|^2)\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi}) = \int_{\mathbb{R}^m} G(|\psi_m(t, \boldsymbol{\xi}_m)|^2) \prod_{j=1}^{m} \phi(\xi_j)\mathrm{d}\boldsymbol{\xi}_m, \tag{2.3}$$

where $\phi(y) = \exp(-y^2/2)/\sqrt{2\pi}$ is the density function of the standard univariate Gaussian distribution.

2.1.2. *Time discretization.* For each fixed $\boldsymbol{\xi} \in U$, (2.1) becomes a deterministic equation, and the second step of QMC-TS lies in the time discretization for (2.1) using the time-splitting scheme. It begins by splitting (2.1) into two subflows Ψ_ρ^{p} and Ψ_ρ^{k} as

$$\Psi_\rho^{\mathrm{p}} : i\partial_t \psi_m = V_m \psi_m, \quad t \in (0, \rho], \tag{2.4a}$$

$$\Psi_\rho^{\mathrm{k}} : i\partial_t \psi_m = -\frac{1}{2}\partial_x^2 \psi_m, \quad t \in (0, \rho]. \tag{2.4b}$$

Note that the above two equations can be integrated exactly in time since V_m is real-valued. Let $\tau > 0$ be the time step size. In view of the Lie–Trotter product formula [58], we employ the following first-order Lie–Trotter splitting method:

$$\psi_m^{n+1} = \Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(\psi_m^n) = \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\mathrm{e}^{-\mathrm{i}\tau V_m}\psi_m^n, \quad n = 0, 1, \ldots, \tag{2.5}$$

where ψ_m^n is the approximation of $\psi_m(t_n)$, with $t_n = n\tau$ and $\psi_m^0 = \psi_{\mathrm{in}}$. The second step of QMC-TS is to approximate $\mathbb{E}[G(|\psi_m(t_n)|^2)]$ by

$$\mathbb{E}[G(|\psi_m^n|^2)] = \int_{\mathbb{R}^m} G(|\psi_m^n(\boldsymbol{\xi}_m)|^2) \prod_{j=1}^m \phi(\xi_j)\mathrm{d}\boldsymbol{\xi}_m. \tag{2.6}$$

Remark 2.1. Let $\psi_m^{n,*} = \Psi_\tau^{\mathrm{p}}(\psi_m^{n-1}) = \mathrm{e}^{-\mathrm{i}\tau V_m}\psi_m^{n-1}$ for $n \geq 1$. Then, $\psi_m^n = \Psi_\tau^{\mathrm{k}}(\psi_m^{n,*}) = \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\psi_m^{n,*}$, and $\psi_m^{n,*} = g_n(\tau)$, where g_n satisfies $g_n(0) = \psi_m^{n-1}$ and

$$\mathrm{i}\partial_t g_n = V_m g_n, \quad t \in (0, \tau]. \tag{2.7}$$

Remark 2.2. We can also use other high-order splitting schemes [57] of the general form

$$\psi_m^{n+1} = \prod_{j=1}^M \mathrm{e}^{\mathrm{i}\alpha_j\tau\partial_x^2/2}\mathrm{e}^{-\mathrm{i}\beta_j\tau V_m}\psi_m^n, \quad n = 0, 1, \ldots, \tag{2.8}$$

where $\alpha_j, \beta_j \in \mathbb{R}$. We devote the analysis to the Lie–Trotter splitting scheme (2.5) for simplicity of presentation, and we will elaborate more on high-order splitting schemes in Section 3.5.

2.1.3. *Quasi-Monte Carlo quadrature.* Let $\Phi(y) = \int_{-\infty}^y \phi(\rho)\mathrm{d}\rho$ be the cumulative distribution function of the standard univariate Gaussian distribution and Φ^{-1} be its inverse. Moreover, we define the vector inverse Gaussian cumulative distribution function $\boldsymbol{\Phi}_m^{-1}$ such that $\boldsymbol{\Phi}_m^{-1}(\boldsymbol{y})$ applies Φ^{-1} to $\boldsymbol{y} \in \mathbb{R}^m$ component-wise. Then, by change of variables $\boldsymbol{\xi}_m = \boldsymbol{\Phi}_m^{-1}(\boldsymbol{y})$, we have

$$\mathbb{E}[G(|\psi_m^n|^2)] = \int_{(0,1)^m} F(\boldsymbol{\Phi}_m^{-1}(\boldsymbol{y}))\mathrm{d}\boldsymbol{y}, \tag{2.9}$$

where $F(\cdot) = G(|\psi_m^n(\cdot)|^2)$. The last step of QMC-TS is to approximate (2.9) by the QMC quadrature

$$Q_{m,N}(F; \boldsymbol{\Delta}) = \frac{1}{N}\sum_{j=1}^N F\left(\boldsymbol{\xi}_m^{(j)}\right), \tag{2.10}$$

where $\{\boldsymbol{\xi}_m^{(j)}\}_{j=1}^N$ are the quadrature points with N the number of samples. In particular, we adopt the randomly shifted (rank-1) lattice rule [38, 45], which generates the quadrature points as

$$\boldsymbol{\xi}_m^{(j)} = \boldsymbol{\Phi}_m^{-1}\left(\mathrm{frac}\left(\frac{j\boldsymbol{z}}{N} + \boldsymbol{\Delta}\right)\right), \quad j = 1, \ldots, N, \tag{2.11}$$

where $\boldsymbol{\Delta} \in [0,1]^m$ is a random shift uniformly distributed over $[0,1]^m$, $\mathrm{frac}(\boldsymbol{y})$ takes the fractional part of $\boldsymbol{y} \in \mathbb{R}^m$ component-wise, and $\boldsymbol{z} \in \mathbb{N}^m$ is known as the generating vector. A specific

Algorithm 1 Quasi-Monte Carlo time-splitting method

Input: truncation dimension m, time step size τ, number of samples N, number of random shifts R.

Construct the generating vector $\boldsymbol{z}$ by the CBC algorithm.

Generate i.i.d. random shifts $\boldsymbol{\Delta}_1, \ldots, \boldsymbol{\Delta}_R$ from the uniform distribution on $[0,1]^m$. For each $k = 1, \ldots, R$, obtain the sample set $\{\boldsymbol{\xi}_m^{(k,j)} = \boldsymbol{\Phi}_m^{-1}\left(\text{frac}\left(\frac{j\boldsymbol{z}}{N} + \boldsymbol{\Delta}_k\right)\right) : j = 1, \ldots, N\}$.

for k = 1:R **do**

  for j = 1:N **do**

    Solve the Schrödinger equation (2.1) via Lie–Trotter splitting (2.5) or other high-order splitting schemes for each $\boldsymbol{\xi}_m^{(k,j)}$ and $n \in \mathbb{N}$, and obtain $\psi_m^n(\boldsymbol{\xi}_m^{(k,j)})$.

  end for

end for

The approximation of the expectation of the physical observable $\mathbb{E}[G(|\psi(t_n, \boldsymbol{\xi}, \cdot)|^2)]$ is given by

$$\overline{Q}_{m,N,R}(G(|\psi_m^n|^2)) = \frac{1}{R}\sum_{k=1}^{R} Q_{m,N}(G(|\psi_m^n|^2); \boldsymbol{\Delta}_k) = \frac{1}{RN}\sum_{k=1}^{R}\sum_{j=1}^{N} G(|\psi_m^n(\boldsymbol{\xi}_m^{(k,j)})|^2). \tag{2.12}$$

Output: $\overline{Q}_{m,N,R}(G(|\psi_m^n|^2))$.

generating vector $\boldsymbol{z}$ for the particular PDE problem can be constructed efficiently by the component-by-component (CBC) algorithm [45]. We will elaborate more on the generating vector $\boldsymbol{z}$ in Section 3.4.

Combining the above three steps, the QMC-TS method is summarized in Algorithm 1.

2.2. **Main result.** Let $s \geq 1$ be fixed. We make the following assumptions to guarantee the convergence of the QMC-TS method.

Assumption 2.1. Assume that $\psi_{\text{in}}, v_0 \in H^s(\mathbb{T})$, $v_j \in H^s(\mathbb{T}) \bigcap W^{1,\infty}(\mathbb{T})$ for $j \in \mathbb{N}^+$, and the linear functional $G \in (H^1(\mathbb{T}))'$, which is the dual space of $H^1(\mathbb{T})$.

Assumption 2.2. Let $a_j = \lambda_j \|v_j\|_{H^s(\mathbb{T})}$ and $b_j = \lambda_j \|v_j\|_{W^{1,\infty}(\mathbb{T})}$ for $j \in \mathbb{N}^+$. Assume that

$$\sum_{j=1}^{\infty} a_j < \infty, \text{ and } \sum_{j=1}^{\infty} b_j^p < \infty, \text{ for some } p \in (0,1].$$

Assumption 2.3. Assume that for some constants $C, \varepsilon, \chi > 0$ independent of m

$$\|V_m - V\|_{L^{2+\varepsilon}_{\boldsymbol{\mu}_\infty}(U, H^1(\mathbb{T}))} \leq Cm^{-\chi}.$$

Remark 2.3. If $v_j \in H^s(\mathbb{T})$ with $s > \frac{3}{2}$, we immediately have $v_j \in W^{1,\infty}(\mathbb{T})$ by Sobolev embedding [1, Chapter 4].

Now we are ready to present the main result of this paper.

Theorem 2.4. *Let Assumptions 2.1–2.3 hold with $s \geq 3$, and we additionally assume* (3.31) *if Assumption 2.2 holds with $p = 1$. If the Lie–Trotter splitting* (2.5) *is used in the QMC-TS method, then there exists a randomly shifted lattice rule* (2.10) *that can be constructed by the CBC algorithm for any fixed T such that the numerical solution ψ_m^n given by the QMC-TS method for $N \leq 10^{30}$*

satisfies the following error estimate:

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[\left|\mathbb{E}[G(|\psi(t_n)|^2)]-Q_{m,N}(G(|\psi_m^n|^2);\boldsymbol{\Delta})\right|^2\right]}\leq C(m^{-\chi}+\tau+N^{-\kappa}), \tag{2.13}$$

for all $t_n=n\tau\in[0,T]$ *and some constant* $C>0$ *independent of* m,τ,N*, where* $\mathbb{E}^{\boldsymbol{\Delta}}$ *denotes the expectation with respect to the random shift* $\boldsymbol{\Delta}$*, and* $\kappa=1/p-1/2$ *for* $p\in(2/3,1]$ *and* $\kappa=1-\delta$ *for* $p\in(0,2/3]$ *with* $\delta>0$ *arbitrarily small.*

3. Convergence analysis

3.1. **Preliminaries.** We need some preliminary results for the proof of our main result. We will frequently use the algebraic property of $H^r(\mathbb{T})$ for $r>1/2$ [1, Chapter 4], which reads that for any $f,g\in H^r(\mathbb{T})$

$$\|fg\|_{H^r(\mathbb{T})}\leq C\|f\|_{H^r(\mathbb{T})}\|g\|_{H^r(\mathbb{T})}, \tag{3.1}$$

where the constant C depends on r. Define the set $U_a:=\{\boldsymbol{\xi}\in\mathbb{R}^{\mathbb{N}}:\sum_{j=1}^{\infty}a_j|\xi_j|<\infty\}$. Then, a minor modification of [49, Lemma 2.28] gives the following lemma.

Lemma 3.1. *Under Assumptions 2.1–2.2, we have* $U_a\in\mathcal{B}(\mathbb{R}^{\mathbb{N}})$ *and* $\boldsymbol{\mu}_\infty(U_a)=1$*.*

We also have the following lemma on the properties of the Gaussian random potentials.

Lemma 3.2. *Let Assumptions 2.1–2.3 hold. Then, for any* $q\geq 1$ *and* $m\in\mathbb{N}^+$*, we have* $V_m\in L^q_{\boldsymbol{\mu}_\infty}(U,H^s(\mathbb{T}))$*, and* $\|V_m\|_{L^q_{\boldsymbol{\mu}_\infty}(U,H^s(\mathbb{T}))}$ *can be bounded uniformly in* m*. Moreover, for* $1\leq q\leq 2+\varepsilon$*, we have* $\lim_{m\to\infty}\|V_m-V\|_{L^q_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))}=0$ *and* $V\in L^q_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))$*.*

Proof. Fix any $m\in\mathbb{N}^+$. It is easy to see that $V_m(\boldsymbol{\xi},\cdot)\in H^s(\mathbb{T})$ for any $\boldsymbol{\xi}\in U_a$, and hence $V_m(\boldsymbol{\xi},\cdot)\in H^s(\mathbb{T})$ a.s. in U by Lemma 3.1. Then, for any $q\geq 1$, we have by Assumption 2.2

$$\|V_m\|_{L^q_{\boldsymbol{\mu}_\infty}(U,H^s(\mathbb{T}))}\leq\|v_0\|_{H^s(\mathbb{T})}+\left(\int_{\mathbb{R}}\rho^q\phi(\rho)\mathrm{d}\rho\right)^{\frac{1}{q}}\sum_{j=1}^{\infty}a_j:=C_q<\infty,$$

where C_q is independent of m. Hence, $V_m\in L^q_{\boldsymbol{\mu}_\infty}(U,H^s(\mathbb{T}))$.

On the other hand, for any $\boldsymbol{\xi}\in U_a$, we have $V_m(\boldsymbol{\xi},\cdot)\to V(\boldsymbol{\xi},\cdot)$ in $H^1(\mathbb{T})$ as $m\to\infty$, and hence $V(\boldsymbol{\xi},\cdot)\in H^1(\mathbb{T})$. By Lemma 3.1, we have $V(\boldsymbol{\xi},\cdot)\in H^1(\mathbb{T})$ a.s. in U. Moreover, for any $1\leq q\leq 2+\varepsilon$, Assumption 2.3 gives $\lim_{m\to\infty}\|V_m-V\|_{L^q_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))}=0$, and hence $V\in L^q_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))$. ◻

In view of Lemmas 3.1–3.2, we can define the solution to (1.3) for a.s. $\boldsymbol{\xi}\in U$ by the Duhamel's formula, which reads

$$\psi(t,\boldsymbol{\xi},x)=\mathrm{e}^{\mathrm{i}t\partial_x^2/2}\psi_{\mathrm{in}}(x)-\mathrm{i}\int_0^t\mathrm{e}^{\mathrm{i}(t-\rho)\partial_x^2/2}V(\boldsymbol{\xi},x)\psi(\rho,\boldsymbol{\xi},x)\mathrm{d}\rho,\quad t\geq 0. \tag{3.2}$$

We will also use the following results.

