Stochastic time-dependent Hartree-Fock methods for fermions: Quasiprobability distributions, master equations, and convergence towards exact quantum dynamics

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The time-dependent fermionic Hartree-Fock equations can be stochastically extended in such a way as to become the exact representation of quantum dynamics. This fact was first observed in the work of Juillet and Chomaz [Phys. Rev. Lett. **88**, 142503 (2002)]. During the past decade, this observation has led to the emergence of a whole family of stochastic wave-function methods for fermions. The common feature of all these methods is that they are based on the expansion of the density operator over the dyadic product of the two fermionic Slater determinant states. In this work, we develop a unified and rigorous foundation for this family of methods. We find a general form of stochastic equations and describe the sufficient conditions under which these methods converge towards exact quantum dynamics. To achieve these goals, we employ the representation of quantum dynamics in generalized phase space. In particular, we consider the quasiprobability distributions which emerge in these stochastic methods and their master equations. It is shown that the convergence towards exact quantum dynamics is controlled by the problem of boundary terms. We provide an example of stochastic Hartree-Fock method which is well-defined and free from this problem.

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I. INTRODUCTION

The time-dependent Hartree-Fock (TDHF) method for fermions is an indispensable tool in computational physics, chemistry, and nuclear physics [1,2]. In the work of Juillet and Chomaz [3], an important observation was made: One can add such a stochastic term (noise) in TDHF that it becomes exact representation of quantum dynamics. By solving TDHF equations for different realizations of the noise, we obtain an ensemble of random trajectories in the space of Slater determinant states. The resulting method, the stochastic fermionic Hartree-Fock, allows one to calculate the exact time evolution of observables through the averaging over this ensemble of trajectories [3].

During the past decade the stochastic fermionic TDHF method of Juillet and Chomaz [3] has led to the emergence of a whole family of stochastic wave-function methods [4–7]. The common feature of all these methods is that they are derived by expanding the density operator over the dyadic products (nondiagonal projection operators) of bra and ket Slater determinant states. The coefficient in this expansion can be chosen real positive. Therefore, this coefficient can be interpreted as an (abstract) probability distribution, and the density operator can be interpreted as the expected value of the dyadic. Then the evolution in time (either real or imaginary) is constructed by assuming that the constituent one-particle orbitals (in the Slater determinant state) evolve according to a certain system of stochastic partial differential equations. The parameters of this system, the drift vectors and the noise matrices, are found from the requirement that the density operator, being represented as the expected value of the dyadic, obeys the exact many-body quantum Liouville equation [8].

All these methods share the same problem. The stochastic evolution in these methods is unconstrained diffusion in the space of Slater determinants. Moreover, the trace of the diffusion matrix grows at least quadratically as the norm of the one-particle orbitals is increased; as a consequence, the spread of the stochastic trajectories grows at least exponentially with time [3,8,9]. Therefore, when we simulate the quantum dynamics using Monte Carlo algorithms based on these methods, after a certain time t_u (called the useful simulation time [10]) the variance of the simulation results becomes prohibitively large. The only exception is the norm-conserving method of Tessieri *et al.* [5]; they have attempted to invent a stochastic representation of quantum dynamics on a domain of finite size in the space of Slater determinants. This way, they would have solved the problem of unconstrained diffusion, and hence the useful simulation time t_u would be significantly increased. However, according to the results presented in [5], it appears that the norm-conserving method has a systematic discrepancy with respect to the exact quantum dynamics. Therefore, the status of this direction of development is unclear.

Currently, all the stochastic TDHF methods are derived from different considerations in the literature [3–7]. This leads to a somewhat fragmented state of the research field, which makes it difficult to make progress in the problem of increasing the useful simulation time t_u and to rigorously study the problem of convergence towards the exact quantum dynamics.

In this work, we consider and rederive all the fermionic stochastic TDHF methods [3,5,6] within a unified framework. As such a framework, we have chosen the generalized phase-space formulation [10–15]. We believe that the generalized phase-space approach and the stochastic wave-function approach are complementary and equivalent pictures of the same subject [9]. The relation between these two approaches is analogous to the relation between the probability-distribution master equations (MEs) and the corresponding stochastic differential equations (SDEs) in the classical probability theory. However, when dealing with a specific task, usually only one of the two approaches is the most appropriate. As it turns out, the task of characterization of all the possible stochastic representations for a given stochastic operator ansatz (which is

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the Slater determinant dyadic in the case treated in our work) is most conveniently performed in the master-equation picture (i.e., within the generalized phase-space approach) [9].

