Exponential integrators for stochastic Schrödinger equations

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We present a class of exponential integrators to compute solutions of the stochastic Schrödinger equations arising from the modeling of open quantum systems. To be able to implement the methods within the same framework as the deterministic counterpart, we express the solution using Kunita's representation. With appropriate truncations, the solution operator can be written as matrix exponentials, which can be efficiently implemented by the Krylov subspace projection. The accuracy is examined in terms of the strong convergence by comparing trajectories, and in terms of the weak convergence by comparing the density-matrix operators. We show that the local accuracy can be further improved by introducing third-order commutators in the exponential. The effectiveness of the proposed methods is tested using the example from Di Ventra *et al.* [J. Phys.: Condens. Matter **16**, 8025 (2004)].

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I. INTRODUCTION

The modeling of open quantum systems has been a subject of immense interest for decades [1–3]. The primary focus is on quantum systems coupled to the environment. While direct computation based on the entire system is infeasible, reduced models where the influence from the bath is implicitly incorporated have shown great promise. One remarkable approach is the stochastic Schrödinger equation (SSE), which can be formally derived from the Schrödinger equation for the entire system by using a projection formalism [4], together with a Markovian approximation. On the other hand, the dynamics of the density-matrix follows a Liouville von Neumann equation that agrees with the Lindblad equation [5]. Therefore, it can be used as a computational approach to obtain the density matrix, especially when the dimension of the problem is high. The SSE has been used in quantum transport to study nonequilibrium transport problems by Di Ventra and coworkers [6] as well as the extension to time-dependent density-functional theory [7,8]. A recent review [9] surveyed many of these aspects.

This paper is primarily concerned with the numerical treatment of the SSE. In the deterministic case, i.e., the time-dependent Schrödinger equation (TDSE), many numerical methods are available. Typically, due to the large number of degrees of freedom in many practical applications, the efficiency has been an important focus in selecting an appropriate method. In addition, the time reversibility and the unitary property of the evolution operator are also desired. These considerations seem to deem classical Runge-Kutta methods unfavorable. Finally, since the timescale associated with electron dynamics is often on the order of attoseconds, there is a stringent limit on the size of the time steps. Although many implicit methods can greatly mitigate this issue, the implementation is often not straightforward. By a comparative study of some existing methods, Castro *et al.* [10] demonstrated that numerical methods can be constructed based on the exponential representation of the solution operator. The Krylov subspace method with Lanczos orthogonalization has been the most efficient in terms of the overall computation cost [10]. This technique approximates the matrix exponential by projecting it onto a subspace [11], and the problem is reduced to computing the matrix exponential of a smaller matrix which can be easily tackled by many existing methods [12].

Unlike the deterministic case, not many methods have been developed, particularly for the SSE. Some of the subtleties in treating stochastic models numerically have been explained in Ref. [13]. The classical Euler-Maruyama and Milstein methods [14] are simple extensions of the Runge-Kutta methods in solving stochastic models and, similar to the deterministic case, they may not be well suited for SSEs. Many of the standard higher-order methods [14] are quite involved in the case of systems of equations with multiplicative noise. In this paper, we propose to extend the framework of exponential integrators for deterministic systems [10,15] to the SSE. We first express the solution operator by using Kunita's notation [16] in the context of stochastic differential equations (SDEs), where the operator in the exponential consists of an infinite series of commutators and multiple stochastic integrals. With truncations, we obtain approximations of the solution operator. We then show that, once the stochastic noise is realized, the truncated operator represents deterministic Schrödinger equations, and a matrix exponential can be used to represent the solution. At this point, the Krylov subspace method can

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again be used. Since the Hamiltonian in this case is no longer Hermitian, we use Arnodi's algorithm [17] to obtain the orthogonal basis.

We also studied the order of accuracy of the proposed methods. We follow two tracks: strong convergence, where the approximate solution is compared with the true solution on a trajectory-wise basis, and the weak convergence, where we study the accuracy in terms of the density matrix. This is particularly important since physical observables, e.g., electron density and current, can be directly obtained from the density matrix.

Some of the key steps in the construction of the algorithms will be summarized as lemmas and theorems. They are presented in this manner not for the purpose of mathematical rigor but to emphasize the mathematical tools and the generality of the formulation, and to clarify the setting under which these methods can be used. It is our hope that interested readers can adapt this approach to other quantum stochastic models and construct useful computational methods.

The remaining part of this paper is organized as follows: in Sec. II, we present the theory behind the construction of the algorithms. We start by defining the solution operator for the SSE, and then derive the exponential integrators as well as the approximation schemes. We examine the accuracy and the extension to nonlinear problems. In Sec. III, we present the numerical results to demonstrate the effectiveness of the exponential schemes.

II. THEORY AND METHODS

Assuming atomic units $\hbar = 1$ and $m = 1$, we consider a SSE as follows:

$$\begin{aligned} d\psi(\mathbf{r},t) &= \left(-i\hat{H} - \tfrac{1}{2}\hat{V}^*\hat{V}\right)\psi(\mathbf{r},t)dt + \hat{V}\psi(\mathbf{r},t)dW_t, \\ \psi(\mathbf{r},0) &= \psi_0. \end{aligned} \tag{1}$$

Here we have chosen to write the SDEs in the conventional form [18], where solutions are interpreted in integral forms. In (1), $\psi(\mathbf{r},t)$ is the wave function in an appropriate Hilbert space. Typically the system has multiple orbitals, each of which would satisfy an equation of this form, but it suffices to describe the case with a single wave function. In equation (1), $\hat{H}$ is a Hermitian operator for the Hamiltonian, and $\hat{V}$ is the bath operator. W_t is the standard one-dimensional Wiener process [18]. Formally $\ell(t) \doteq \frac{dW_t}{dt}$ can be interpreted as white noise. In applications, the system could be coupled with multiple environments; then there would a set of heat baths $\hat{V}_\alpha$, corresponding to a set of stochastic noises $\{l_\alpha(t)\}$. The Markovian assumption embodies the following properties:

$$\begin{aligned} \overline{\ell_\alpha(t)} &= 0, \\ \overline{\ell_\alpha(t)\ell_\beta(t')} &= \delta_{\alpha,\beta}\delta(t-t'), \end{aligned} \tag{2}$$

where the overline indicates the stochastic average over an ensemble of realizations of the Brownian motion. Finally, as emphasized numerous times in the literature, the SSE (1) is interpreted in the Itô sense [18].