Lemma 3.3. *Let Assumptions 2.1–2.3 hold. Then, we have* $\exp(K\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})})\in L^q_{\boldsymbol{\mu}_\infty}(U)$ *for any* $K>0$ *and* $q\geq 1$*.*

Proof. Lemma 3.2 indicates that $V_{\mathrm{r}}(\boldsymbol{\xi},x)$ is an $H^1(\mathbb{T})$-valued centered Gaussian random variable, and $H^1(\mathbb{T})$ is a separable Hilbert space. Then, by Fernique's theorem [11, 18] (see also [8, Theorem 2.2]), there exists a constant $\beta>0$ such that $\int_U \exp\left(\beta\|V_{\mathrm{r}}(\boldsymbol{\xi})\|^2_{H^1(\mathbb{T})}\right)\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi})<\infty$. Then, we have by Young's inequality that

$$\int_U \exp(qK\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})})\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi})\le C_{K,q},$$

where $C_{K,q}=\exp\left(qK\|v_0\|_{H^1(\mathbb{T})}+q^2K^2/(4\beta)\right)\int_U\exp\left(\beta\|V_{\mathrm{r}}(\boldsymbol{\xi})\|^2_{H^1(\mathbb{T})}\right)\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi})<\infty$. Hence, for any $K>0$ and $q\ge1$, we have $\exp(K\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})})\in L^q_{\boldsymbol{\mu}_\infty}(U)$. □

Lemma 3.4. *Let Assumptions 2.1–2.2 hold. Then, for any $K>0$ and $q\ge1$, it holds that $\exp(K\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})})\in L^q_{\boldsymbol{\mu}_\infty}(U)$, and $\|\exp(K\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})})\|_{L^q_{\boldsymbol{\mu}_\infty}(U)}$ can be bounded uniformly in m.*

Proof. We have from the proof of [25, Theorem 16] that for any $C\ge0$

$$\int_{\mathbb{R}}\exp(C|\xi|)\phi(\xi)\mathrm{d}\xi=2\exp\left(\frac{C^2}{2}\right)\Phi(C),\quad \Phi(C)\le\frac12\exp\left(\frac{2C}{\sqrt{2\pi}}\right). \tag{3.3}$$

Then,

$$\begin{aligned}\int_U\exp(qK\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})})\mathrm{d}\boldsymbol{\mu}_\infty(\boldsymbol{\xi})\le&\exp(qK\|v_0\|_{H^s(\mathbb{T})})\prod_{j=1}^m\int_{\mathbb{R}}\exp(qKa_j|\xi_j|)\phi(\xi_j)\mathrm{d}\xi_j\\ \le&\exp\left(qK\|v_0\|_{H^s(\mathbb{T})}+\frac{2qK}{\sqrt{2\pi}}\sum_{j=1}^\infty a_j+\frac{q^2K^2}{2}\sum_{j=1}^\infty a_j^2\right),\end{aligned}$$

where the upper bound on the right-hand side is finite due to Assumption 2.2 and is independent of m. Hence, we have $\exp(K\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})})\in L^q_{\boldsymbol{\mu}_\infty}(U)$. □

3.2. **Dimension truncation error.** We first need the regularity of the solution in the physical domain.

Lemma 3.5. *Let Assumptions 2.1–2.3 hold. Then, for any $T>0$ and $\boldsymbol{\xi}\in U_a$, we have*

$$\|\psi(t,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\le\|\psi_{\mathrm{in}}\|_{H^1(\mathbb{T})}\exp\left(CT\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\right),\quad 0\le t\le T, \tag{3.4}$$

where C comes from the algebraic property of $H^1(\mathbb{T})$. Moreover, for any $1\le q<\infty$, we have $\psi\in L^q_{\boldsymbol{\mu}_\infty}(U,L^\infty((0,T),H^1(\mathbb{T})))$.

Proof. Fix any $T>0$ and $\boldsymbol{\xi}\in U_a$. By the algebraic property of $H^1(\mathbb{T})$ (see (3.1)) and the fact that $\mathrm{e}^{\mathrm{i}t\partial_x^2/2}$ is an isometry on $H^1(\mathbb{T})$ for all $t\in\mathbb{R}$, we take the H^1-norm on both sides of (3.2) and obtain

$$\|\psi(t,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\le\|\psi_{\mathrm{in}}\|_{H^1(\mathbb{T})}+C\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\int_0^t\|\psi(\rho,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\mathrm{d}\rho. \tag{3.5}$$

Then, a bootstrap-type argument [56] will give the local well-posedness of (1.3) in $H^1(\mathbb{T})$ for $\boldsymbol{\xi}$ (see also [63, Appendix A] for details of the bootstrap-type argument). Moreover, by Gronwall's inequality, we can deduce (3.4) from (3.5). In addition, by Lemma 3.3, we have $\psi\in L^q_{\boldsymbol{\mu}_\infty}(U,L^\infty((0,T),H^1(\mathbb{T})))$ for any $1\le q<\infty$. □

Lemma 3.6. *Let Assumptions 2.1–2.2 hold. Then, for any $T>0$ and $\boldsymbol{\xi}\in U_a$, we have*

$$\|\psi_m(t,\boldsymbol{\xi})\|_{H^s(\mathbb{T})}\le\|\psi_{\mathrm{in}}\|_{H^s(\mathbb{T})}\exp\left(CT\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})}\right),\quad 0\le t\le T,\tag{3.6}$$

where C comes from the algebraic property of $H^s(\mathbb{T})$. Moreover, for any $1\le q<\infty$, we have $\psi_m\in L^q_{\boldsymbol{\mu}_\infty}(U,L^\infty((0,T),H^s(\mathbb{T})))$, and $\|\psi_m\|_{L^q_{\boldsymbol{\mu}_\infty}(U,L^\infty((0,T),H^s(\mathbb{T})))}$ can be bounded uniformly in m.

Proof. The proof uses Lemma 3.4 and is similar to that of Lemma 3.5, so we omit it here. □

Now we give the dimension truncation error of the solution and the expectation of the physical observable.

Lemma 3.7. *Under Assumptions 2.1–2.3, we have for any $T>0$*

$$\|\psi_m-\psi\|_{L^2_{\boldsymbol{\mu}_\infty}(U,L^\infty((0,T),H^1(\mathbb{T})))}\le Cm^{-\chi},\tag{3.7}$$

where C is independent of m.

Proof. Let $\delta\psi=\psi_m-\psi$. Taking the difference between (1.3) and (2.1), we have

$$\begin{cases}\mathrm{i}\partial_t\delta\psi=-\dfrac{1}{2}\partial_x^2\delta\psi+V\delta\psi+(V_m-V)\psi_m, & x\in\mathbb{T},\boldsymbol{\xi}\in U,t>0,\\ \delta\psi(t=0)=0, & x\in\mathbb{T}.\end{cases}$$

For any $\boldsymbol{\xi}\in U_a$, the Duhamel formula gives

$$\delta\psi(t,\boldsymbol{\xi})=-\mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}(t-\rho)\partial_x^2/2}\left(V(\boldsymbol{\xi})\delta\psi(\rho,\boldsymbol{\xi})+(V_m(\boldsymbol{\xi})-V(\boldsymbol{\xi}))\psi_m(\rho,\boldsymbol{\xi})\right)\mathrm{d}\rho,\quad 0\le t\le T,$$

which by the algebraic property of $H^1(\mathbb{T})$ gives

$$\begin{aligned}\|\delta\psi(t,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\le& C\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\int_0^t\|\delta\psi(\rho,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\mathrm{d}\rho\\ &+Ct\|\psi_m(\boldsymbol{\xi})\|_{L^\infty((0,T),H^1(\mathbb{T}))}\|V_m(\boldsymbol{\xi})-V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})},\quad 0\le t\le T.\end{aligned}$$

By Gronwall's inequality, we have for any $0\le t\le T$ and $\boldsymbol{\xi}\in U_a$

$$\|\delta\psi(t,\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\le CT\|\psi_m(\boldsymbol{\xi})\|_{L^\infty((0,T),H^1(\mathbb{T}))}\|V_m(\boldsymbol{\xi})-V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\exp\left(CT\|V(\boldsymbol{\xi})\|_{H^1(\mathbb{T})}\right).\tag{3.8}$$

Then, (3.8) gives (3.7) by Lemmas 3.3 and 3.6, Assumption 2.3 and Hölder's inequality. □

Lemma 3.8. *Under Assumptions 2.1–2.3, we have for any $T>0$*

$$|\mathbb{E}[G(|\psi(t)|^2)]-\mathbb{E}[G(|\psi_m(t)|^2)]|\le Cm^{-\chi},\quad 0\le t\le T,\tag{3.9}$$

where C is independent of m.

Proof. We have $\||\psi(t)|^2-|\psi_m(t)|^2\|_{H^1(\mathbb{T})}\le C\|\psi(t)+\psi_m(t)\|_{H^1(\mathbb{T})}\|\psi(t)-\psi_m(t)\|_{H^1(\mathbb{T})}$ by the algebraic property of $H^1(\mathbb{T})$. Then,

$$\begin{aligned}|\mathbb{E}[G(|\psi(t)|^2)]-\mathbb{E}[G(|\psi_m(t)|^2)]|\le&\mathbb{E}[|G(|\psi(t)|^2-|\psi_m(t)|^2)|]\\ \le&\|G\|_{H^1(\mathbb{T})'}\mathbb{E}[\||\psi(t)|^2-|\psi_m(t)|^2\|_{H^1(\mathbb{T})}]\\ \le&C\|G\|_{H^1(\mathbb{T})'}\mathbb{E}[\|\psi(t)+\psi_m(t)\|_{H^1(\mathbb{T})}\|\psi(t)-\psi_m(t)\|_{H^1(\mathbb{T})}]\\ \le&C\|G\|_{H^1(\mathbb{T})'}\left(\|\psi(t)\|_{L^2_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))}+\|\psi_m(t)\|_{L^2_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))}\right)\\ &\times\|\psi(t)-\psi_m(t)\|_{L^2_{\boldsymbol{\mu}_\infty}(U,H^1(\mathbb{T}))},\end{aligned}$$

where we have used the Cauchy-Schwarz inequality in the last inequality. The above equation gives (3.9) by Lemmas 3.5–3.7. □

3.3. **Temporal error.** We first give two lemmas on the regularity of $\partial_t \psi_m$ and the semi-discrete solution ψ_m^n in the physical domain, respectively.

Lemma 3.9. *Let Assumptions 2.1–2.2 hold with $s \geq 3$. Then, for any $T > 0$ and $\boldsymbol{\xi} \in U_a$,*

$$\|\partial_t \psi_m(t, \boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})} \leq (\|\psi_{\rm in}\|_{H^s(\mathbb{T})} + C\psi_{\rm in}\|_{H^{s-2}(\mathbb{T})}\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\|) \exp\left(CT\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\right) \tag{3.10}$$

where $0 \leq t \leq T$ and C comes from the algebraic property of $H^{s-2}(\mathbb{T})$. Moreover, for any $1 \leq q < \infty$, we have $\partial_t \psi_m \in L^q_{\boldsymbol{\mu}_\infty}(U, L^\infty((0,T), H^{s-2}(\mathbb{T})))$ and $\|\partial_t \psi_m\|_{L^q_{\boldsymbol{\mu}_\infty}(U, L^\infty((0,T), H^{s-2}(\mathbb{T})))}$ can be bounded uniformly in m.

Proof. Fix any $T > 0$ and $\boldsymbol{\xi} \in U_a$. We take the partial derivative of both sides of (2.1) with respect to t and obtain

$$\mathrm{i}\partial_t \partial_t \psi_m = -\frac{1}{2}\partial_x^2 \partial_t \psi_m + V_m \partial_t \psi_m,$$

and hence the Duhamel's formula gives

$$\partial_t \psi_m(t, \boldsymbol{\xi}, x) = \mathrm{e}^{\mathrm{i}t\partial_x^2/2}\partial_t \psi_m(0, \boldsymbol{\xi}, x) - \mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}(t-\rho)\partial_x^2/2} V_m(\boldsymbol{\xi}, x)\partial_t \psi_m(\rho, \boldsymbol{\xi}, x)\mathrm{d}\rho, \quad 0 \leq t \leq T.$$

We take the H^{s-2}-norm on both sides of the above equation, and similar arguments to those in the proof of Lemma 3.5 give

$$\|\partial_t \psi_m(t, \boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})} \leq \|\partial_t \psi_m(0, \boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})} \exp\left(CT\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\right), \quad 0 \leq t \leq T, \tag{3.11}$$

where C comes from the algebraic property of $H^{s-2}(\mathbb{T})$. Note that

$$\partial_t \psi_m(0, \boldsymbol{\xi}, x) = \frac{1}{2}\mathrm{i}\partial_x^2 \psi_{\rm in}(x) - \mathrm{i}V_m(\boldsymbol{\xi}, x)\psi_{\rm in}(x). \tag{3.12}$$

We can obtain (3.10) by combining (3.11)–(3.12). Moreover, for any $1 \leq q < \infty$, we have $\partial_t \psi_m \in L^q_{\boldsymbol{\mu}_\infty}(U, L^\infty((0,T), H^{s-2}(\mathbb{T})))$ and $\|\partial_t \psi_m\|_{L^q_{\boldsymbol{\mu}_\infty}(U, L^\infty((0,T), H^{s-2}(\mathbb{T})))}$ can be bounded uniformly in m, by Lemmas 3.2 and 3.4 and Hölder's inequality. ☐

Lemma 3.10. *Let Assumptions 2.1–2.2 hold. Then, for any $0 < \tau \leq T$ and $\boldsymbol{\xi} \in U_a$,*

$$\|\psi_m^n(\boldsymbol{\xi})\|_{H^s(\mathbb{T})} \leq \|\psi_{\rm in}\|_{H^s(\mathbb{T})} \exp(CT\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})}), \quad 0 \leq n \leq \lfloor T/\tau \rfloor, \tag{3.13}$$

where C comes from the algebraic property of $H^s(\mathbb{T})$. Moreover, for any $1 \leq q < \infty$ and $0 \leq n \leq \lfloor T/\tau \rfloor$, we have $\psi_m^n \in L^q_{\boldsymbol{\mu}_\infty}(U, H^s(\mathbb{T}))$ and $\|\psi_m^n\|_{L^q_{\boldsymbol{\mu}_\infty}(U, H^s(\mathbb{T}))}$ can be bounded uniformly in m and n.