In Sec. II, we review the conventional Hartree-Fock method and discuss the ideas behind its stochastic extension. We illustrate how this leads to the expansion of the density operator over the Slater determinant dyadics. In Sec. III, we study the properties of the nondiagonal Slater-determinant-state projections. We show that they form an overcomplete basis in the space of N-particle density operators. The expansion coefficient of the density operator in this basis can be chosen real positive. Therefore, we can interpret it as a probability distribution in the double Slater space. Then we discuss the action of normally ordered number-conserving products of creation and annihilation operators on the Slater projection. This helps us to compute the expected value of any observable in the double Slater space. In Sec. IV, we consider the time evolution of a quantum system with pairwise interactions. The master equation for the quasiprobability distribution in double Slater space, which corresponds to this time evolution, is derived. The conditions for its correctness are described. In Sec. IV G, we show how one can use the analyticity of Slater projections in order to perform the stochastic unraveling of the master equation. In Sec. V, we describe the equivalent transformations of the master equations and of the corresponding SDE. In Sec. VI, we illustrate how all the currently known in literature stochastic Hartree-Fock methods can be obtained by applying a suitable equivalent transformation. In Sec. VII, we discuss the status of stochastic TDHF methods with respect to the convergence towards the exact quantum dynamics. In particular, we present a variant of the stochastic TDHF method, for which we explicitly prove that it correctly reproduces the exact dynamics. We conclude in Sec. VIII.

II. THE STOCHASTIC TIME-DEPENDENT HARTREE-FOCK METHOD

Suppose we are given a system of N particles with a general Hamiltonian,

$$\widehat{H} = \sum_{r,s=1}^{\mathcal{N}} T_{rs}\widehat{a}_r^\dagger\widehat{a}_s - \frac{1}{4}\sum_{r,s,u,v=1}^{\mathcal{N}} V_{rsuv}\widehat{a}_r^\dagger\widehat{a}_s^\dagger\widehat{a}_u\widehat{a}_v, \tag{1}$$

containing a two-body interaction; here the matrix elements of Hermitian operators $T_{rs} = \langle r|\widehat{T}|s\rangle$ and $V_{rsuv} = (r,s|\widehat{V}|u,v)$, where by $|r,s)$ and $(u,v|$ we denote the two-particle wave functions without antisymmetrization (distinguishable particles). Note that we can always choose $\widehat{V}$ such that $V_{rsuv} = V_{srvu}$. The creation $\widehat{a}^\dagger(\mathbf{x}_r) \equiv \widehat{a}_r^\dagger$ and annihilation $\widehat{a}(\mathbf{x}_r) \equiv \widehat{a}_r$ operators obey the standard anticommutation relations

$$[\widehat{a}_r, \widehat{a}_s^\dagger]_+ = \delta_{rs}, \tag{2}$$

where δ_{rs} is the Kronecker δ. The exact time evolution is governed by the quantum Liouville equation

$$\frac{\partial}{\partial t}\widehat{\rho}_N(t) = \frac{1}{i\hbar}[\widehat{H}, \widehat{\rho}_N(t)], \tag{3}$$

where the density operator $\widehat{\rho}_N(t)$ represents the state of the quantum system.

A. The conventional Hartree-Fock method

In the conventional Hartree-Fock method, we approximate the state of the system by the antisymmetrized product of one-body orbitals,

$$\widehat{\rho}_N(t) = |\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N\rangle\langle\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N|, \tag{4}$$

where

$$|\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N\rangle = \prod_{l=1}^{N}\left[\sum_{r=1}^{\mathcal{N}}\phi_l(\mathbf{x}_r)\widehat{a}^\dagger(\mathbf{x}_r)\right]|0\rangle \tag{5}$$