In the following discussion, we generally assume that the Hamiltonian $\hat{H}$ is linear. In the case where $\hat{H}$ is nonlinear, we adopt the operator-splitting method (e.g., see Refs. [19,20]), which separates the Hamiltonian into linear and nonlinear parts. This will be discussed in detail in Sec. II C. Throughout this paper, we also assume that the operators $\hat{H}$ and $\hat{V}$ have been discretized spatially.

Before we present approximation schemes, we first discuss how the *exact* solution can be represented.

A. Solution operators for general deterministic and stochastic systems

We start by considering the deterministic case, i.e., where the stochastic bath operator $V \equiv 0$. Inspired by the idea of the Koopman operator [21–23], we give a representation of the solution in the form of an exponential operator. More specifically, for a general n-dimensional autonomous dynamical system,

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{3}$$

the Koopman operator $\mathcal{U}(t)$ describes the evolution of an observable A,

$$A\,\mathbf{x}(t) = \mathcal{U}(t)A(\mathbf{x}_0).$$

It can be expressed in an exponential form,

$$\mathcal{U}(t) = e^{\mathcal{L}t}, \quad \mathcal{L} = \mathbf{F}(\mathbf{x}_0)\cdot\nabla_{\mathbf{x}_0}. \tag{4}$$

By applying this result to the deterministic Schrödinger equation, we have the following formula:

Lemma II.1. When $\hat{V} \equiv 0$, the solution of the SSE (1) can be represented by the exponential operator

$$\psi(\mathbf{r},t) = \exp(\hat{D}_t)\psi_0, \tag{5}$$

where $\hat{D}_t$ is a differential operator given by

$$\hat{D}_t = -it\hat{H}\left(\psi_0\frac{\partial}{\partial\psi_0} - \psi_0^*\frac{\partial}{\partial\psi_0^*}\right). \tag{6}$$

Here ψ^* denotes the complex conjugate of ψ.

Furthermore, due to the linearity of the SSE (1), the solution can also be expressed as a matrix or operator exponential,

$$\psi(\mathbf{r},t) = \exp(-it\hat{H})\psi_0. \tag{7}$$

The matrix exponential is defined by the Taylor series of the exponential function.

A short derivation can be found in Appendix A. We should point out that, in principle, the Koopman's solution form (5) holds for general nonlinear systems, and it can be regarded as the foundation of operator-splitting algorithms, e.g., those for classical molecular dynamics models [20] and quantum mechanics models [20]. Although it is not directly relevant to the discussions here, the Koopman operator can be applied to functions of the state variable. For nonautonomous systems, the Koopman operator can be extended by including the term ∂_{t_0}, where t_0 is the initial time. This bypasses the use of time-ordered time evolution operators, and it has been used in Ref. [20] to incorporate a time-dependent potential.

Now we turn to the stochastic case. We first introduce Kunita's results for a general SDE [16]. More specifically, we have:

Theorem II.1 (Kunita 1980, Lemma 2.1). For an autonomous SDE of the Stratonovich type,

$$dz_t = a(z_t)dt + b(z_t) \circ dW_t, \tag{8}$$

the solution with an initial value $z(0) = z_0$ can be represented as

$$z(t) = \exp(\hat{D}_t) z_0, \tag{9}$$

where the differential operator $\hat{D}_t$ is given by

$$\hat{D}_t = tX_0 + W_t X_1 + \frac{1}{2}(J_{(0,1)} - J_{(1,0)})[X_0, X_1] + \sum_{J;3\leqslant|J|} \left\{ \sum_{\Delta J}^{*} c_{\Delta J} W^{\Delta J}(t) \right\} X^J. \tag{10}$$

Here X_0 and X_1 are differential operators defined by

$$X_0 \doteq \sum_{i=1}^{n} a^i \partial_i, \quad X_1 \doteq \sum_{i=1}^{n} b^i \partial_i, \quad \partial_i \doteq \frac{\partial}{\partial z_{0,i}}. \tag{11}$$

In addition, $J_{(0,1)}$ and $J_{(1,0)}$ are Stratonovich stochastic integrals defined respectively as

$$J_{(0,1)} \doteq \int_0^t s dW_s, \qquad J_{(1,0)} \doteq \int_0^t W_s ds. \tag{12}$$

The notation $[X_0, X_1]$ is the usual Lie bracket defined by $X_0X_1 - X_1X_0$; $J = (j_1, \ldots, j_m)$ indicates multi-indices, and $X^J = [\cdots[X_{j_1}, X_{j_2}]\cdots X_{j_m}]$ are high-order commutators. The rest of the notation has been defined explicitly in Kunita's work [16].

Note that, in this lemma, the stochastic equations are of the Stratonovich type [18]. But SDEs of this type can be converted from (and to) Itô SDEs. More specifically, for a general n-dimensional Itô SDE

$$dz_t = a(t, z_t)dt + b(t, z_t)dW_t, \tag{13}$$

where $a, z_t \in \mathbb{R}^n$, $b \in \mathbb{R}^{n\times m}$, and $W_t \in \mathbb{R}^m$. The corresponding Stratonovich SDEs are given by [18]

$$dz_t = \underline{a}(t, z_t)dt + b(t, z_t) \circ dW_t. \tag{14}$$

Here the modified drift term is defined componentwise by

$$\underline{a}^i(t, z) = a^i(t, z) - \frac{1}{2}\sum_{j=1}^{n}\sum_{k=1}^{m} b^{j,k}(t, z)\frac{\partial b^{i,k}}{\partial x_j}(t, z). \tag{15}$$

Therefore, to use Kunita's notation, we first need to switch our Itô-type SSE (1) to the corresponding Stratonovich type,

$$d\psi(\mathbf{r}, t) = \left[-i\hat{H} - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]\psi(\mathbf{r}, t)dt + \hat{V}\psi(\mathbf{r}, t) \circ dW_t. \tag{16}$$

Effectively, this introduces the additional drift term $-\frac{1}{2}\hat{V}^2\psi$.

Now we apply Kunita's lemma [16] to (16) and, by direct computation, we have the following corollary:

Corollary II.1. The solution of equation (1) [or equivalently (16)] can be represented as

$$\psi(\mathbf{r}, t) = \exp(\hat{D}_t)\psi(\mathbf{r}, 0), \tag{17}$$

where the solution operator $\hat{D}_t$ can be approximated by

$$\hat{D}_t \approx \hat{D}_t^I \doteq \left[-i\hat{H} - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]t + \hat{V}W_t, \tag{18}$$

by keeping the first-order Stratonovich integrals, and

$$\hat{D}_t \approx \hat{D}_t^{\mathrm{II}} \doteq \left[-i\hat{H} - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]t + \hat{V}W_t + \tfrac{1}{2}[J_{(0,1)}(t) - J_{(1,0)}(t)]\left(\tfrac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} + i[\hat{H}, \hat{V}]\right). \tag{19}$$

by retaining the second-order Stratonovich integrals.