Proof. Fix $T > 0$ and $\boldsymbol{\xi} \in U_a$. Recall $\psi_m^{n,*}$ defined in Remark 2.1. Since $\mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}$ is a linear isometry on $H^s(\mathbb{T})$, we have $\|\psi_m^n\|_{H^s(\mathbb{T})} = \|\psi_m^{n,*}\|_{H^s(\mathbb{T})}$. Furthermore, we consider g_n introduced in Remark 2.1. Taking the $H^s(\mathbb{T})$-norm on both sides of (2.7), we have by the algebraic property of $H^s(\mathbb{T})$ and the Gronwall's inequaliy that $\|g(\tau)\|_{H^s(\mathbb{T})} \leq \|g(0)\|_{H^s(\mathbb{T})} \exp(C\tau\|V_m\|_{H^s(\mathbb{T})})$, i.e.,

$$\|\psi_m^n(\boldsymbol{\xi})\|_{H^s(\mathbb{T})} = \|\psi_m^{n,*}(\boldsymbol{\xi})\|_{H^s(\mathbb{T})} \leq \|\psi_m^{n-1}(\boldsymbol{\xi})\|_{H^s(\mathbb{T})} \exp(C\tau\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})}), \tag{3.14}$$

where C comes from the algebraic property of $H^s(\mathbb{T})$. We have (3.13) by iterating (3.14) from n to 1. Moreover, for any $1 \leq q < \infty$ and $0 \leq n \leq \lfloor T/\tau \rfloor$, we have $\psi_m^n \in L^q_{\boldsymbol{\mu}_\infty}(U, H^s(\mathbb{T}))$ and $\|\psi_m^n\|_{L^q_{\boldsymbol{\mu}_\infty}(U, H^s(\mathbb{T}))}$ can be bounded independently of m and n, by Lemma 3.4. ☐

Now we can give the temporal error of the solution and the expectation of the physical observable.

Lemma 3.11. *Let Assumptions 2.1–2.2 hold with $s \geq 3$. Then, for any $0 < \tau \leq T$,*

$$\|\psi_m(t_n) - \psi_m^n\|_{L^2_{\boldsymbol{\mu}_\infty}(U, H^{s-2}(\mathbb{T}))} \leq C\tau, \quad 0 \leq t_n = n\tau \leq T, \tag{3.15}$$

where C is independent of m and τ.

Proof. The proof largely follows the analysis in [54, Section 3] for the Lie–Trotter splitting. For any $f, g \in H^{s-2}(\mathbb{T})$, we have

$$\|\Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(f) - \Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(g)\|_{H^{s-2}(\mathbb{T})} = \|\Psi_\tau^{\mathrm{p}}(f) - \Psi_\tau^{\mathrm{p}}(g)\|_{H^{s-2}(\mathbb{T})},$$

since $\mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}$ is an isometry on $H^{s-2}(\mathbb{T})$. Let $\widetilde{f}(t) = \Psi_t^{\mathrm{p}}(f)$ and $\widetilde{g}(t) = \Psi_t^{\mathrm{p}}(g)$. Then, by the Duhamel's formula and the algebraic property of $H^{s-2}(\mathbb{T})$, we have for $0 \leq t \leq \tau$

$$\|\widetilde{f}(t) - \widetilde{g}(t)\|_{H^{s-2}(\mathbb{T})} \leq \|f - g\|_{H^{s-2}(\mathbb{T})} + C\int_0^t \|V\|_{H^{s-2}(\mathbb{T})}\|\widetilde{f}(\rho) - \widetilde{g}(\rho)\|_{H^{s-2}(\mathbb{T})}\mathrm{d}\rho.$$

By Gronwall's inequality, we have

$$\|\Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(f) - \Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(g)\|_{H^{s-2}(\mathbb{T})} = \|\widetilde{f}(\tau) - \widetilde{g}(\tau)\|_{H^{s-2}(\mathbb{T})} \leq \mathrm{e}^{C\tau\|V\|_{H^{s-2}(\mathbb{T})}}\|f - g\|_{H^{s-2}(\mathbb{T})}.$$

On the other hand, by Taylor expansion, we have

$$\begin{aligned}\Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(\psi_m(t_{n-1})) =& \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\mathrm{e}^{-\mathrm{i}\tau V_m}\psi_m(t_{n-1}) \\ =& \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\left(1 - \mathrm{i}\tau V_m - \tau^2 V_m^2\int_0^1 (1-\theta)\mathrm{e}^{-\mathrm{i}\theta\tau V_m}\mathrm{d}\theta\right)\psi_m(t_{n-1}).\end{aligned}$$

Moreover, the Duhamel's formular gives

$$\begin{aligned}\psi_m(t_n) =& \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\psi_m(t_{n-1}) - \mathrm{i}\int_0^\tau \mathrm{e}^{\mathrm{i}(\tau-\rho)\partial_x^2/2}V_m\psi_m(t_{n-1}+\rho)\mathrm{d}\rho \\ =& \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\psi_m(t_{n-1}) - \mathrm{i}\tau\mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}V_m\psi_m(t_{n-1}) \\ &- \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\int_0^\tau\int_0^1 \mathrm{e}^{-\mathrm{i}\theta\rho\partial_x^2/2}\mathrm{d}\theta(\rho\partial_x^2/2)[V_m\psi_m(t_{n-1}+\rho)]\mathrm{d}\rho \\ &- \mathrm{i}\mathrm{e}^{\mathrm{i}\tau\partial_x^2/2}\int_0^\tau V_m(\psi_m(t_{n-1}+\rho) - \psi_m(t_{n-1}))\mathrm{d}\rho.\end{aligned}$$

Then, the local error reads

$$\begin{aligned}&\|\psi_m(t_n,\boldsymbol{\xi}) - \Psi_\tau^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}}(\psi_m(t_{n-1},\boldsymbol{\xi}),\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})} \\ &\quad\leq C\tau^2\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}^2\|\psi_m(t_{n-1},\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\sup_{0\leq\theta\leq1}\|\mathrm{e}^{-\mathrm{i}\theta\tau V_m(\boldsymbol{\xi})}\|_{H^{s-2}(\mathbb{T})} \\ &\qquad + C\tau^2\sup_{0\leq\rho\leq\tau}\|\psi_m(t_{n-1}+\rho,\boldsymbol{\xi})\|_{H^s(\mathbb{T})}\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})} \\ &\qquad + C\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\int_0^\tau \|\psi_m(t_{n-1}+\rho,\boldsymbol{\xi}) - \psi_m(t_{n-1},\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\mathrm{d}\rho.\end{aligned}$$

The Faà di Bruno's formula (see, e.g., [29]) gives

$$\begin{aligned}
&\sup_{0\le\theta\le 1}\|\mathrm{e}^{-\mathrm{i}\theta\tau V_m(\boldsymbol{\xi})}\|_{H^{s-2}(\mathbb{T})}\\
&\le \sup_{0\le\theta\le 1} C(1+\sum_{j=1}^{s-2}\|\partial_x^j \mathrm{e}^{-\mathrm{i}\theta\tau V_m(\boldsymbol{\xi})}\|_{L^2(\mathbb{T})})\\
&\le \sup_{0\le\theta\le 1} C\left(1+\sum_{j=1}^{s-2}\sum_{k=1}^{j}\|B_{j,k}(-\mathrm{i}\theta\tau\partial_x V_m(\boldsymbol{\xi}), -\mathrm{i}\theta\tau\partial_x^2 V_m(\boldsymbol{\xi}),\dots,-\mathrm{i}\theta\tau\partial_x^{j-k+1}V_m(\boldsymbol{\xi}))\|_{L^2(\mathbb{T})}\right)\\
&:= K_1(\boldsymbol{\xi}),
\end{aligned}$$

where $\{B_{j,k}\}_{k=1}^{j}$, $j=1,\dots,s-2$, are the Bell polynomials [5], and by Lemma 3.2 $K_1(\boldsymbol{\xi})\in L^q_{\boldsymbol{\mu}_\infty}(U)$ and $\|K_1\|_{L^q_{\boldsymbol{\mu}_\infty}(U)}$ can be bounded uniformly in m and τ for any $1\le q<\infty$. Some additional calculations give

$$\begin{aligned}
\int_0^\tau \|\psi_m(t_{n-1}+\rho)-\psi_m(t_{n-1})\|_{H^{s-2}(\mathbb{T})} =& \int_0^\tau \left\|\int_0^\rho \partial_t\psi_m(t_{n-1}+y)\mathrm{d}y\right\|_{H^{s-2}(\mathbb{T})}\mathrm{d}\rho\\
\le& \tau^2\sup_{0\le\rho\le\tau}\|\partial_t\psi_m(t_{n-1}+\rho)\|_{H^{s-2}(\mathbb{T})}.
\end{aligned}$$

Therefore, we have

$$\|\psi_m(t_n,\boldsymbol{\xi})-\Psi_\tau^{\mathrm{k}}\circ\Psi_\tau^{\mathrm{p}}(\psi_m(t_{n-1},\boldsymbol{\xi}),\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\le K_2(\boldsymbol{\xi})\tau^2,$$

where

$$\begin{aligned}
K_2(\boldsymbol{\xi}) =& C\tau^2\Big(K_1(\boldsymbol{\xi})\|V_m(\boldsymbol{\xi})\|^2_{H^{s-2}(\mathbb{T})}\|\psi_m(\boldsymbol{\xi})\|_{L^\infty((0,T),H^{s-2}(\mathbb{T}))}\\
&+\|V_m(\boldsymbol{\xi})\|_{H^s(\mathbb{T})}\|\psi_m(\boldsymbol{\xi})\|_{L^\infty((0,T),H^s(\mathbb{T}))}\\
&+\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\|\partial_t\psi_m(\boldsymbol{\xi})\|_{L^\infty((0,T),H^{s-2}(\mathbb{T}))}\Big).
\end{aligned}$$

By Lemmas 3.2, 3.6 and 3.9 and Hölder's inequality, $K_2(\boldsymbol{\xi})\in L^q_{\boldsymbol{\mu}_\infty}(U)$ and $\|K_2\|_{L^q_{\boldsymbol{\mu}_\infty}(U)}$ can be bounded uniformly in m and τ for any $1\le q<\infty$.

Finally, we have

$$\begin{aligned}
&\|\psi_m(t_n,\boldsymbol{\xi})-\psi_m^n(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\\
&\quad\le \|\psi_m(t_n,\boldsymbol{\xi})-\Psi_\tau^{\mathrm{k}}\circ\Psi_\tau^{\mathrm{p}}(\psi_m(t_{n-1},\boldsymbol{\xi}),\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\\
&\qquad+\|\Psi_\tau^{\mathrm{k}}\circ\Psi_\tau^{\mathrm{p}}(\psi_m(t_{n-1},\boldsymbol{\xi}),\boldsymbol{\xi})-\Psi_\tau^{\mathrm{k}}\circ\Psi_\tau^{\mathrm{p}}(\psi_m^{n-1}(\boldsymbol{\xi}),\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}\\
&\quad\le \mathrm{e}^{C\tau\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}}\|\psi_m(t_{n-1},\boldsymbol{\xi})-\psi_m^{n-1}(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}+K_2(\boldsymbol{\xi})\tau^2\\
&\quad\le \mathrm{e}^{CT\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}}\|\psi_m(0,\boldsymbol{\xi})-\psi_m^0(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}+K_2(\boldsymbol{\xi})\tau^2\sum_{j=0}^{n-1}\mathrm{e}^{Cj\tau\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}}\\
&\quad\le T\mathrm{e}^{CT\|V_m(\boldsymbol{\xi})\|_{H^{s-2}(\mathbb{T})}}K_2(\boldsymbol{\xi})\tau,
\end{aligned}$$

and we can obtain (3.15) by Lemma 3.4 and Hölder's inequality. □

Lemma 3.12. *Let Assumptions 2.1–2.2 hold with $s\ge 3$. Then, for any $0<\tau\le T$,*

$$|\mathbb{E}[G(|\psi_m(t_n)|^2)]-\mathbb{E}[G(|\psi_m^n|^2)]|\le C\tau,\quad 0\le t_n=n\tau\le T,\tag{3.16}$$

where C is independent of m and τ.

Proof. The proof uses Lemmas 3.6, 3.10 and 3.11, and is similar to that of Lemma 3.8. Hence, we omit it here. ☐

3.4. **QMC quadrature error.** The analysis of the QMC quadrature error is closely related to the mixed first derivatives of ψ_m^n with respect to ξ_m, whose growth as $|\boldsymbol{\xi}_m| \to \infty$ has a direct impact on the convergence rate of QMC. Let $\nu = (\nu_1, \nu_2, \dots, \nu_m) \in \mathcal{J} := \{0,1\}^m$ with $|\nu| = \sum_{j=1}^m \nu_j$, $\mathcal{I}_\nu = \{j : \nu_j = 1\}$, and $\mathcal{I}_\nu^\dagger = \{1, 2, \dots, m\} \setminus \mathcal{I}_\nu$. The following notation is adopted to denote the mixed first derivative:

$$\partial^\nu \psi_m^n = \partial_{\xi_1}^{\nu_1} \dots \partial_{\xi_m}^{\nu_m} \psi_m^n, \quad \nu \in \mathcal{J}.$$

Before proceeding further, we give bounds on the $L^2(\mathbb{T})$-norms of g_n and $\partial_x g_n$ introduced in Remark 2.1.

Lemma 3.13. *Under Assumptions 2.1–2.2, we have for any* $0 < \tau \le T$ *and* $\boldsymbol{\xi} \in U_a$

$$\|g_n(\rho, \boldsymbol{\xi})\|_{L^2(\mathbb{T})} = \|\psi_{\rm in}\|_{L^2(\mathbb{T})}, \tag{3.17}$$

$$\|\partial_x g_n(\rho, \boldsymbol{\xi})\|_{L^2(\mathbb{T})} \le \|\partial_x \psi_{\rm in}\|_{L^2(\mathbb{T})} + T\|\partial_x V_m(\boldsymbol{\xi})\|_{L^\infty(\mathbb{T})}\|\psi_{\rm in}\|_{L^2(\mathbb{T})}, \tag{3.18}$$

where $0 \le \rho \le \tau$ *and* $1 \le n \le \lfloor T/\tau \rfloor$.