is the Slater determinant state, in which each of the N orbitals $\boldsymbol{\phi}_l = [\phi_l(\mathbf{x}_1),\ldots,\phi_l(\mathbf{x}_\mathcal{N})]$, $l = 1\ldots N$, is occupied exactly by one particle. The values of the orbitals $\phi_l(\mathbf{x}_r) \equiv \phi_{lr}$ are defined on a certain lattice of sites $\mathbf{x}_r$, $r = 1,\ldots,\mathcal{N}$, in the n-dimensional coordinate space $\mathbb{R}^n$; the orbitals $\boldsymbol{\phi}_l$ belong to the one-body Hilbert space $H \equiv \mathbb{C}^\mathcal{N}$. Then we look for such deterministic evolution,

$$\boldsymbol{\phi}_l = \boldsymbol{\phi}_l(t), \tag{6}$$

that the exact quantum evolution (3) is approximated in the most optimal way. The optimality criterion is given by a certain action functional [2,16]. Minimizing the action functional with respect to the trajectories (6), one can obtain the well-known TDHF equations

$$i\frac{\partial}{\partial t}\langle\mathbf{x}_r|\boldsymbol{\phi}_l\rangle = \langle\mathbf{x}_r|\widehat{h}|\boldsymbol{\phi}_l\rangle - \frac{1}{2}\sum_m(\mathbf{x}_r,\boldsymbol{\phi}_m|\widehat{V}\{|\boldsymbol{\phi}_m,\boldsymbol{\phi}_l) - |\boldsymbol{\phi}_l,\boldsymbol{\phi}_m)\}, \tag{7}$$

for the case when the orbitals $\boldsymbol{\phi}_l$ are orthonormal.

B. The stochastic Hartree-Fock method

Now let us enlarge the optimization space: We consider nondeterministic (stochastic) evolutions [3,8]

$$d|\boldsymbol{\phi}_l\rangle = \widehat{A}_l|\boldsymbol{\phi}_l\rangle dt + \sum_m \widehat{B}_{lm}|dW_m\rangle. \tag{8}$$

Then the pure state $|\Psi(t)\rangle$ is approximated as the expected value,

$$|\Psi(t)\rangle = \mathrm{E}[|\boldsymbol{\phi}_1(t)\cdots\boldsymbol{\phi}_N(t)\rangle]. \tag{9}$$

Because now we have more degrees of freedom, we expect that the exact quantum evolution Eq. (3) can be approximated better. In fact, it turns out that in the case of pairwise interactions, the quantum evolution can be represented exactly by Eqs. (8) and (9) [3,8].

To find the operator-valued coefficients $\widehat{A}_l$ and $\widehat{B}_{lm}$ in Eq. (8), one might apply a certain stochastic generalization of the minimum action principle [6,17], in full analogy with the conventional TDHF method. However, as experience shows, the resulting stochastic equations are not guaranteed to reproduce the exact quantum dynamics [5,6,8]. Moreover, this way we obtain only one particular choice of $\widehat{A}_l$ and $\widehat{B}_{lm}$, whereas we would like to describe the whole family of possible choices of $\widehat{A}_l$ and $\widehat{B}_{lm}$ in order to choose among them the most appropriate for the problem at hand. Therefore, in this work we choose another approach: We consider the probability

distributions in the space of tuples $(\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_N)$, which are generated by the stochastic process (8), and the corresponding master equations.

The representation (9) implies that we should be able to expand the wave function as

$$|\Psi(t)\rangle = \int d\vec{\boldsymbol{\phi}}\, d\vec{\boldsymbol{\phi}}^{\,*} \mathcal{P}(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}^{\,*}, t) |\vec{\boldsymbol{\phi}}\rangle, \tag{10}$$

where, for brevity, we introduce the notation $\vec{\boldsymbol{\phi}} = (\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_N)^T$ to denote the dependence on the whole set of orbitals (this definition is inspired by the notation used in [14,15]). The volume element is $d\vec{\boldsymbol{\phi}} = \prod_{l=1}^{N} \prod_{r=1}^{\mathcal{N}} d\phi_{lr}$. Since the density operator of pure state is $\widehat{\rho}_N(t) = |\Psi(t)\rangle\langle\Psi(t)|$, we conclude that the stochastic evolution (8) leads to an expansion of general (nonpure) density operator,