The truncation is justified on the grounds that the stochastic integrals have decreasing variance [14]. Interested readers can find the detailed derivation in Appendix B.

B. Exponential integrators

Based on the truncated Kunita notation of the solution operator, one can construct numerical methods [19,24,25]. Here we focus on one-step methods, where the solution at the next step is updated based only on the solution at the current step [14]. The same procedure would be repeated at each time step. In this case, it is enough to illustrate the methods within one step, e.g., from $t = 0$ to $t = \Delta t$, with Δt being the step length. To this end, we first sample W_t and write

$$\Delta W = W_{\Delta t} - W_0. \tag{20}$$

For later steps, we define $\Delta W_n = W_{t_{n+1}} - W_{t_n}$, and simply replace ΔW by ΔW_n and apply the same procedure. In the following context we also use $\psi(t_n) \approx \psi_n$ as the numerical approximation of the state vector ψ at time t_n.

With this notation, the first-order truncation, when applied to the initial condition, becomes,

$$\hat{D}_{\Delta t}^I = \left\{\left[-i\hat{H} - \frac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]\Delta t + \hat{V}\Delta W\right\}\psi\frac{\partial}{\partial\psi} + \left\{\left[i\hat{H} - \frac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]\Delta t + \hat{V}\Delta W\right\}\psi^*\frac{\partial}{\partial\psi^*}. \tag{21}$$

Since ΔW has been realized, the operator above can be viewed as a deterministic operator, and in light of the Koopman's notation (5), it generates a solution of the following ordinary differential equations (ODEs):

$$\frac{\partial}{\partial\tau}\phi = \left[-i\hat{H} - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]\phi\Delta t + \hat{V}\phi\Delta W, \quad \tau \in [0, \Delta t]. \tag{22}$$

In particular, Lemma II.1 implies that the solution can be written as an exponential,

$$\phi(\Delta t) = \exp(-i\Delta t\hat{\mathcal{H}}_{\mathrm{I}})\phi(0), \tag{23}$$

where

$$\hat{\mathcal{H}}_{\mathrm{I}} = \hat{H} - \frac{i}{2}(\hat{V}^* + \hat{V})\hat{V} + i\frac{\Delta W}{\Delta t}\hat{V}. \tag{24}$$

Using (23) we construct the follow exponential scheme,

$$\psi_{n+1} = \exp(-i\Delta t\hat{\mathcal{H}}_{\rm I})\psi_n. \tag{25}$$

We later refer to this scheme as Scheme I. The matrix exponential in (23) will be treated by using Krylov subspace projection method together with the Arnoldi's method [15,17]. In general, this algorithm yields

$$A \approx V_m H_m V_m^*, \tag{26}$$

where m is the dimension of the Krylov subspace, $H_m \in \mathbb{C}^{m\times m}$ is a Hessenberg matrix, and $V_m \in \mathbb{C}^{N\times m}$ consists of m orthonormal column vectors. Thus the matrix exponential is approximated by

$$\exp(A)v \approx V_m \exp(H_m)e_1, \tag{27}$$

where e_1 is the first unit vector in $\mathbb{C}^m$.

Since m is relatively small, $\exp(H_m)$ is much easier to compute than the original matrix exponential and can be computed by any of the current methods that computes a matrix exponential [12]. In our numerical experiment (Sec. III), even $m = 3$ is adequate.

We should note that, although we only take the first-order terms in the exponent in Scheme I, this method is different from the Euler-Maruyama method. In fact, a direct expansion yields the term $\frac{1}{2}(\nabla b)b\Delta W^2$, which appears in the Milsteins scheme, a first-order method (rather than 0.5 order).

Similarly, we construct an integrator by the truncation of the solution operator $\hat{D}_t$ up to the second-order Stratonovich integral,

$$\begin{aligned}\hat{D}^{\rm II}_{\Delta t} = &\left[\left\{-i\hat{H} - \frac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right\}\Delta t + \hat{V}\Delta W + \Delta U\left(\frac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} + i[\hat{H}, \hat{V}]\right)\right]\psi\frac{\partial}{\partial\psi}\\ &+\left[\left\{i\hat{H} - \frac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right\}\Delta t + \hat{V}\Delta W + \Delta U\left(\frac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} - i[\hat{H}, \hat{V}]\right)\right]\psi^*\frac{\partial}{\partial\psi^*},\end{aligned} \tag{28}$$

where $\Delta U = \frac{1}{2}(J_{(0,1)} - J_{(1,0)})$ is a Gaussian random variable [14] with mean zero and variance $\frac{\Delta t^3}{12}$.

Once ΔW and ΔU are realized, the solution corresponds to that of the following ODEs:

$$\begin{aligned}\frac{\partial}{\partial\tau}\psi = &\left[-i\hat{H} - \frac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\right]\psi\Delta t + \hat{V}\psi\Delta W\\ &+\left(\frac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} + i[\hat{H}, \hat{V}]\right)\psi\Delta U, \quad \tau \in [0, \Delta t].\end{aligned} \tag{29}$$

An exponential scheme can then be constructed accordingly:

$$\psi_{n+1} = \exp(-i\Delta t\hat{\mathcal{H}}_{\rm II})\psi_n, \tag{30}$$

where the matrix $\hat{\mathcal{H}}_{\rm II}$ is given by

$$\begin{aligned}\hat{\mathcal{H}}_{\rm II} = &\hat{H} - \frac{i}{2}(\hat{V}^* + \hat{V})\hat{V} + i\frac{\Delta W}{\Delta t}\hat{V}\\ &+ i\frac{\Delta U}{\Delta t}\left(\frac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} + i[\hat{H}, \hat{V}]\right).\end{aligned} \tag{31}$$

We later refer to this scheme as Scheme II. Scheme II has one more term in the exponential than Scheme I.