Proof. Fix $0 \le \rho \le \tau \le T, 1 \le n \le \lfloor T/\tau \rfloor$ and $\boldsymbol{\xi} \in U_a$. First, we have $g_n(\rho) = \mathrm{e}^{-\mathrm{i}\rho V_m} \psi_m^{n-1} = \mathrm{e}^{-\mathrm{i}\rho V_m} \mathrm{e}^{\mathrm{i}\tau \partial_x^2/2} g_{n-1}(\tau)$, and thus

$$\|g_n(\rho)\|_{L^2(\mathbb{T})} = \|g_{n-1}(\tau)\|_{L^2(\mathbb{T})} = \dots = \|g_1(\tau)\|_{L^2(\mathbb{T})} = \|\psi_{\rm in}\|_{L^2(\mathbb{T})}.$$

On the other hand, taking the partial derivative of (2.7) with respect to x, we have

$$\mathrm{i}\partial_t \partial_x g_n = V_m \partial_x g_n + \partial_x V_m g_n.$$

Multiplying the above equation by $\overline{\partial_x g_n}$, integrating it with respect to x over $\mathbb{T}$, and taking the imaginary part of it, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\partial_x g_n\|_{L^2(\mathbb{T})}^2 = \mathrm{Im}\left(\int_{\mathbb{T}} \overline{\partial_x g_n} \partial_x V_m g_n\right).$$

The Cauchy-Schwarz inequality gives

$$\|\partial_x g_n\|_{L^2(\mathbb{T})} \frac{\mathrm{d}}{\mathrm{d}t}\|\partial_x g_n\|_{L^2(\mathbb{T})} \le \|\partial_x g_n\|_{L^2(\mathbb{T})}\|\partial_x V_m\|_{L^\infty(\mathbb{T})}\|g_n\|_{L^2(\mathbb{T})}.$$

Dropping the term of $\|\partial_x g_n\|_{L^2(\mathbb{T})}$ in the above equation, integrating it with respect to t over $(0, \rho)$ and using (3.17), we have

$$\|\partial_x g_n(\rho)\|_{L^2(\mathbb{T})} \le \|\partial_x g_n(0)\|_{L^2(\mathbb{T})} + \rho\|\partial_x V_m\|_{L^\infty(\mathbb{T})}\|\psi_{\rm in}\|_{L^2(\mathbb{T})}. \tag{3.19}$$

Note that $\|\partial_x \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2} f\|_{L^2(\mathbb{T})} = \|\partial_x f\|_{L^2(\mathbb{T})}$ for any $f \in H^1(\mathbb{T})$. Then, we deduce from (3.19)

$$\|\partial_x g_n(\rho)\|_{L^2(\mathbb{T})} \le \|\partial_x g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \tau\|\partial_x V_m\|_{L^\infty(\mathbb{T})}\|\psi_{\rm in}\|_{L^2(\mathbb{T})}. \tag{3.20}$$

Finally, we obtain (3.18) by iterating (3.20) from n to 2 and using (3.19) for g_1. ☐

Let $C_T = \max\{1, T\}$ and $\Upsilon_m(\boldsymbol{\xi}) = \max\{1, \|V_m(\boldsymbol{\xi})\|_{W^{1,\infty}(\mathbb{T})}\}$. Now we give bounds on $\partial^\nu \psi_m^n$ and $\partial^\nu G(|\psi_m^n|^2)$.

Lemma 3.14. *Under Assumptions 2.1–2.2, we have for any* $0 < \tau \le T$ *and* $\boldsymbol{\xi} \in U_a$

$$\|\partial^\nu \psi_m^n(\boldsymbol{\xi})\|_{H^1(\mathbb{T})} \le |\nu|! 4^{|\nu|+1} C_T^{|\nu|+1} \|\psi_{\rm in}\|_{H^1(\mathbb{T})} \Upsilon_m(\boldsymbol{\xi}) \prod_{j \in \mathcal{I}_\nu} b_j, \quad 1 \le n \le \lfloor T/\tau \rfloor. \tag{3.21}$$

Proof. Fix $T > 0$ and $\boldsymbol{\xi} \in U_a$. We shall prove that for any $0 \le n \le \lfloor T/\tau \rfloor$ and $0 \le \rho \le \tau$

$$\|\partial^\nu g_n(\rho, \boldsymbol{\xi})\|_{L^2(\mathbb{T})} \le |\nu|! C_T^{|\nu|} \|\psi_{\rm in}\|_{L^2(\mathbb{T})} \prod_{j \in \mathcal{I}_\nu} b_j, \tag{3.22}$$

$$\|\partial_x \partial^\nu g_n(\rho, \boldsymbol{\xi})\|_{L^2(\mathbb{T})} \le |\nu|! 4^{|\nu|} C_T^{|\nu|+1} \|\psi_{\rm in}\|_{H^1(\mathbb{T})} \Upsilon_m(\boldsymbol{\xi}) \prod_{j \in \mathcal{I}_\nu} b_j, \tag{3.23}$$

and then (3.21) follows from the above two equations and the relations that $\|\partial^\nu \psi_m^n\|_{L^2(\mathbb{T})} = \|\partial^\nu g_n(\tau)\|_{L^2(\mathbb{T})}$ and $\|\partial_x \partial^\nu \psi_m^n\|_{L^2(\mathbb{T})} = \|\partial_x \partial^\nu g_n(\tau)\|_{L^2(\mathbb{T})}$ for any $|\nu| \ge 1$, which are due to the fact that $\partial^\nu \psi_m^n = \mathrm{e}^{\mathrm{i}\tau \partial_x^2/2} \partial^\nu g_n(\tau)$. Now we prove (3.22) and (3.23) by induction on $|\nu|$.

For $|\nu| = 1$, we differentiate (2.7) with respect to ξ_j and obtain

$$\mathrm{i}\partial_t \partial_j g_n = V_m \partial_j g_n + \partial_j V_m g_n.$$

where we denote $\partial_j = \partial_{\xi_j}$ for short. Similar arguments to the proof of (3.18) in Lemma 3.13 give

$$\begin{aligned}
\|\partial_j g_n(\rho)\|_{L^2(\mathbb{T})} \le& \|\partial_j g_n(0)\|_{L^2(\mathbb{T})} + \int_0^\rho \|\partial_j V_m\|_{L^\infty(\mathbb{T})} \|g_n(y)\|_{L^2(\mathbb{T})} \mathrm{d}y \\
\le& \|\partial_j g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \tau \lambda_j \|v_j\|_{L^\infty(\mathbb{T})} \|\psi_{\rm in}\|_{L^2(\mathbb{T})},
\end{aligned}$$

where we have used (3.17) and the fact that $g_n(0) = \psi_m^{n-1} = \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2} g_{n-1}(\tau)$ in the second inequality. We obtain (3.22) for $|\nu| = 1$ by iterating the above equation from n to 2 and the fact that $\partial_j g_1(0) = \partial_j \psi_{\rm in} = 0$. Then, differentiating (2.7) with respect to ξ_j and x, we have

$$\mathrm{i}\partial_t \partial_x \partial_j g_n = V_m \partial_x \partial_j g_n + \partial_x V_m \partial_j g_n + \partial_j V_m \partial_x g_n + \partial_x \partial_j V_m g_n.$$

Following a similar procedure, we obtain

$$\begin{aligned}
\|\partial_x \partial_j g_n(\tau)\|_{L^2(\mathbb{T})} \le& \|\partial_x \partial_j g_n(0)\|_{L^2(\mathbb{T})} + \int_0^\tau \Big(\|\partial_x V_m\|_{L^\infty(\mathbb{T})} \|\partial_j g_n(y)\|_{L^2(\mathbb{T})} \\
&+ \|\partial_j V_m\|_{L^\infty(\mathbb{T})} \|\partial_x g_n(y)\|_{L^2(\mathbb{T})} + \|\partial_x \partial_j V_m\|_{L^\infty(\mathbb{T})} \|g_n(y)\|_{L^2(\mathbb{T})} \Big) \mathrm{d}y \\
\le& \|\partial_x \partial_j g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + C_T \tau b_j \|\partial_x V_m\|_{L^\infty(\mathbb{T})} \|\psi_{\rm in}\|_{L^2(\mathbb{T})} \\
&+ \tau \lambda_j \|v_j\|_{L^\infty(\mathbb{T})} \|\partial_x \psi_{\rm in}\|_{L^2(\mathbb{T})} + T\tau \lambda_j \|v_j\|_{L^\infty(\mathbb{T})} \|\partial_x V_m\|_{L^\infty(\mathbb{T})} \|\psi_{\rm in}\|_{L^2(\mathbb{T})} \\
&+ \tau \lambda_j \|\partial_x v_j\|_{L^\infty(\mathbb{T})} \|\psi_{\rm in}\|_{L^2(\mathbb{T})} \\
\le& \|\partial_x \partial_j g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + 4\tau C_T \|\psi_{\rm in}\|_{H^1(\mathbb{T})} \Upsilon_m b_j,
\end{aligned}$$

where we have used Lemma 3.13, (3.22) for $|\nu| = 1$ and the fact that $g_n(0) = \psi_m^{n-1} = \mathrm{e}^{\mathrm{i}\tau\partial_x^2/2} g_{n-1}(\tau)$ in the second inequality. We obtain (3.23) for $|\nu| = 1$ by iterating the above equation from n to 2 and the fact that $\partial_x \partial_j g_1(0) = \partial_x \partial_j \psi_{\rm in} = 0$.

For $|\nu| \ge 2$, the Leibniz rule gives

$$\begin{aligned}
\mathrm{i}\partial_t \partial^\nu g_n =& \sum_{\mu \preceq \nu} \binom{\nu}{\mu} \partial^{\nu-\mu} V_m \partial^\mu g_n = V_m \partial^\nu g_n + \sum_{|\nu-\mu|=1, \mu \prec \nu} \partial^{\nu-\mu} V_m \partial^\mu g_n, \\
\mathrm{i}\partial_t \partial_x \partial^\nu g_n =& \sum_{\mu \preceq \nu} \binom{\nu}{\mu} (\partial^{\nu-\mu} V_m \partial_x \partial^\mu g_n + \partial_x \partial^{\nu-\mu} V_m \partial^\mu g_n) \\
=& V_m \partial_x \partial^\nu g_n + \partial_x V_m \partial^\nu g_n + \sum_{|\nu-\mu|=1, \mu \prec \nu} (\partial^{\nu-\mu} V_m \partial_x \partial^\mu g_n + \partial_x \partial^{\nu-\mu} V_m \partial^\mu g_n),
\end{aligned}$$

where $\binom{\nu}{\mu} = \prod_{j=1}^{m} \binom{\nu_j}{\mu_j}$, and the second equalities in the above two equation are both due to the fact that $\partial^\nu V_m = 0$ for $|\nu| \geq 2$. We can then deduce in the aforementioned way that

$$\|\partial^\nu g_n(\rho)\|_{L^2(\mathbb{T})} \leq \|\partial^\nu g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \int_0^\tau \left(\sum_{|\nu-\mu|=1,\mu\prec\nu} \|\partial^{\nu-\mu} V_m\|_{L^\infty(\mathbb{T})} \|\partial^\mu g_n(y)\|_{L^2(\mathbb{T})} \right) \mathrm{d}y, \tag{3.24}$$

$$\begin{aligned}\|\partial_x\partial^\nu g_n(\rho)\|_{L^2(\mathbb{T})} \leq& \|\partial_x\partial^\nu g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \int_0^\tau \Bigg(\|\partial_x V_m\|_{L^\infty(\mathbb{T})} \|\partial^\nu g_n(y)\|_{L^2(\mathbb{T})} \\ &+ \sum_{|\nu-\mu|=1,\mu\prec\nu} \big(\|\partial^{\nu-\mu} V_m\|_{L^\infty(\mathbb{T})} \|\partial_x\partial^\mu g_n(y)\|_{L^2(\mathbb{T})} \\ &+ \|\partial_x\partial^{\nu-\mu} V_m\|_{L^\infty(\mathbb{T})} \|\partial^\mu g_n(y)\|_{L^2(\mathbb{T})} \big) \Bigg) \mathrm{d}y. \end{aligned} \tag{3.25}$$

Note that we have $|\mu| = |\nu| - 1$ for $|\nu - \mu| = 1$ and $\#\{\mu : |\nu - \mu| = 1\} = |\nu|$. Then, inserting the assumption (3.22) for $\partial^\mu g_n$ with $|\mu| = |\nu| - 1$ into (3.24), we can obtain (3.22) for $|\nu|$ by iterating (3.24) from n to 2. Finally, inserting (3.22) for $\partial^\nu g_n, \partial^\mu g_n$ and the assumption (3.23) for $\partial_x \partial^\mu g_m$ with $|\mu| = |\nu| - 1$ into (3.25), we can obtain

$$\begin{aligned}\|\partial_x\partial^\nu g_n(\rho)\|_{L^2(\mathbb{T})} \leq& \|\partial_x\partial^\nu g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \tau|\nu|! C_T^{|\nu|} \|\psi_{\mathrm{in}}\|_{L^2(\mathbb{T})} \|\partial_x V_m\|_{L^\infty(\mathbb{T})} \prod_{j\in\mathcal{I}_\nu} b_j \\ &+ \tau \sum_{|\nu-\mu|=1,\mu\prec\nu} \Bigg((|\nu|-1)! 4^{|\nu|-1} C_T^{|\nu|} \|\psi_{\mathrm{in}}\|_{H^1(\mathbb{T})} \Upsilon_m(\boldsymbol{\xi}) \prod_{j\in\mathcal{I}_\nu} b_j \\ &+ (|\nu|-1)! C_T^{|\nu|-1} \|\psi_{\mathrm{in}}\|_{L^2(\mathbb{T})} \prod_{j\in\mathcal{I}_\nu} b_j \Bigg) \\ \leq& \|\partial_x\partial^\nu g_{n-1}(\tau)\|_{L^2(\mathbb{T})} + \tau|\nu|! 4^{|\nu|} C_T^{|\nu|} \|\psi_{\mathrm{in}}\|_{H^1(\mathbb{T})} \Upsilon_m(\boldsymbol{\xi}) \prod_{j\in\mathcal{I}_\nu} b_j. \end{aligned}$$

We obtain (3.23) for $|\nu|$ by iterating the above equation from n to 2. □

Lemma 3.15. *Under Assumptions 2.1–2.2, we have for any $T > 0$ and $\boldsymbol{\xi} \in U_a$*

$$|\partial^\nu G\left(|\psi_m^n(\boldsymbol{\xi})|^2\right)| \leq C(|\nu|+1)! 4^{|\nu|+2} C_T^{|\nu|+2} \|G\|_{H^1(\mathbb{T})'} \|\psi_{\mathrm{in}}\|_{H^1(\mathbb{T})}^2 (\Upsilon_m(\boldsymbol{\xi}))^2 \prod_{j\in\mathcal{I}_\nu} b_j, \tag{3.26}$$

where $1 \leq n \leq \lfloor T/\tau \rfloor$ and the constant C comes from the algebraic property of $H^1(\mathbb{T})$.