The higher-order Stratonovich integral terms from Kunita's expansion are complicated. But we discovered that, by incorporating two more commutator terms in our truncation, we get better convergence results with respect to the density-matrix operator. This will be referred to as Scheme III. It is as follows:

$$\psi_{n+1} = \exp(-i\Delta t\hat{\mathcal{H}}_{\rm III})\psi_n, \tag{32}$$

where

$$\hat{\mathcal{H}}_{\rm III} = \hat{\mathcal{H}}_{\rm II} + i\Delta t\left(\frac{1}{24}[\hat{V}, [\hat{V}^*, \hat{V}]\hat{V}] + \frac{i}{12}[\hat{V}, [\hat{H}, \hat{V}]]\right). \tag{33}$$

C. The extension to nonlinear stochastic Schrödinger equations

In the discussion above we have assumed that the Hamiltonian is linear and independent of time. The extension to nonlinear problems, e.g., those that resemble the Kohn-Sham equations in the time-dependent density-functional theory [26,27] with an external potential, is straightforward. Following Watanabe and Ksukada [20], we can separate the Hamiltonian as

$$H = H_0 + H_1(t), \tag{34}$$

where H_0 is the linear part and $H_1(t)$ contains the nonlinear contribution. We assume that the nonlinearity appears in the potential as a local operator. Then, a one-step can method be constructed by using an operator-splitting method [20],

$$\begin{aligned}\psi_{n+1} = &\exp\left(\frac{\Delta t}{2}\partial_{t_n}\right)\exp\left(-i\frac{\Delta t}{2}H_1\right)\exp(-i\Delta t H_0)\\ &\times\exp\left(-i\frac{\Delta t}{2}H_1\right)\exp\left(\frac{\Delta t}{2}\partial_{t_n}\right)\psi_n.\end{aligned} \tag{35}$$

The operator ∂_{t_n} operates on quantities that explicitly depend on the time variable. The exponential associated with the linear Hamiltonian was discussed in the previous section. On the other hand, the exponential for the nonlinear part, due to the fact that H_1 is diagonal, is also straightforward. The error associated with the splitting, which can be analyzed by using the Baker-Campbell-Hausdorff (BCH) formula [28], is locally $O(\Delta t^3)$.

D. The accuracy of the exponential integrators

Now we discuss the accuracy of our schemes as $\Delta t \to 0$. Unlike the deterministic case, the convergence of numerical

methods for stochastic models can be formulated in both the strong and weak sense [14].

Strong convergence. The strong convergence of these schemes is summarized as follows:

Theorem II.2. Let ψ_T be the exact solution of model (1) at time T. Let $\tilde{\psi}_T^{\Delta t}$ be the approximation by the exponential integrator discussed above at time T, with time discretization Δt. Then

$$\overline{\left|\tilde{\psi}_T^{\Delta t} - \psi_T\right|} \leqslant K_1 \Delta t^{\gamma} \tag{36}$$

holds, where the constants K_1, K_2 do not depend on Δt. Here $\gamma = 1$ for Scheme I, and $\gamma = 1.5$ for Scheme II.

Following the idea in the proof of Theorem 2.1 in Ref. [29], we can verify the accuracy by comparing the schemes to the stochastic Taylor expansion and utilizing Lemma 5.7.3 and Theorem 10.6.3 in Ref. [14].

Weak convergence. Following the notations in Kleoden and Platern [14], the weak convergence is in the sense of averages. As we alluded to in the introduction, a primary quantity of interest in open quantum systems is the density matrix. In the stochastic case, the density matrix is defined as the following ensemble average [8]:

$$\hat{\rho}(t) \doteq \overline{|\psi(t)\rangle\langle\psi(t)|}. \tag{37}$$

In general, the analysis of the weak convergence relies on the Dynkin's formula and the Kolmogorov backward equation [14]. However, for the SSE (1), one can actually write down an exact equation for the density matrix, known as the Lindblad equation [30]:

$$i\partial_t \rho = [H, \rho] - \frac{i}{2}(\hat{V}^*\hat{V}\rho + \rho\hat{V}^*\hat{V} - 2\hat{V}\rho\hat{V}^*). \tag{38}$$

This can be derived from SSE (1) by using the Itô's formula [18].

With the Lindblad equation, one can expand the density matrix at time $t = t_n$ as a power series in Δt. Meanwhile, all our schemes can be written in terms of ODEs (with random coefficients) and the corresponding approximate density matrix can also be expanded in the same manner. With direct comparison, we obtain the order of local consistency error, summarized as follows:

Theorem II.3. If ρ is the exact density matrix and $\hat{\rho}_{\rm I}$, $\hat{\rho}_{\rm II}$, $\hat{\rho}_{\rm III}$ are the approximations from Schemes I–III, respectively, then we have

$$\begin{aligned}
\rho(\Delta t) - \hat{\rho}_{\rm I}(\Delta t) &= O(\Delta t^2),\\
\rho(\Delta t) - \hat{\rho}_{\rm II}(\Delta t) &= O(\Delta t^2),\\
\rho(\Delta t) - \hat{\rho}_{\rm III}(\Delta t) &= O(\Delta t^3).
\end{aligned} \tag{39}$$

This suggests that Schemes I and II have order 1 weak convergence while Scheme III is second order. Surprisingly, Scheme II, which has higher strong order, does not have better convergence in terms of the density matrix. This problem is addressed by adding another term to the exponential integrator, and which hence leads to Scheme III. See Appendix C for details.

III. NUMERICAL RESULTS

We consider the example used by Di Ventra *et al.* [8] to demonstrate the performance of the proposed methods. The underlying Schrödinger equation, describing the dynamics of a one-dimensional gas of excited bosons confined in a harmonic potential and in contact with an external bath, is given in atomic units (a.u.) ($\hbar = m = 1$ throughout this section),

$$\begin{aligned}
d\psi(x,t) = &-i\left(-\frac{1}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2 + \tilde{g}n(x,t)\right)\psi(x,t)dt\\
&-\frac{1}{2}\hat{V}^*\hat{V}\psi(x,t)dt + \hat{V}\psi(x,t)dW_t.
\end{aligned} \tag{40}$$

Using the same treatment as in Di Ventra *et al.* [8], we first pick $\tilde{g} = 0$ and we choose the Hilbert space spanned by the basis set $\{\varphi_j : j = 1, \ldots, d\}$, consisting of the eigenfunctions of the quantum harmonic oscillators. The projection makes the Hamiltonian diagonal, and we choose $d = 20$. To test our schemes, we conducted simulations over the time interval $t \in [0, 1]$, with step size $\Delta t = 10^{-3}$. We also take the same bath operator,

$$\hat{V} \equiv \delta \begin{pmatrix} 0 & 1 & 1 & 1 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & \cdots \end{pmatrix}, \tag{41}$$

where δ is interpreted as a coupling constant.

Before we discuss the convergence results, we should mention that our schemes have shown good numerical stability. We computed the system with the bath operator defined above for different step sizes, and our schemes are stable for $\Delta t \leqslant 10^{-3}$, while the Euler-Maruyama method is stable only for $\Delta t \leqslant 10^{-5}$.

First we examine strong convergence. In Fig. 1 we compare the following error:

$$e(t) = \overline{\|\psi(t) - \hat{\psi}(t)\|}, \tag{42}$$

from the numerical methods. The expectation is approximated by an average over 100 runs. Here in our test, the exact solution ψ is computed by the 1.0 order Milstein scheme performed with a much smaller time step ($\delta t = 10^{-2}\Delta t$). We observe that Scheme II, with expected 1.5 order strong convergence, exhibits a much smaller error than Scheme I, which has 1.0 strong order.

Next we examine the weak convergence in terms of the density matrix. In particular, we compare the first entry of the density matrix, which is the square of the coefficient of the ground state when projecting the state vector to the basis of the eigenvectors of the Hamiltonian. We find that, due to the fact that the bath operator $\hat{V}$ (41) satisfies $[[\hat{V}^*, \hat{V}]\hat{V}, \hat{V}] = [[\hat{H}, \hat{V}], \hat{V}] = 0$, Schemes II and III are identical. Therefore, we pick another bath operator $\hat{V}_1$, as follows:

$$\hat{V}_1 \equiv \delta \begin{pmatrix} 0 & 1 & 1 & 1 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix}. \tag{43}$$

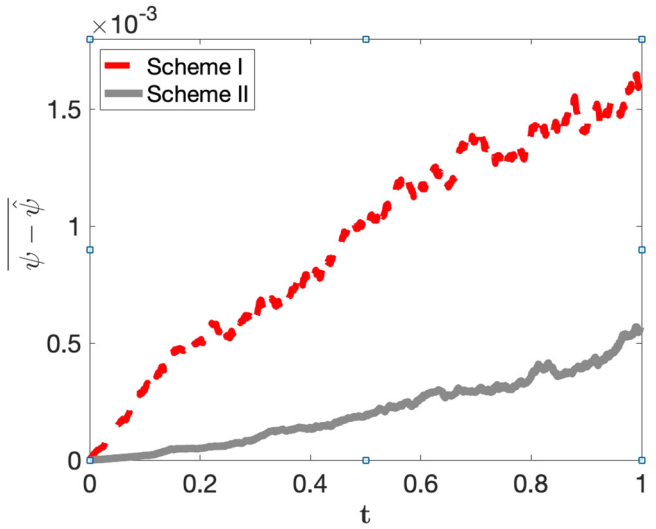

FIG. 1. A comparison of the strong order accuracy of Schemes I and II. The dashed red line depicts the error from Scheme I, and the solid gray line shows the error from Scheme II. The linear case $\tilde{g} = 0$ is considered.

We consider the error of the first entry of the density matrix $\rho_{11} = \overline{|\psi_0|}^2$ from Schemes I, II, and III. The results are displayed in Fig. 2. We approximated the expectation using 100 runs. Again the exact density matrix ρ is computed by the Milstein scheme with a much smaller time step. We observe that Scheme II has a moderate improvement over Scheme I, and Scheme III offers significantly better accuracy. This can be attributed to the higher-order weak convergence property that we demonstrated in the previous section.

In Mora [31], an exponential scheme called the Euler-exponential for SSE (1) is proposed, which has weak 1.0 order convergence. It can be written as

$$\psi^{n+1} = \mathcal{P}\left\{\exp\left[\left(-iH - \tfrac{1}{2}\hat{V}^*\hat{V}\right)\Delta t\right](\psi^n + \hat{V}\,\Delta W\,\psi^n)\right\}, \quad (44)$$

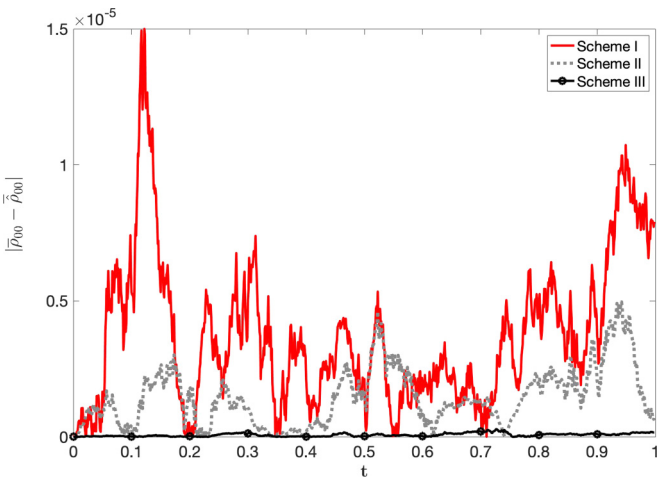

FIG. 2. The error in the ρ_{00} entry of the density-matrix: Scheme I (solid red upper line), Scheme II (dotted gray line), Scheme III (solid black lower line).

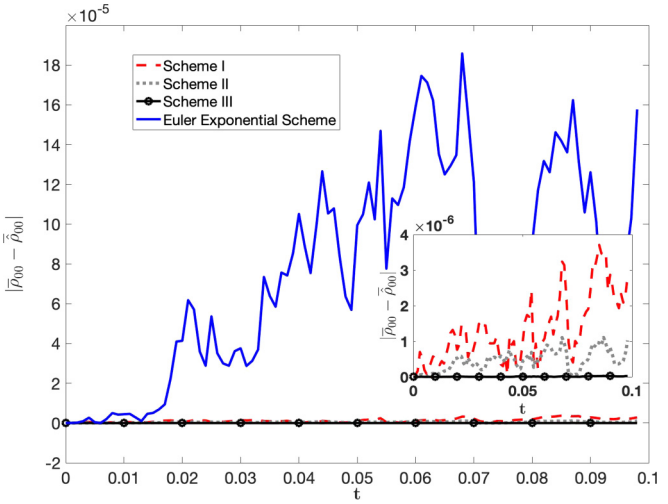

FIG. 3. A comparison with the Euler-exponential scheme (solid blue line) constructed by Mora [31], Scheme I (dashed red line), II (dotted gray line), and III (solid black line with circles).

where $\mathcal{P}$ is the projection to the unit ball to ensure the norm-preserving property. As a comparison, Fig. 3 depicts the error from the Euler-exponential method (the blue solid line on top), compared with our schemes. Our schemes yield significantly smaller error than the Euler-exponential method.