Proof. Fix $T > 0$ and $\boldsymbol{\xi} \in U_a$. For $1 \leq n \leq \lfloor T/\tau \rfloor$, we have

$$|\partial^\nu G\left(|\psi_m^n|^2\right)| = |G\left(\partial^\nu |\psi_m^n|^2\right)| \leq \|G\|_{H^1(\mathbb{T})'} \|\partial^\nu |\psi_m^n|^2\|_{H^1(\mathbb{T})}.$$

By the algebraic property of $H^1(\mathbb{T})$, we find

$$|\partial^\nu G\left(|\psi_m^n(\boldsymbol{\xi})|^2\right)| \leq \|G\|_{H^1(\mathbb{T})'} \sum_{\mu\preceq\nu} C \left\|\partial^{\nu-\mu} \overline{\psi_m^n}\right\|_{H^1(\mathbb{T})} \|\partial^\mu \psi_m^n\|_{H^1(\mathbb{T})}.$$

We obtain (3.26) from the above equation by Lemma 3.14. □

Lemma 3.15 shows that $|\partial^\nu G\left(|\psi_m^n(\boldsymbol{\xi})|^2\right)|$ grows at most quadratically in $|\boldsymbol{\xi}_m|$. For the analysis of QMC quadrature error, we work with the non-standard weighted unanchored Sobolev space

$\mathcal{W}_{m,\gamma,w} := \{F(\xi) : \mathbb{R}^m \to \mathbb{R} \mid \|F\|_{\mathcal{W}_{m,\gamma,w}} < \infty\}$ [45] with the norm

$$\|F\|_{\mathcal{W}_{m,\gamma,w}} := \left[\sum_{\nu\in\mathcal{J}} \gamma_\nu^{-1} \int_{\mathbb{R}^{|\nu|}} \left(\int_{\mathbb{R}^{m-|\nu|}} \partial^\nu F(\xi) \prod_{j\in\mathcal{I}_\nu^\dagger} \phi(\xi_j) \mathrm{d}\xi_\nu^\dagger\right)^2 \prod_{j\in\mathcal{I}_\nu} w_j(\xi_j)^2 \mathrm{d}\xi_\nu\right]^{1/2}, \tag{3.27}$$

where by the notation, ξ is split into the active part ξ_ν for differentiation and the inactive part $\xi_\nu^\dagger$, i.e., ξ_ν consists of ξ_j with $j \in \mathcal{I}_\nu$ and $\xi_\nu^\dagger$ consists of ξ_k with $k \in \mathcal{I}_\nu^\dagger$. The notation γ_ν denotes the product and order-dependent (POD) weight parameter, i.e., $\gamma_\nu = \Gamma_{|\nu|} \prod_{j\in\mathcal{I}_\nu} \gamma_j$ with $\gamma_{(0,\ldots,0)} = 1$ for some sequences $\Gamma_0 = \Gamma_1 = 1, \Gamma_2, \ldots$ and $\gamma_1 \geq \gamma_2 \geq \ldots > 0$, which will be chosen in Lemma 3.17, and $\gamma := \{\gamma_\nu \,|\, \nu \in \mathcal{J}\}$. The function w_j in (3.27) is a positive continuous decaying weight function that serves to counteract the growth of $|\partial^\nu G(|\psi_m^n(\boldsymbol{\xi})|^2|)|$, and $w := \{w_j : j = 1, \ldots, m\}$. The quadratic growth of the bound in (3.26) allows us to choose the favorable weight functions in the form of

$$w_j(\xi) = \exp\left(-\theta_j|\xi|\right), \tag{3.28}$$

which can lead to a dimension-independent and almost linear convergence rate of QMC [38, 45]; see Lemmas 3.16–3.17. Here, we assume that $\max\{b_j, \theta_{\min}\} < \theta_j < \theta_{\max}$ for $j \in \mathbb{N}^+$ and some constants $0 < \theta_{\min} < \theta_{\max} < \infty$, and we will specify θ_j in Lemma 3.17. We also let $\mathcal{D} = \inf_{j\in\mathbb{N}}(\theta_j - b_j)$.

Recall the randomly shifted QMC lattice rule (2.10) with the generating vector $\boldsymbol{z}$ and the random shift $\boldsymbol{\Delta}$, and we have from [25, 45] that for a general $F \in \mathcal{W}_{m,\gamma,w}$

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[\left|\mathbb{E}[F] - Q_{m,N}(F;\boldsymbol{\Delta})\right|^2\right]} \leq e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})\|F\|_{\mathcal{W}_{m,\gamma,w}},$$

where $e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})$ is referred to as the shift averaged worst case error. Note that $\|F\|_{\mathcal{W}_{m,\gamma,w}}$ does not depend on $\boldsymbol{z}$, and thus we can construct $\boldsymbol{z}$ by making $e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})$ as small as possible. Moreover, we know from [45] that $e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})$ depends on the weight functions w and the POD weight parameters γ, and that once w and γ are chosen a generating vector $\boldsymbol{z}$ can be constructed by the CBC algorithm. That is, we set $z_1 = 1$ and then determine z_j for $j = 2, \ldots, m$ sequentially by minimizing $e_{j,N}^{\mathrm{sh}}(z_1, \ldots, z_{j-1}, z_j)$ over $z_j \in \{z \in \mathbb{N} : 1 \leq z \leq N-1, \gcd(z,N) = 1\}$. We refer to [45] for the explicit expression of $e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})$ and more details on the CBC algorithm. More importantly, it is proved in [45] that we can obtain almost linear convergence in N for $e_{m,N}^{\mathrm{sh}}(\boldsymbol{z})$ with the standard multivariate Gaussian distribution and our choice of weight functions in (3.28). We present a relevant result from [25, Theorem 15] in Lemma 3.16. Based on it, we prove the dimension-independent and almost linear convergence rate in N of the QMC-TS scheme in Lemma 3.17.

Lemma 3.16 ([25, Theorem 15]). *Let $m, N \in \mathbb{N}^+$, the weight parameters γ be fixed, the weight functions w be given in the form of* (3.28)*, and $F \in \mathcal{W}_{m,\gamma,w}$. Then, there exists a randomly shifted lattice rule* (2.10) *that can be constructed by the CBC algorithm such that*

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[|\mathbb{E}[F] - Q_{m,N}(F;\boldsymbol{\Delta})|^2\right]} \leq \left[\sum_{\nu\in\mathcal{J}\backslash\{(0,\ldots,0)\}} \gamma_\nu^\lambda \prod_{j\in\mathcal{I}_\nu} \varrho_j(\lambda)\right]^{\frac{1}{2\lambda}} \varphi_{\mathrm{tot}}(N)^{-\frac{1}{2\lambda}}\|F\|_{W_{m,\gamma,w}}, \tag{3.29}$$

for any $\lambda \in (\frac{1}{2}, 1]$, with

$$\varrho_j(\lambda) = 2\left(\frac{\sqrt{2\pi}\exp(\theta_j^2/\eta_*)}{\pi^{2-2\eta_*}(1-\eta_*)\eta_*}\right)^\lambda \zeta\left(\lambda + \frac{1}{2}\right), \quad \eta_* = \frac{2\lambda - 1}{4\lambda} \tag{3.30}$$

where ζ is the Riemann zeta function and $\varphi_{\rm tot}$ is the Euler totient function with the property that $1/\varphi_{\rm tot}(N) \le 9/N$ for $N \le 10^{30}$.

Lemma 3.17. *Let Assumptions 2.1–2.2 hold. If Assumption 2.2 holds with $p = 1$, we additionally assume that*

$$\sum_{j=1}^{\infty} b_j < \frac{\mathcal{D}^{1/2}}{4C_T \varrho_{\max}(1)^{1/2}}, \tag{3.31}$$

where $\varrho_{\max}(\lambda)$ is defined by replacing θ_j in (3.30) by $\theta_{\max}$. Choose the weight parameters

$$\gamma_\nu = \left(C_{|\nu|} \prod_{j\in\mathcal{I}_\nu} \frac{b_j^2}{(\theta_j - b_j)\varrho_j(\lambda^*)} \right)^{1/(1+\lambda^*)}, \tag{3.32}$$

where $C_{|\nu|} = ((|\nu|+1)!)^2 (4C_T)^{2|\nu|}$,

$$\lambda^* = \begin{cases} \dfrac{1}{2-2\delta}, & \text{when } 0 < p \le \dfrac{2}{3}, \\ \dfrac{p}{2-p}, & \text{when } \dfrac{2}{3} < p \le 1, \end{cases} \tag{3.33}$$

with arbitrary $\delta \in (0, 1/2]$, and θ_j is the parameter in weight function $w_j(\xi_j)$ in (3.28) with

$$\theta_j = \frac{1}{2}\left(b_j + \sqrt{b_j^2 + 1 - \frac{1}{2\lambda^*}} \right), \quad j \in \mathbb{N}^+. \tag{3.34}$$

Then, there exists a randomly shifted lattice rule (2.10) that can be constructed by the CBC algorithm such that for $N \le 10^{30}$

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[|\mathbb{E}[G(|\psi_m^n|^2)] - Q_{m,N}(G(|\psi_m^n|^2);\boldsymbol{\Delta})|^2 \right]} \le \begin{cases} CN^{-(1-\delta)}, & \text{when } 0 < p \le \dfrac{2}{3}, \\ CN^{-(1/p-1/2)}, & \text{when } \dfrac{2}{3} < p \le 1, \end{cases} \tag{3.35}$$

where C is independent of m, τ, N, but depends on p and, when relevant, δ.

Proof. With the elementary inequality $\max\{1, \rho^2\} \le \exp(\rho)$ for $\rho \ge 0$, we can deduce from Lemma 3.15 that

$$|\partial^\nu G\left(|\psi_m^n(\boldsymbol{\xi})|^2\right)| \le \widetilde{C}(|\nu|+1)!(4C_T)^{|\nu|} \exp\left(\sum_{j=1}^m b_j|\xi_j|\right) \prod_{j\in\mathcal{I}_\nu} b_j, \quad 1 \le n \le \lfloor T/\tau \rfloor, \boldsymbol{\xi} \in U_a,$$

where $\widetilde{C} = 16CC_T^2\|G\|_{H^1(\mathbb{T})'}\|\psi_{\rm in}\|_{H^1(\mathbb{T})}^2 \exp(\|v_0\|_{W^{1,\infty}(\mathbb{T})})$, with C from the algebraic property of $H^1(\mathbb{T})$. In addition, from the proof of [25, Theorem 16], we have (3.3), $2\exp(b_j^2/2)\Phi(b_j) \ge 1$, and $\int_{\mathbb{R}} \exp(2b_j|\xi_j|) w_j^2(\xi_j) \mathrm{d}\xi_j = 1/(\theta_j - b_j)$. Then, we obtain by the definition (3.27) of the $\mathcal{W}_{m,\gamma,w}$-norm that

$$\begin{aligned} \|G\left(|\psi_m^n|^2\right)\|_{\mathcal{W}_{m,\gamma,w}}^2 \le& \widetilde{C}^2 \prod_{j=1}^m (2\exp(b_j^2/2)\Phi(b_j)) \left(\sum_{\nu\in\mathcal{J}} \gamma_\nu^{-1} C_{|\nu|} \prod_{j\in\mathcal{I}_\nu} \frac{b_j^2}{2\exp(b_j^2/2)\Phi(b_j)(\theta_j - b_j)} \right) \\ \le& (\breve{C})^2 \sum_{\nu\in\mathcal{J}} \gamma_\nu^{-1} C_{|\nu|} \prod_{j\in\mathcal{I}_\nu} \frac{b_j^2}{\theta_j - b_j}, \end{aligned} \tag{3.36}$$

where $C_{|\nu|} = ((|\nu|+1)!)^2(4C_T)^{2|\nu|}$ and $\breve{C} = \widetilde{C}\exp\left(\frac{1}{4}\sum_{j=1}^\infty b_j^2 + \frac{1}{\sqrt{2\pi}}\sum_{j=1}^\infty b_j\right)$.

The rest of the proof is similar to that of [25, Theorem 20 and Corollary 21], and we only provide the main idea here. In view of Lemma 3.16 and (3.36), to derive a dimension-independent bound on the QMC quadrature error, we need to bound the quantity

$$C_{\gamma,m} := \left(\sum_{\nu \in \mathcal{J} \setminus \{(0,\dots,0)\}} \gamma_\nu^\lambda \prod_{j \in \mathcal{I}_\nu} \varrho_j(\lambda) \right)^{1/\lambda} \left(\sum_{\nu \in \mathcal{J}} \gamma_\nu^{-1} C_{|\nu|} \prod_{j \in \mathcal{I}_\nu} \frac{b_j^2}{\theta_j - b_j} \right)$$

independently of m. To this end, we first choose

$$\gamma_\nu = \left(C_{|\nu|} \prod_{j \in \mathcal{I}_\nu} \frac{b_j^2}{(\theta_j - b_j)\varrho_j(\lambda)} \right)^{1/(1+\lambda)},$$

which minimizes $C_{\gamma,m}$ for fixed θ_j and λ by [37, Lemma 6.2 and Theorem 6.4]. Then, we further find that $\lambda \in (1/2, 1]$ needs to be bounded from below, depending on the value of p in Assumption 2.2. For $\lambda \in (1/2, 1)$, we need $\lambda \geq p/(2-p)$. We want λ to be as small as possible in view of (3.29). So we can choose $\lambda = \lambda^* = 1/(2-2\delta)$ for some $\delta \in (0, 1/2)$ when $p \in (0, 2/3]$ and $\lambda = \lambda^* = p/(2-p)$ when $p \in (2/3, 1)$. When $p = 1$, we need to additionally assume (3.31), and then we can choose $\lambda = \lambda^* = 1$. Finally, the choice of $\{\theta_j\}_{j=1}^\infty$ in (3.34) minimizes $C_{\gamma,m}$ given the above choices of γ_ν and λ. These choices of γ_ν, λ and $\{\theta_j\}_{j=1}^\infty$ give the error estimate (3.35) by Lemma 3.16. □

Now we are ready to prove the main result presented in Section 2.2.