Now we consider the nonlinear case, and we pick $\tilde{g} = 1$ in (40). As discussed in Sec. II B, we adopted the symmetric splitting scheme. The exact solution is computed by the Euler-Maruyama method with a much smaller time step $\delta t = 10^{-3}\Delta t$. We approximate the expectation using 100 runs. From Figs. 4 and 5, we make similar observations as in Figs. 1 and 2.

Now we test the errors as a function of two important parameters of this method, i.e., time step size Δt and coupling constant δ. We compare our solution to the exact solution (the wave function approximated by the Euler-Maruyama method

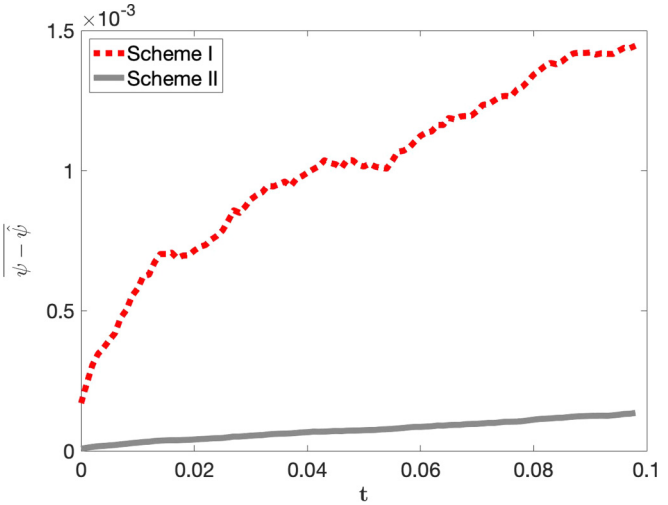

FIG. 4. A comparison of the strong order of Schemes I and II in the nonlinear case: $\tilde{g} = 1$. Scheme I (dotted red line), Scheme II (solid gray line).

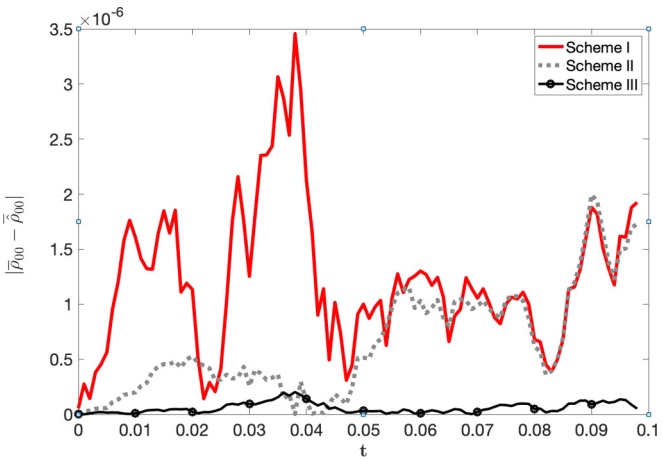

FIG. 5. The error of the entry ρ_{11} of the density matrix in the nonlinear case: $\tilde{g} = 1$. Scheme I (solid red upper line), Scheme II (dotted gray line), Scheme III (solid black lower line).

on the much smaller time step of $\Delta t = 10^{-5}$) of the quantum system, and the error is measured in the L^∞ norm in the time interval [0,1], i.e., $\|e(t)\|_{L^\infty(0,1)}$ from (42). We take the ensemble size of 100, enough for the Monte Carlo errors to be negligible.

The numerical error will depend on the choice of the step size. Figure 6 depicts the error of the wave functions from the numerical schemes, including Schemes I, II, and III, for various choices of time step size Δt. We compared the accuracy with the backward Euler-Maruyama (BEM) method, since the explicit Euler-Maruyama method is only stable with

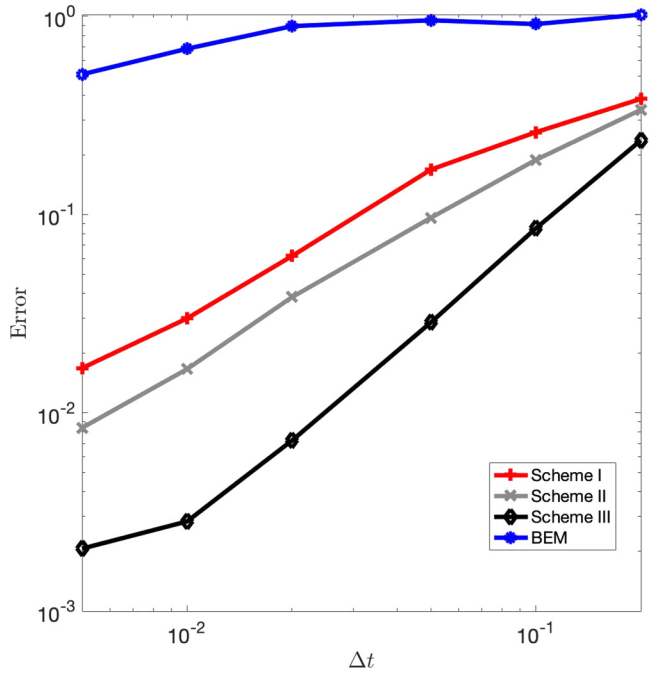

FIG. 6. A comparison of error from Schemes I, II, III and the Euler-Maruyama method with various choices of step size. The error, measured as the L^∞ norm in the time interval [0,1] of the local error (42), is shown on log scales.

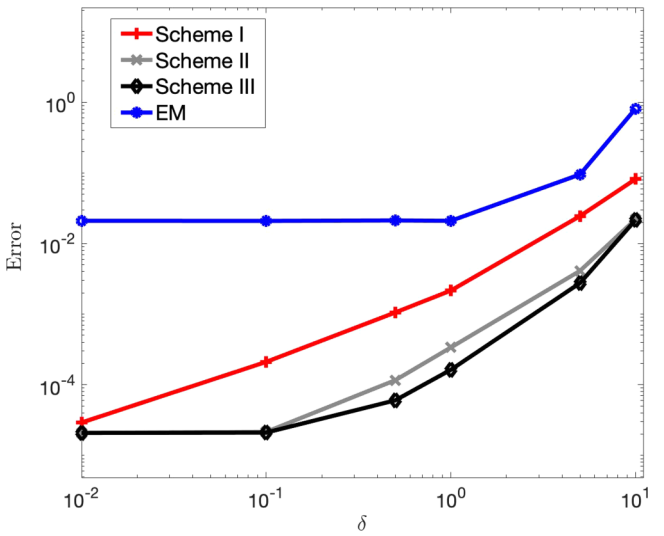

FIG. 7. A comparison of error of Schemes I, II, III and the Euler-Maruyama method for different choices of coupling constant. $\delta = 0$ corresponds to the bath-free case. The error, measured as the L^∞ norm in the time interval [0,1] of the local error (42), is shown on log scales.

much smaller step sizes. The slopes of the lines confirm the orders of convergence discussed in the previous section. Among these methods, the error from Scheme III decreases the fastest with step size.

In the SSE, the parameter δ represents the coupling coefficient, which would arise when deriving the SSE from the entire system by using perturbative expansions [4]. In particular, the case with $\delta = 0$ represents a bath-free scenario, and the SSE becomes deterministic. Fig. 7 depicts the numerical error from the four methods with different choices of the coupling coefficient δ. We find that the error tends to decrease with weaker coupling, and reaches a minimum when $\delta = 0$. This is the consequence of the fact that the error bounds of the stochastic numerical schemes involve higher-order stochastic integrals, which would disappear and only deterministic terms from the Taylor expansion affect the error. In this case, Schemes I, II, and III are still more accurate than the Euler-Maruyama method.

One of the crucial properties of the SSE is mass conservation. This implies that $\overline{\|\psi(t)\|^2}$ should remain constant. To test this property, we implemented the exponential integrators on a long time period and compare it with the Euler-Maruyama method. We choose the following bath operator:

$$\hat{V}_2 \equiv \frac{1}{10}\begin{pmatrix} 0 & 1 & 1 & 1 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix}. \tag{45}$$

We pick the time step $\Delta t = 10^{-4}$, ensuring that the Euler-Maruyama method is stable under this setting. We evolve the system for 10^5 steps up to $T = 10$. The ensemble average is approximated by averaging over 1000 runs, and doing a larger ensemble size did not result in noticeable changes. We depict

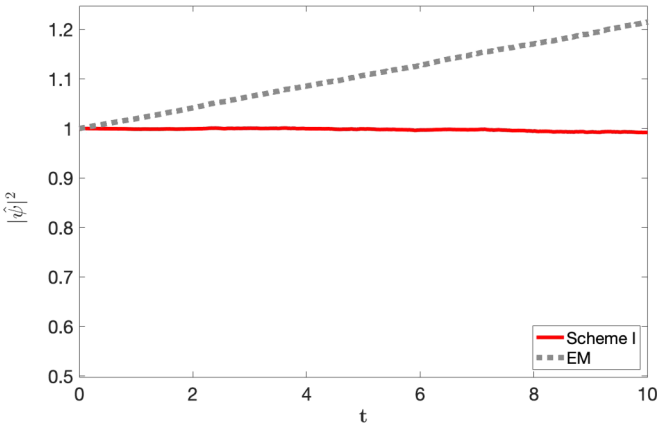

FIG. 8. The ensemble average of the norm of state vector (total mass). Scheme I (solid red line); Euler-Maruyama (dotted gray line).

the squared norm from the two methods in Fig. 8. The norms from Schemes II and III are very close to Scheme I so we omit them in the figure. We observe that the Euler-Maruyama method causes the norm to increase quite quickly, while the norm from Schemes I, II, and III seems to decrease, but it remains much closer to 1.

IV. SUMMARY AND DISCUSSION

In this paper we proposed exponential integrators for the stochastic Schrödinger equation based on Kunita's representation [16], which can be efficiently implemented by using the Krylov subspace method. Our schemes I and II have been verified to have order 1.0 and order 1.5, respectively, in the sense of strong convergence. We also discussed their convergence in terms of the density matrix. This analysis also suggests that the accuracy can be improved by adding two commutators in Scheme II. The nonlinear case is addressed by adopting an operator-splitting method [19,20,24], where the linear and nonlinear parts are treated separately.

In our numerical tests, we have found that our exponential schemes have better stability property, when compared with the Euler-Maruyama and Milstein's methods. They are also much better at preserving the square norm (mass) of the wave function. Overall, these schemes are good alternatives in the computation of the stochastic Schrödinger equation. Meanwhile, unlike some of the methods for deterministic Schrödinger equations, these methods do not exactly preserve the norm. It is still an open challenge to find a norm-preserving integrator.

ACKNOWLEDGMENT

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APPENDIX A: THE PROOF OF THEOREM II.1

Proof. We can actually use Theorem II.2 to prove this lemma. $\hat{V} \equiv 0$ gives the deterministic case. Since the Itô formula [18] is defined for real-valued equations, a simple idea is to separate the state vector into real and imaginary parts,

$$d\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & H \\ -H & 0 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} dt, \tag{A1}$$

where u and v are respectively the real and imaginary part of $\psi(x,t)$. Theorem II.2 gives the following representation to the solution of (A1):

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \exp(D_t)\begin{bmatrix} u \\ v \end{bmatrix}, \tag{A2}$$

where

$$D_t = tHv\frac{\partial}{\partial u} - tHu\frac{\partial}{\partial v}. \tag{A3}$$

By taking $f(u,v) = u + iv = \psi$, we have,

$$\psi(x,t) = \exp D_t \psi. \tag{A4}$$

According to the chain rule [20],

$$\begin{aligned} \frac{\partial}{\partial u} &= \frac{\partial \psi}{\partial u}\frac{\partial}{\partial \psi} + \frac{\partial \psi^*}{\partial u}\frac{\partial}{\partial \psi^*} = \frac{\partial}{\partial \psi} + \frac{\partial}{\partial \psi^*}, \\ \frac{\partial}{\partial v} &= \frac{\partial \psi}{\partial v}\frac{\partial}{\partial \psi} + \frac{\partial \psi^*}{\partial v}\frac{\partial}{\partial \psi^*} = i\frac{\partial}{\partial \psi} - i\frac{\partial}{\partial \psi^*}, \end{aligned} \tag{A5}$$

and a substitution into (A3), one gets

$$\begin{aligned} D_t &= tHv\left(\frac{\partial}{\partial \psi} + \frac{\partial}{\partial \psi^*}\right) - tHu\left(i\frac{\partial}{\partial \psi} - i\frac{\partial}{\partial \psi^*}\right), \\ &= -itH(u+iv)\frac{\partial}{\partial \psi} + (-itH)(-u+iv)\frac{\partial}{\partial \psi^*}, \\ &= -itH\left(\psi\frac{\partial}{\partial \psi} - \psi^*\frac{\partial}{\partial \psi^*}\right). \end{aligned} \tag{A6}$$