Proof of Theorem 2.4. By the triangle inequality, we have

$$\begin{aligned} &\sqrt{\mathbb{E}^{\boldsymbol{\Delta}} \left[\left| \mathbb{E}[G(|\psi(t_n)|^2)] - Q_{m,N}(G(|\psi_m^n|^2); \boldsymbol{\Delta}) \right|^2 \right]} \\ &\quad \leq |\mathbb{E}[G(|\psi(t_n)|^2)] - \mathbb{E}[G(|\psi_m(t_n)|^2)]| + |\mathbb{E}[G(|\psi_m(t_n)|^2)] - \mathbb{E}[G(|\psi_m^n|^2)]| \\ &\quad\quad + \sqrt{\mathbb{E}^{\boldsymbol{\Delta}} \left[|\mathbb{E}[G(|\psi_m^n|^2)] - Q_{m,N}(G(|\psi_m^n|^2); \boldsymbol{\Delta})|^2 \right]}. \end{aligned}$$

Then, we prove the theorem using Lemmas 3.8, 3.12, and 3.17. □

3.5. **Some discussions.** We end this section with a few comments on our main result.

(1) The time discretization scheme has a direct impact on the performance of the randomly shifted lattice-based QMC quadrature rule. If the semi-discrete solution grows too fast in $|\boldsymbol{\xi}|$, we may have to choose weight functions that decay faster than (3.28) and the resulting QMC quadrature may not achieve almost linear convergence [38, 45].
(2) Theorem 2.4 can be generalized to d-space-dimensional case ($d \geq 1$) by additionally assuming that $G \in (H^r(\mathbb{T}))'$, $v_j \in W^{r,\infty}(\mathbb{T})$ for $j \in \mathbb{N}^+$, $\sum_{j=1}^\infty (b_{j,r})^p < \infty$ for some $p \in (0, 1]$ with $b_{j,r} = \lambda_j \|v_j\|_{W^{r,\infty}(\mathbb{T})}$, and $\|V_m - V\|_{L^{2+\varepsilon}_{\mu_\infty}(U, H^r(\mathbb{T}))} \leq C m^{-\chi}$ for some constants C, χ, ε independent of m, where $r > d/2$. Then, the error estimate (2.13) still holds for QMC-TS.
(3) We can use a general splitting scheme of the form (2.8) for time discretization. In particular, we can adopt the Strang splitting [53]

$$\psi_m^{n+1} = \Psi_{\tau/2}^{\mathrm{k}} \circ \Psi_\tau^{\mathrm{p}} \circ \Psi_{\tau/2}^{\mathrm{k}}(\psi_m^n) = \mathrm{e}^{\mathrm{i}\tau\partial_x^2/4} \mathrm{e}^{-\mathrm{i}\tau V_m} \mathrm{e}^{\mathrm{i}\tau\partial_x^2/4} \psi_m^n, \quad n = 0.1, \dots, \tag{3.37}$$

which is known to be second-order and is one of the most popular splitting schemes. In this case, if we additionally assume that Assumptions 2.1–2.3 hold with $s \geq 5$, then under the conditions of Theorem 2.4 we can prove by following the analysis in [54, Section 4] that the following error estimate holds for QMC-TS:

$$\sqrt{\mathbb{E}^{\boldsymbol{\Delta}}\left[\left|\mathbb{E}[G(|\psi(t_n)|^2)] - Q_{m,N}(G(|\psi_m^n|^2);\boldsymbol{\Delta})\right|^2\right]} \leq C(m^{-\chi} + \tau^2 + N^{-\kappa}), \tag{3.38}$$

where C is independent of m, τ, N and κ is the same as in Theorem 2.4.

(4) Following the third comment, for the Lie–Trotter splitting (2.5) (resp. the Strang splitting (3.37)), the time convergence of order 1 (resp. order 2) will be achieved as long as Assumption 2.1 holds with $s \geq 3$ (resp. $s \geq 5$), while the summability of $\{a_j\}_{j=1}^{\infty}$ with $s \geq 3$ (resp. $s \geq 5$) in Assumption 2.2 guarantees that the time convergence is independent of m.

(5) Following the second and third comments, the QMC quadrature achieves the dimension-independent $\mathcal{O}(N^{-\kappa})$ convergence as long as $\sum_{j=1}^{\infty}(b_{j,r})^p < \infty$ for some $p \in (0,1]$, regardless of the choice of the splitting scheme for time discretization.

(6) The fully discrete scheme can be obtained by combining the QMC-TS scheme with some spatial dicretization, e.g., the Fourier pseudospectral method [50], the finite difference method [43, 44], etc. The crucial step to obtain the QMC convergence rate for the fully discrete scheme is to derive a bound on the mixed first derivatives of the fully discrete solution with respect to $\boldsymbol{\xi}$, which turns out to be non-trivial. But we believe that the QMC convergence rate in Theorem 2.4 would hold provided that the spatial mesh size is sufficiently small; see the numerical examples in Section 4. We will address this issue in future works.

(7) A more challenging problem is the nonlinear Schrödinger equation with a Gaussian random potential

$$\mathrm{i}\partial_t\psi(t,\omega,x) = -\frac{1}{2}\partial_x^2\psi(t,\omega,x) + V(\omega,x)\psi(t,\omega,x) + \alpha|\psi(t,\omega,x)|^2\psi(t,\omega,x), \tag{3.39}$$

where $V(\omega, x)$ is a Gaussian random field and $\alpha \neq 0$. The well-posedness of the solution ψ, particularly the integrability of ψ in the random space, is non-trivial due to the cubic nonlinearity. We will study the problem in the future.

4. Numerical examples

In this section, we give some convergence tests of the QMC-TS method to verify our theoretical findings. To implement the QMC-TS method, we use the Fourier pseudospectral method with mesh size h for spatial discretization, and the generating vector for QMC is constructed using the code from [47] (see also [35]). We consider two primary physical observables: the position density S and the current density J, where

$$S(t,\boldsymbol{\xi},x) = S(\psi(t,\boldsymbol{\xi},x)) = |\psi(t,\boldsymbol{\xi},x)|^2, \tag{4.1}$$

$$J(t,\boldsymbol{\xi},x) = J(\psi(t,\boldsymbol{\xi},x)) = \mathrm{Im}(\overline{\psi(t,\boldsymbol{\xi},x)}\nabla\psi(t,\boldsymbol{\xi},x)). \tag{4.2}$$

The first example tests the convergence rates of different time-splitting schemes and sampling methods.

Example 4.1. Consider the Schrödinger equation (2.1) with $\mathbb{T} = [-\pi, \pi]$, $T = 1$, the initial data

$$\psi_{\mathrm{in}}(x) = \sqrt{\frac{8}{\pi}}\exp(-8x^2), \tag{4.3}$$

and the random potential

$$V_m(\boldsymbol{\xi}, x) = 1 + \sum_{j=1}^{m} \frac{1}{j^{\frac{9}{2}}} \xi_j \cos(jx). \tag{4.4}$$

We consider $m = 4$.

To test the convergence rates, we consider the L^2 relative errors for S and J, i.e.,

$$\mathrm{err}_{L^2}(S) = \frac{\|\mathbb{E}_{\mathrm{num}}[S(\psi_{m,\mathrm{num}}(t))] - \mathbb{E}_{\mathrm{ref}}[S(\psi_{m,\mathrm{ref}}(t))]\|_{L^2(\mathbb{T})}}{\|\mathbb{E}_{\mathrm{ref}}[S(\psi_{m,\mathrm{ref}}(t))]\|_{L^2(\mathbb{T})}}, \tag{4.5}$$

$$\mathrm{err}_{L^2}(J) = \frac{\|\mathbb{E}_{\mathrm{num}}[J(\psi_{m,\mathrm{num}}(t))] - \mathbb{E}_{\mathrm{ref}}[J(\psi_{m,\mathrm{ref}}(t))]\|_{L^2(\mathbb{T})}}{\|\mathbb{E}_{\mathrm{ref}}[J(\psi_{m,\mathrm{ref}}(t))]\|_{L^2(\mathbb{T})}}. \tag{4.6}$$

Here, $\mathbb{E}_{\mathrm{ref}}[S(\psi_{m,\mathrm{ref}}(t,x))]$ and $\mathbb{E}_{\mathrm{ref}}[J(\psi_{m,\mathrm{ref}}(t,x))]$ are the reference solutions, which are computed using the Strang splitting and the Fourier pseudospectral method combined with the stochastic collocation method, where we choose $\tau = 5 \times 10^{-5}, h = \frac{\pi}{128}$ and 20 collocation points in each of the m dimensions of $\boldsymbol{\xi}_m$. Moreover, $\psi_{m,\mathrm{num}}$ is the numerical solution obtained by some numerical scheme in time and space for fixed m and $\boldsymbol{\xi}_m$. If we consider QMC as the sampling method, $\mathbb{E}_{\mathrm{num}}[F]$ for a general $F(\boldsymbol{\xi}_m)$ reads

$$\mathbb{E}_{\mathrm{num}}[F] = \overline{Q}_{m,N,R}(F) = \frac{1}{R} \sum_{k=1}^{R} Q_{m,N}(F; \boldsymbol{\Delta}_k),$$

where $Q_{m,N}(F; \boldsymbol{\Delta}_k)$ is defined in (2.10) with $\boldsymbol{\Delta}_k$ the k-th independent random shift. We will also consider MC as the sampling method, and in the case $\mathbb{E}_{\mathrm{num}}[F]$ reads

$$\mathbb{E}_{\mathrm{num}}[F] = \frac{1}{N_{\mathrm{MC}}} \sum_{j=1}^{N_{\mathrm{MC}}} F(\boldsymbol{\xi}_{m,\mathrm{MC}}^{(j)}),$$

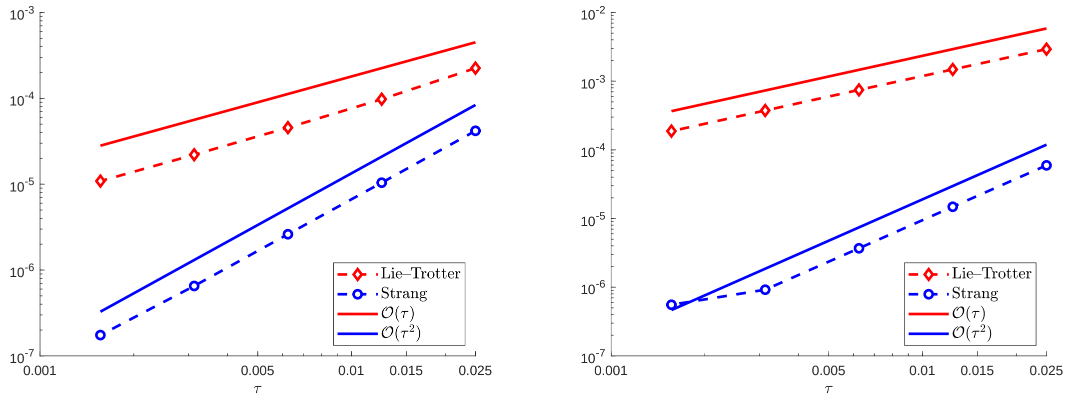
where $\{\boldsymbol{\xi}_{m,\mathrm{MC}}^{(j)}\}_{j=1}^{N_{\mathrm{MC}}}$ are the MC sample points with N_{MC} the total number.

For time convergence tests, we use the Lie–Trotter and Strang splittings in QMC-TS, where we fix $R = 50, N = 2^{18}, h = \frac{\pi}{64}$ and choose $\tau = \frac{1}{40}, \frac{1}{80}, \frac{1}{160}, \frac{1}{320}, \frac{1}{640}$. By the discussion in Section 3.5, we should observe first-order and second-order convergence in τ for the Lie–Trotter and Strang splittings, respectively. The numerical results are shown in Figure 1, where the optimal convergence rates in time are observed for both splitting schemes.

For tests of convergence in the number of samples, we compare QMC and MC as the sampling method, and we use the Strang splitting and the Fourier pseudospectral method for time and spatial discretization, respectively. We fix $\tau = 10^{-4}$ and $h = \frac{\pi}{64}$. For a fair comparison of QMC and MC, we let $N_{\mathrm{tot}} = N_{\mathrm{MC}} = RN$, and we choose $R = 50$ and $N = 2^{10}, 2^{11}, \ldots, 2^{16}$. The L^2 relative errors of S and J are shown in Figure 2, and the fitted convergence rates of QMC and MC are shown in Table 1a. We observe that the convergence rates of QMC are approximately linear, which is consistent with the discussion in Section 3.5, while the convergence rates of MC are slightly lower than the theoretical $\frac{1}{2}$ order.

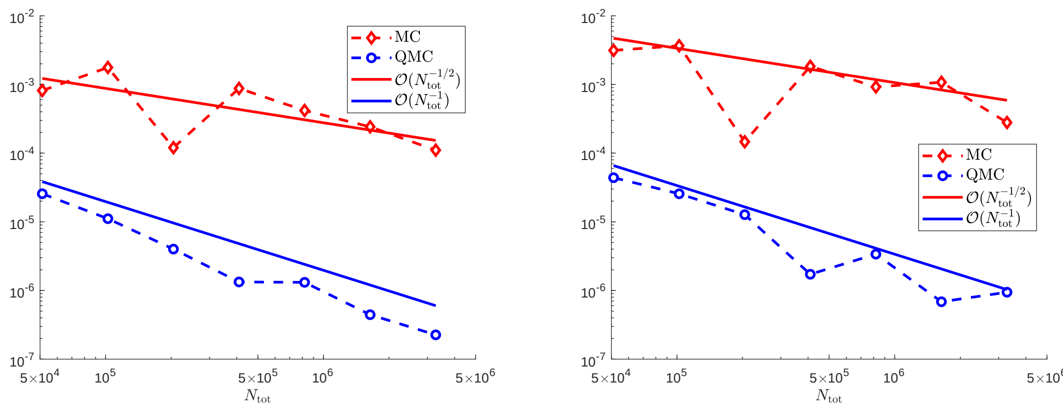
The second example shows the dimension-independence of the convergence in time and the number of QMC samples.