For the second part, since H is linear and $\frac{\partial}{\partial \psi^*}\psi = 0$,

$$\begin{aligned} \exp(D_t)\psi &= \sum_{j=0}^{\infty}\frac{1}{j!}\left[-itH\left(\psi\frac{\partial}{\partial \psi} - \psi^*\frac{\partial}{\partial \psi^*}\right)\right]^j\psi \\ &= \exp(-itH)\psi. \end{aligned} \tag{A7}$$

■

APPENDIX B: PROOF OF COROLLARY II.3

Proof. We first rewrite the equation as

$$d\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} -M & H \\ -H & -M \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} dt + \begin{bmatrix} \hat{V} & 0 \\ 0 & \hat{V} \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} \circ dW, \tag{B1}$$

where

$$M := \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}. \tag{B2}$$

Theorem II.2 gives the following representation to the solution of (B1):

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \exp\tilde{D}_t\begin{bmatrix} u \\ v \end{bmatrix}, \tag{B3}$$

where $\tilde{D}_t$ is expressed as a Magnus expansion. If we take the truncation of the first two terms, we have

$$\tilde{D}_t^{\mathrm{I}} = \left\{\begin{bmatrix} -M & H \\ -H & -M \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} J_{(0)} + \begin{bmatrix} \hat{V} & 0 \\ 0 & \hat{V} \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix} J_{(1)}\right\}\cdot\nabla. \tag{B4}$$

To be concise, we let

$$\begin{aligned} A &:= -Mt + \hat{V}W_t, \\ B &:= Ht. \end{aligned} \tag{B5}$$

As a result, the truncated operator can be written in a more compact form,

$$\tilde{D}_t^{\mathrm{I}} = \begin{bmatrix} A & B \\ -B & A \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \cdot \nabla = (Au + Bv)\frac{\partial}{\partial u} + (-Bu + Av)\frac{\partial}{\partial v}. \tag{B6}$$

Following the same idea in Theorem II.1, we get

$$\begin{aligned} \tilde{D}_t^{\mathrm{I}} &= (Au + Bv)\left(\frac{\partial}{\partial \psi} + \frac{\partial}{\partial \psi^*}\right) + (-Bu + Av)\left(i\frac{\partial}{\partial \psi} - i\frac{\partial}{\partial \psi^*}\right) \\ &= (A - iB)\psi\frac{\partial}{\partial \psi} + (A + iB)\psi^*\frac{\partial}{\partial \psi^*}. \end{aligned} \tag{B7}$$

Since $\frac{\partial}{\partial \psi^*}\psi = 0$, we have

$$\begin{aligned} \psi^I(x,t) = \exp(\tilde{D}_t^{\mathrm{I}})\psi = \exp\big\{\big[-iH - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\big]t \\ + \hat{V}W_t\big\}\psi. \end{aligned} \tag{B8}$$

Similarly, if we include the third term of the expansion of $\tilde{D}_t$ in (B3), i.e.,

$$\begin{aligned} A &:= -MJ_{(0)} + \hat{V}J_{(1)} + \tfrac{1}{2}\{J_{(0,1)} - J_{(1,0)}\}[\hat{V}, M], \\ B &:= HJ_{(0)} + \tfrac{1}{2}\{J_{(0,1)} - J_{(1,0)}\}[\hat{V}, H], \end{aligned} \tag{B9}$$

we have

$$\begin{aligned} \psi^{\mathrm{II}}(x,t) &= \exp\left(\tilde{D}_t^{\mathrm{I}}\right)\psi \\ &= \exp\big\{\big[-iH - \tfrac{1}{2}(\hat{V}^* + \hat{V})\hat{V}\big]t + \hat{V}W_t \\ &\quad + \tfrac{1}{2}(J_{(0,1)} - J_{(1,0)})\big(\tfrac{1}{2}[\hat{V}^*, \hat{V}]\hat{V} + i[H, \hat{V}]\big)\big\}\psi. \end{aligned} \tag{B10}$$

This verifies the claim. ■

APPENDIX C: THE PROOF OF THEOREM II.5

Proof. We can write the equation for the density matrix,

$$\begin{aligned} \partial_t\hat{\rho} = \exp(A\Delta t + B\Delta W + C\Delta U)\hat{\rho}_{t_0}\exp(A^*\Delta t + B^*\Delta W \\ + C^*\Delta U), \end{aligned} \tag{C1}$$

from the exponential integrators. We can expand the exponential, and using

$$\overline{\Delta W \Delta W} = \Delta t, \tag{C2}$$

we have

$$\begin{aligned} \partial_t\hat{\rho}(0) = A\rho(0) + \rho(0)A^* + B\rho(0)B^* + \tfrac{1}{2}BB\rho(0) \\ + \tfrac{1}{2}\rho(0)B^*B^* := \mathcal{L}\rho(0). \end{aligned} \tag{C3}$$

This agrees with the first derivative of the density-matrix computed from the Lindblad equation. Since the ΔU term does not contribute to the $O(\Delta t)$ term, we have $\partial_t\rho(0) = \partial_t\hat{\rho}_{\mathrm{I}}(0) = \partial_t\hat{\rho}_{\mathrm{II}}(0)$.

From the Lindblad equation, we can also compute the second derivative of the density-matrix:

$$\partial_{tt}\rho(0) = \mathcal{L}\mathcal{L}\rho(0). \tag{C4}$$

We can expand it with some lengthy calculation:

$$\begin{aligned} \partial_{tt}\rho = AA\rho + \rho A^*A^* + 2A\rho A^* + AB\rho B^* + BA\rho B^* \\ + A\rho B^*B^* + B\rho B^*A^* + B\rho A^*B^* + B\rho B^*A^* \\ + \tfrac{1}{2}ABB\rho + \tfrac{1}{2}BBA\rho + \tfrac{1}{2}\rho A^*B^*B^* + \tfrac{1}{2}\rho B^*B^*A^* \\ + \tfrac{1}{4}BBBB\rho + BBB\rho B^* + \tfrac{3}{2}BB\rho B^*B^* + B\rho B^*B^*B^* \\ + \tfrac{1}{4}\rho B^*B^*B^*B^*. \end{aligned} \tag{C5}$$

This is the same as $\partial_{tt}\hat{\rho}_{\mathrm{III}}(0)$. Thus we have $\partial_{tt}\rho(0) = \partial_{tt}\hat{\rho}_{\mathrm{III}}(0)$. ■

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