Example 4.2. Consider the Schrödinger equation (2.1) with $\mathbb{T} = [-\pi, \pi], T = 1$, the initial condition (4.3) and the random potential (4.4). We consider $m = 2, 4, 6$.



(a) L^2 relative error of S at $T = 1$ (b) L^2 relative error of J at $T = 1$

FIGURE 1. Convergence in time for Example 4.1



(a) L^2 relative error of S at $T = 1$ (b) L^2 relative error of J at $T = 1$

FIGURE 2. Convergence in the number of samples for Example 4.1

	QMC	MC
S	1.1206	0.4499
J	1.0349	0.4052

(a) Example 4.1

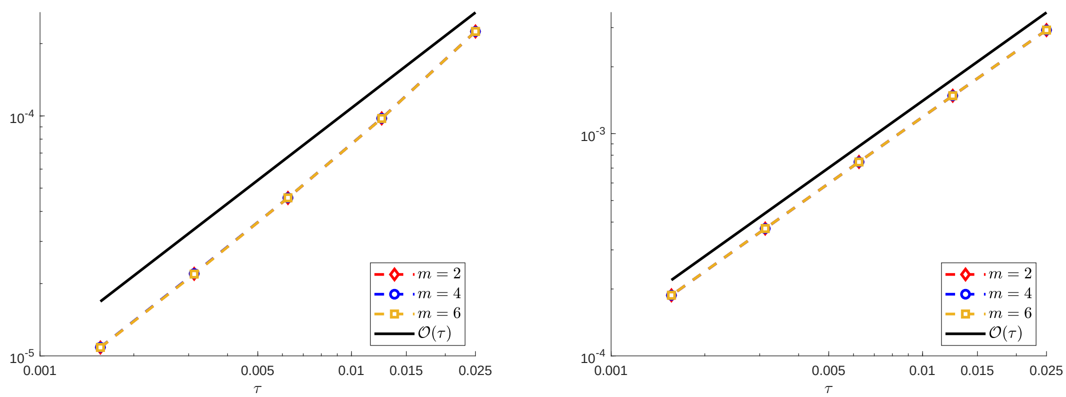
	$m = 2$	$m = 4$	$m = 6$
S	1.1598	1.1206	1.0844
J	1.1740	1.0349	1.1775

(b) Example 4.2

TABLE 1. Fitted convergence rates in N_{tot} of L^2 relative errors for Examples 4.1–4.2

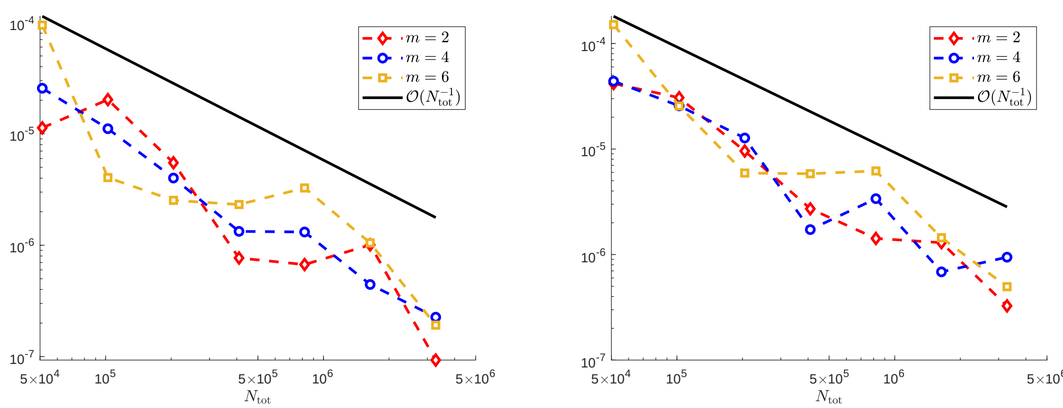
We still consider the L^2 relative errors (4.5)–(4.6) for S and J, respectively. The reference solutions are computed in the same way as in the previous example.

For time convergence tests, we use the Lie–Trotter splitting in QMC-TS. We should observe dimension-independent and first-order convergence in time by Theorem 2.4. We fix $R = 50, N = 2^{18}, h = \frac{\pi}{64}$ and choose $\tau = \frac{1}{40}, \frac{1}{80}, \frac{1}{160}, \frac{1}{320}, \frac{1}{640}$. The results are shown in Figure 3. The L^2 relative errors decay at a rate of $\mathcal{O}(\tau)$ and are nearly the same for different m, which is consistent with Theorem 2.4.



(a) L^2 relative error of S at $T = 1$ (b) L^2 relative error of J at $T = 1$

FIGURE 3. Convergence in time for Example 4.2



(a) L^2 relative error of S at $T = 1$ (b) L^2 relative error of J at $T = 1$

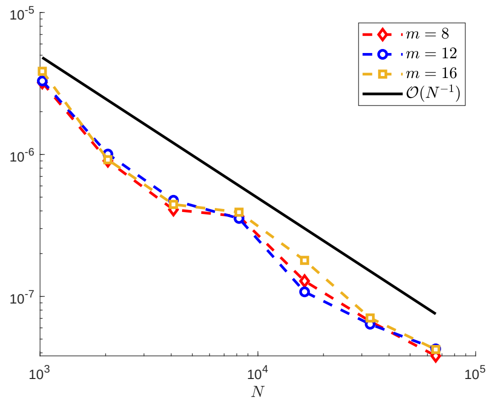
FIGURE 4. Convergence in the number of samples for Example 4.2

For convergence tests of QMC, we use the Strang splitting in QMC-TS. We should observe dimension-independent and almost linear convergence in the number of samples by the discussion in Section 3.5. We fix $\tau = 10^{-4}, h = \frac{\pi}{64}$ and let $N_{\text{tot}} = RN$, where we choose $R = 50$ and $N = 2^{10}, 2^{11}, \ldots, 2^{16}$. The L^2 relative errors of S and J and shown in Figure 4, and the fitted convergence rates are shown in Table 1b. The dimension-independence of the QMC quadrature error is confirmed by Figure 4 and Table 1b shows that the convergence rates in N_{tot} are all around 1 for different m, which verifies our theories.

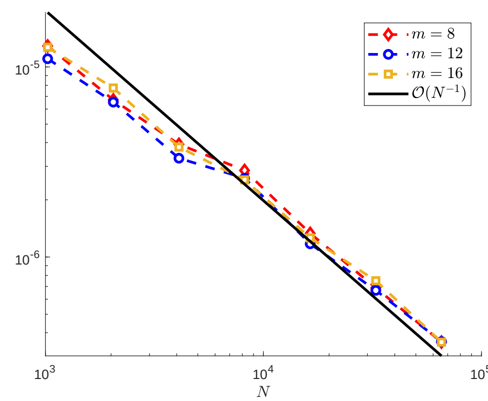
The next example shows the dimension-independence of the convergence of QMC in high dimensions.

Example 4.3. Consider the Schrödinger equation (2.1) with $\mathbb{T} = [-\pi, \pi], T = 1$, the initial condition (4.3) and the random potential (4.4). We consider $m = 8, 12, 16$.

Since m is large in this example, it is prohibitively expensive to compute a reference solution, and hence we cannot test the time convergence. However, we can still test the convergence of QMC



(a) Standard error of $S_T(\frac{\pi}{4})$ at $T=1$



(b) Standard error of $J_T(\frac{\pi}{4})$ at $T=1$

FIGURE 5. Convergence of QMC in Example 4.3

	$m=8$	$m=12$	$m=16$
$S_T(\frac{\pi}{4})$	1.0738	0.9912	1.0989
$J_T(\frac{\pi}{4})$	0.9951	0.9379	0.9253

(a) Example 4.3

	$m=8$	$m=12$	$m=16$
$S_T(\frac{\pi}{4})$	0.7732	0.7850	0.7578
$J_T(\frac{\pi}{4})$	0.7890	0.8074	0.8737

(b) Example 4.4 with $\alpha = 9/4$

	$m=8$	$m=12$	$m=16$
$S_T(\frac{\pi}{4})$	1.1881	1.1551	1.1459
$J_T(\frac{\pi}{4})$	0.9119	0.9201	0.9381

(c) Example 4.4 with $\alpha = 5/2$

TABLE 2. Fitted convergence rates in N of standard errors for Examples 4.3–4.4

using the following fact: for a general $F(\boldsymbol{\xi}_m)$

$$\sqrt{\frac{1}{R(R-1)}\sum_{k=1}^{R}\left(Q_{m,N}(F;\boldsymbol{\Delta}_k)-\overline{Q}_{m,N,R}(F)\right)^2} \approx \sqrt{\mathbb{E}^{\boldsymbol{\Delta}}[|\mathbb{E}[F]-Q_{m,N}(F;\boldsymbol{\Delta})|^2]}, \tag{4.7}$$

where the left-hand side is called the standard error of F and is an unbiased estimator for the right-hand side, which is the root mean square error of F. Therefore, we can use the standard error to test the convergence of QMC. The same idea is adopted in [24, 25, 63]. Let $S_T(x) = S(\psi_{m,\text{num}}(t=T,\boldsymbol{\xi}_m,x))$ and $J_T(x) = J(\psi_{m,\text{num}}(t=T,\boldsymbol{\xi}_m,x))$. We consider the standard errors of $S_T(\frac{\pi}{4})$ and $J_T(\frac{\pi}{4})$.

We use Lie–Trotter splitting in QMC-TS. We should observe dimension-indpendent and almost linear convergence of QMC by Theorem 2.4. We fix $\tau = 2\times 10^{-5}, h=\frac{\pi}{64}$ and choose $R=50$ and $N = 2^{10}, 2^{11}, \ldots, 2^{16}$. The standard errors are shown in Figure 5. The convergence rates of the standard errors, which are fitted using errors corresponding to $N = 2^{13}, 2^{14}, 2^{15}, 2^{16}$, are shown in Table 2a. The standard errors do not vary much as m changes, which confirms the dimension-independence of QMC quadrature error, and the convergence rates are close to 1. These results validate our theories.

The last example shows the effect of the decay rate of the randomness on the convergence rate of QMC.

Example 4.4. Consider the Schrödinger equation (2.1) with $\mathbb{T} = [-\pi, \pi], T = 1$, the initial condition (4.3) and the random potential

$$V_m(\boldsymbol{\xi}, x) = 1 + \sum_{j=1}^{m} \frac{1}{j^\alpha} \xi_j \cos(jx). \tag{4.8}$$

We consider $\alpha = \frac{9}{4}, \frac{5}{2}$ and $m = 8, 12, 16$.

By the discussion in Section 3.5, we would obtain dimension-independent convergence of QMC regardless of the splitting scheme for time discretization. Furthermore, Theorem 2.4 shows that the convergence rate of QMC would be $\frac{3}{4}$ if $\alpha = \frac{9}{4}$ and would be almost linear if $\alpha = \frac{5}{2}$. We still consider the standard errors of $S_T(\frac{\pi}{4})$ and $J_T(\frac{\pi}{4})$.

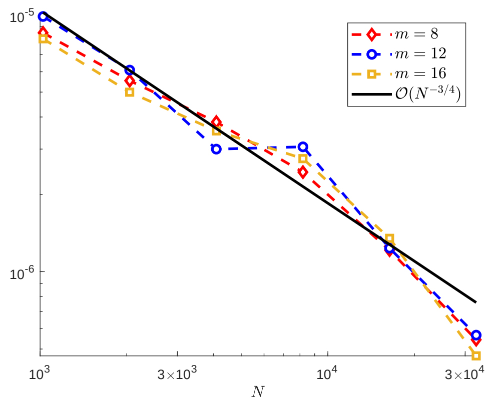
We use the Strang splitting in QMC-TS. We fix $\tau = 10^{-4}, h = \frac{\pi}{64}$ and choose $R = 50$ and $N = 2^{10}, 2^{11}, \ldots, 2^{15}$. The standard errors are shown in Figure 6, and the fitted convergence rates are shown in Tables 2b and 2c. We still see from Figure 6 that the standard errors do not vary much with different values of m, which again confirms the dimension-independence of convergence of QMC. Furthermore, we see from Table 2b that for $\alpha = \frac{9}{4}$ the fitted convergence rate of the standard error of $S_T(\frac{\pi}{4})$ is around the theoretical value $\frac{3}{4}$ and that of $J_T(\frac{\pi}{4})$ is slightly larger than $\frac{3}{4}$. On the other hand, we see from Table 2c for $\alpha = \frac{5}{2}$, the fitted convergence rates of the standard errors of both $S_T(\frac{\pi}{4})$ and $J_T(\frac{\pi}{4})$ are around the theoretical value 1. These results show that faster decay of randomness in the potential leads to faster convergence of QMC, which is consistent with Theorem 2.4.

Acknowledgement

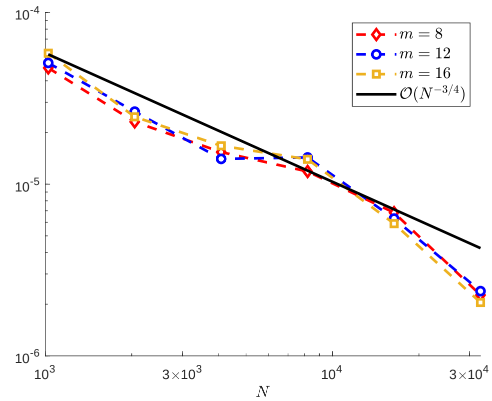
X. Zhao is supported by National Key Research and Development Program of China (Project 2024YFE03240400) and National Natural Science Foundation of China (Projects 42450275 and 12271413). Z. Zhang was supported by the National Natural Science Foundation of China (Projects 92470103 and 12171406), the Hong Kong RGC grant (Projects 17307921 and 17304324), seed funding from the HKU-TCL Joint Research Center for Artificial Intelligence, and the Outstanding Young Researcher Award of HKU (2020-21). The authors would like to thank Professor Ivan G. Graham (University of Bath), Professor Frances Kuo (University of New South Wales), and Doctor James A. Nichols (Australian National University) for helpful discussions on the coding for constructing the generating vector by the CBC algorithm. The computations were performed using research computing facilities provided by Information Technology Services, the University of Hong Kong.

References

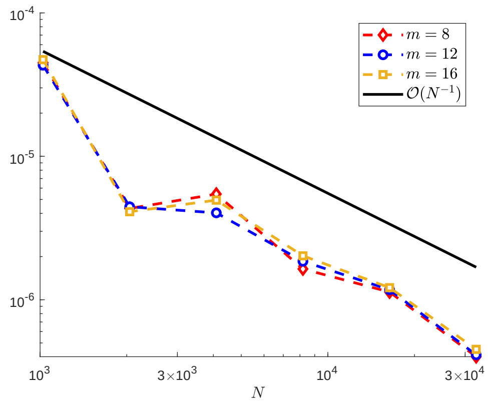
[1] R. A. Adams and J. J. Fournier, *Sobolev spaces*, Academic Press, 2021.
[2] P. W. Anderson, *Absence of diffusion in certain random lattices*, Phys. Rev., 109 (1958), p. 1492.
[3] I. Babuška, F. Nobile, and R. Tempone, *A stochastic collocation method for elliptic partial differential equations with random input data*, SIAM J. Numer. Anal., 45 (2007), pp. 1005–1034.
[4] W. Bao and Y. Cai, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Models, 6 (2013), pp. 1–135.
[5] E. T. Bell, *Exponential polynomials*, Ann. Math., 35 (1934), pp. 258–277.
[6] V. I. Bogachev, *Gaussian measures*, vol. 62, American Mathematical Society, 1998.



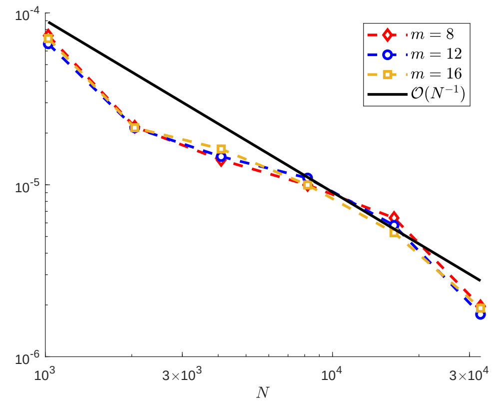
(a) Standard error of $S_T(\frac{\pi}{4})$ with $\alpha = \frac{9}{4}$



(b) Standard error of $J_T(\frac{\pi}{4})$ with $\alpha = \frac{9}{4}$



(c) Standard error of $S_T(\frac{\pi}{4})$ with $\alpha = \frac{5}{2}$



(d) Standard error of $J_T(\frac{\pi}{4})$ with $\alpha = \frac{5}{2}$

FIGURE 6. Convergence of QMC in Example 4.4, with $T = 1$

[7] R. E. CAFLISCH, *Monte Carlo and quasi-Monte Carlo methods*, Acta Numer., 7 (1998), pp. 1–49.

[8] J. CHARRIER, *Strong and weak error estimates for elliptic partial differential equations with random coefficients*, SIAM J. Numer. Anal., 50 (2012), pp. 216–246.

[9] A. COHEN, R. DEVORE, AND C. SCHWAB, *Convergence rates of best N-term Galerkin approximations for a class of elliptic sPDEs*, Found. Comput. Math., 10 (2010), pp. 615–646.

[10] C. CONTI, *Solitonization of the Anderson localization*, Phys. Rev. A, 86 (2012), p. 061801.

[11] G. DA PRATO AND J. ZABCZYK, *Stochastic equations in infinite dimensions*, Cambridge university press, 2014.

[12] A. DEBUSSCHE AND J. MARTIN, *Solution to the stochastic Schrödinger equation on the full space*, Nonlinearity, 32 (2019), p. 1147–1174.

[13] A. DEBUSSCHE AND H. WEBER, *The Schrödinger equation with spatial white noise potential*, Electron. J. Probab., 23 (2018), p. 1–16.

[14] J. DICK, *On the convergence rate of the component-by-component construction of good lattice rules*, J. Complexity, 20 (2004), pp. 493–522.

[15] J. DICK, F. Y. KUO, AND I. H. SLOAN, *High-dimensional integration: the quasi-Monte Carlo way*, Acta Numer., 22 (2013), pp. 133–288.

[16] L. DUMAZ AND C. LABBÉ, *Localization of the continuous Anderson Hamiltonian in 1-D*, Probab. Theory Relat. Fields, 176 (2020), p. 353–419.

[17] T. P. EGGARTER, *Schrödinger equation with a random potential: A functional approach*, J. Math. Phys., 14 (1973), pp. 1308–1313.

[18] X. FERNIQUE, *Regularite des trajectoires des fonctions aleatoires gaussiennes*, in Ecole d'Eté de Probabilités de Saint-Flour IV—1974, P. L. Hennequin, ed., Berlin, Heidelberg, 1975, Springer Berlin Heidelberg, pp. 1–96.

[19] S. Fishman, A. Iomin, and K. Mallick, *Asympotic localization of stationary states in the nonlinear Schrödinger equation*, Phys. Rev. E, 78 (2008), p. 066605.

[20] S. Flach, D. Krimer, and C. Skokos, *Universal spreading of wave packets in disordered nonlinear systems*, Phys. Rev. Lett., 102 (2009), p. 024101.

[21] M. Ganesh, F. Y. Kuo, and I. H. Sloan, *Quasi-Monte Carlo finite element analysis for wave propagation in heterogeneous random media*, SIAM/ASA J. Uncertain. Quantif., 9 (2021), pp. 106–134.

[22] F. Germinet and A. Klein, *A comprehensive proof of localization for continuous Anderson models with singular random potentials*, J. Eur. Math. Soc., 15 (2013), p. 53–143.

[23] R. G. Ghanem and P. D. Spanos, *Stochastic finite elements: a spectral approach*, Springer, New York, 1991.

[24] A. D. Gilbert, I. G. Graham, F. Y. Kuo, R. Scheichl, and I. H. Sloan, *Analysis of quasi-Monte Carlo methods for elliptic eigenvalue problems with stochastic coefficients*, Numer. Math., 142 (2019), pp. 863–915.

[25] I. G. Graham, F. Y. Kuo, J. A. Nichols, R. Scheichl, C. Schwab, and I. H. Sloan, *Quasi-Monte Carlo finite element methods for elliptic PDEs with lognormal random coefficients*, Numer. Math., 131 (2015), pp. 329–368.

[26] I. G. Graham, F. Y. Kuo, D. Nuyens, I. H. Sloan, and E. A. Spence, *Quasi-Monte Carlo methods for uncertainty quantification of wave propagation and scattering problems modelled by the Helmholtz equation*, arXiv preprint arXiv:2502.12451, (2025).

[27] P. A. Guth, V. Kaarnioja, F. Y. Kuo, C. Schillings, and I. H. Sloan, *A quasi-Monte Carlo method for optimal control under uncertainty*, SIAM/ASA J. Uncertain. Quantif., 9 (2021), pp. 354–383.

[28] ———, *Parabolic PDE-constrained optimal control under uncertainty with entropic risk measure using quasi-Monte Carlo integration*, Numer. Math., 156 (2024), pp. 565–608.

[29] M. Hardy, *Combinatorics of partial derivatives*, Electron. J. Combin., 13 (2006), pp. 1–13.

[30] J. Hu, S. Jin, and D. Xiu, *A stochastic Galerkin method for Hamilton–Jacobi equations with uncertainty*, SIAM J. Sci. Comput., 37 (2015), pp. A2246–A2269.

[31] S. Jin, P. Markowich, and C. Sparber, *Mathematical and computational methods for semiclassical Schrödinger equations*, Acta Numer., 20 (2011), pp. 121–209.

[32] O. Kallenberg, *Foundations of modern probability*, Springer, 2021.

[33] K. Karhunen, *Über lineare methoden in der wahrscheinlichkeitsrechnung*, Ann. Acad. Sci. Fenn., 37 (1947), pp. 3–79.

[34] F. Y. Kuo, *Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces*, J. Complexity, 19 (2003), pp. 301–320.

[35] F. Y. Kuo and D. Nuyens, *Application of quasi-Monte Carlo methods to elliptic PDEs with random diffusion coefficients: a survey of analysis and implementation*, Found. Comput. Math., 16 (2016), pp. 1631–1696.

[36] F. Y. Kuo, C. Schwab, and I. H. Sloan, *Quasi-Monte Carlo methods for high-dimensional integration: the standard (weighted Hilbert space) setting and beyond*, ANZIAM J., 53 (2011), pp. 1–37.

[37] F. Y. Kuo, C. Schwab, and I. H. Sloan, *Quasi-Monte Carlo finite element methods for a class of elliptic partial differential equations with random coefficients*, SIAM J. Numer. Anal., 50 (2012), pp. 3351–3374.

[38] F. Y. Kuo, I. H. Sloan, G. W. Wasilkowski, and B. J. Waterhouse, *Randomly shifted lattice rules with the optimal rate of convergence for unbounded integrands*, J. Complexity, 26 (2010), pp. 135–160.

[39] F. Y. Kuo, G. W. Wasilkowski, and B. J. Waterhouse, *Randomly shifted lattice rules for unbounded integrands*, J. Complexity, 22 (2006), pp. 630–651.

[40] I. Lifshits, L. Gredeskul, and L. Pastur, *Introduction to the theory of disordered systems*, Wiley-Interscience, New York, 1988.

[41] M. Loève, *Fonctions aleatoire du second ordre*, in Processus stochastiques et mouvement brownien, Gauthier-Villars, 1948.

[42] C. Lubich, *On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations*, Math. Comp., 77 (2008), pp. 2141–2153.

[43] P. A. Markowich, P. Pietra, and C. Pohl, *Numerical approximation of quadratic observables of Schrödinger-type equations in the semi-classical limit*, Numer. Math., 81 (1999), pp. 595–630.

[44] P. A. Markowich, P. Pietra, C. Pohl, and H. P. Stimming, *A Wigner-measure analysis of the Dufort–Frankel scheme for the Schrödinger equation*, SIAM J. Numer. Anal., 40 (2002), pp. 1281–1310.

[45] J. A. Nichols and F. Y. Kuo, *Fast CBC construction of randomly shifted lattice rules achieving $\mathcal{O}(n-1+\delta)$ convergence for unbounded integrands over $\mathbb{R}^s$ in weighted spaces with POD weights*, J. Complexity, 30 (2014), pp. 444–468.

[46] F. Nobile, R. Tempone, and C. G. Webster, *A sparse grid stochastic collocation method for partial differential equations with random input data*, SIAM J. Numer. Anal., 46 (2008), pp. 2309–2345.
[47] D. Nuyens, *QMC4PDE*. `https://people.cs.kuleuven.be/~dirk.nuyens/qmc4pde/`. webpage.
[48] D. Nuyens and R. Cools, *Fast algorithms for component-by-component construction of rank-1 lattice rules in shift-invariant reproducing kernel Hilbert spaces*, Math. Comp., 75 (2006), pp. 903–920.
[49] C. Schwab and C. J. Gittelson, *Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs*, Acta Numer., 20 (2011), pp. 291–467.
[50] J. Shen, T. Tang, and L.-L. Wang, *Spectral methods: algorithms, analysis and applications*, vol. 41, Springer Science & Business Media, 2011.
[51] R. Shu, J. Hu, and S. Jin, *A stochastic Galerkin method for the Boltzmann equation with multi-dimensional random inputs using sparse wavelet bases*, Numer. Math. Theory Methods Appl., 10 (2017), pp. 465–488.
[52] I. H. Sloan, F. Y. Kuo, and S. Joe, *Constructing randomly shifted lattice rules in weighted Sobolev spaces*, SIAM J. Numer. Anal., 40 (2002), pp. 1650–1665.
[53] G. Strang, *On the construction and comparison of difference schemes*, SIAM J. Numer. Anal., 5 (1968), pp. 506–517.
[54] C. Su and X. Zhao, *On time-splitting methods for nonlinear Schrödinger equation with highly oscillatory potential*, ESAIM Math. Model. Numer. Anal., 54 (2020), pp. 1491–1508.
[55] T. Tang and T. Zhou, *Convergence analysis for stochastic collocation methods to scalar hyperbolic equations with a random wave speed*, Commun. Comput. Phys, 8 (2010), pp. 226–248.
[56] T. Tao, *Nonlinear dispersive equations: local and global analysis*, American Mathematical Soc., 2006.
[57] M. Thalhammer, *High-order exponential operator splitting methods for time-dependent schrödinger equations*, SIAM J. Numer. Anal., 46 (2008), pp. 2022–2038.
[58] H. F. Trotter, *On the product of semi-groups of operators*, Proc. Amer. Math. Soc., 10 (1959), pp. 545–551.
[59] X. Wang, *Strong tractability of multivariate integration using quasi–Monte Carlo algorithms*, Math. Comp., 72 (2003), pp. 823–838.
[60] B. J. Waterhouse, F. Y. Kuo, and I. H. Sloan, *Randomly shifted lattice rules on the unit cube for unbounded integrands in high dimensions*, J. Complexity, 22 (2006), pp. 71–101.
[61] Z. Wu and Z. Huang, *A Bloch decomposition-based stochastic Galerkin method for quantum dynamics with a random external potential*, J. Comput. Phys., 317 (2016), pp. 257–275.
[62] ———, *Convergence analysis on stochastic collocation methods for the linear Schrodinger equation with random inputs*, Adv. Appl. Math. Mech., 12 (2020), pp. 30–56.
[63] Z. Wu, Z. Zhang, and X. Zhao, *Error estimate of a quasi-Monte Carlo time-splitting pseudospectral method for nonlinear Schrödinger equation with random potentials*, SIAM/ASA J. Uncertain. Quantif., 12 (2024), pp. 1–29.
[64] D. Xiu and G. E. Karniadakis, *The Wiener–Askey polynomial chaos for stochastic differential equations*, SIAM J. Sci. Comput., 24 (2002), pp. 619–644.
[65] X. Zhao, *Numerical integrators for continuous disordered nonlinear Schrödinger equation*, J. Sci. Comput., 89 (2021), p. 40.

Z. Wu: Department of Mathematics, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China.

Email address: `wuzz@hku.hk`

Z. Zhang: Department of Mathematics, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China. Materials Innovation Institute for Life Sciences and Energy (MILES), HKU-SIRI, Shenzhen, China.

Email address: `zhangzw@hku.hk`

X. Zhao: School of Mathematics and Statistics & Computational Sciences Hubei Key Laboratory, Wuhan University, Wuhan, 430072, China.

Email address: `matzhxf@whu.edu.cn`

URL: `http://jszy.whu.edu.cn/zhaoxiaofei/en/index.htm`