$$\widehat{\rho}_N = \int \prod_{\alpha=1}^{2} d\vec{\boldsymbol{\phi}}^{\,(\alpha)} d\vec{\boldsymbol{\phi}}^{\,(\alpha)*} \mathcal{P}(\vec{\boldsymbol{\phi}}^{\,(1)}, \vec{\boldsymbol{\phi}}^{\,(2)*}, \vec{\boldsymbol{\phi}}^{\,(1)*}, \vec{\boldsymbol{\phi}}^{\,(2)}) \times |\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}|, \tag{11}$$

over nondiagonal unnormalized Slater-determinant-state projections,

$$\widehat{\Lambda}(\vec{\boldsymbol{\phi}}^{\,(1)}, \vec{\boldsymbol{\phi}}^{\,(2)*}) = |\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}|. \tag{12}$$

We call operators $\widehat{\Lambda}$ the unnormalized projections because of the property $\widehat{\Lambda}^2 = \langle\vec{\boldsymbol{\phi}}^{\,(2)}|\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\widehat{\Lambda}$. Here we must make an important observation that in order to represent the exact dynamical evolution of arbitrary density operator, we need to propagate stochastically a pair of states, not just one state. In fact, this conclusion applies to all the currently known stochastic wave-function methods [3,8,13,18–20].

C. General implications of stochastic representation

Let us discuss a few implications of the stochastic representations (8)–(11). First of all, it should be possible to choose the non-negative coefficients $\mathcal{P}(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}^{\,*}, t)$ and $\mathcal{P}(\vec{\boldsymbol{\phi}}^{\,(1)}, \vec{\boldsymbol{\phi}}^{\,(2)*}, \vec{\boldsymbol{\phi}}^{\,(1)*}, \vec{\boldsymbol{\phi}}^{\,(2)})$ in the expansions (10) and (11), correspondingly. Otherwise, it would be impossible to represent the state of quantum system as a probability distribution.

Another important implication follows from the fact that we are trying to represent the reversible quantum evolution (3) by the irreversible stochastic process, Eq. (8). Indeed, let us consider the following thought experiment. We start from a certain initial state $\Psi(0)$ with the corresponding probability distribution $\mathcal{P}(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}^{\,*}, 0)$ according to (10). Then we propagate this state forward in time during a time interval Δt. According to (8), the resulting probability distribution $\mathcal{P}(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}^{\,*}, \Delta t)$ will experience a drift and will be smeared out due to diffusion. Now, we apply the complex conjugation to the propagated wave function $\Psi(\Delta t)$, which corresponds to the mapping $\mathcal{P}(\vec{\boldsymbol{\phi}}, \vec{\boldsymbol{\phi}}^{\,*}, t) \to \mathcal{P}(\vec{\boldsymbol{\phi}}^{\,*}, \vec{\boldsymbol{\phi}}, t)$. If we propagate $\Psi^*(\Delta t)$ once more during a time interval Δt, we will return to the original state $\Psi^*(0)$. Nevertheless, the probability distribution after this propagation will not coincide with the initial one, $\mathcal{P}(\vec{\boldsymbol{\phi}}^{\,*}, \vec{\boldsymbol{\phi}}, \Delta t, \Delta t) \neq \mathcal{P}(\vec{\boldsymbol{\phi}}^{\,*}, \vec{\boldsymbol{\phi}}, 0)$, since it gets irreversibly smeared out (however, the drift contributions may cancel). Therefore, we conclude that the expansion coefficients in Eq. (10) should be nonunique. This is possible only if the states $|\vec{\boldsymbol{\phi}}\rangle$ form a basis whose elements are not linearly independent. The basis which is complete but whose elements are not linearly independent is called overcomplete. The same observations apply to the representation (11): The basis $|\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}|$ should be overcomplete.

III. THE SLATER-DETERMINANT-STATE PROJECTIONS

In accordance with the reasoning of previous section, the derivation of the stochastic fermionic Hartree-Fock method by Juillet and Chomaz [3] is centered on the nondiagonal Slater-determinant-state projections (hereinafter, for brevity, we call them the "Slater projections"). In this section, we review the properties of these projections. We demonstrate that they satisfy the discussed-above general necessary conditions of stochastic representability. We also derive other useful identities which will help us to construct the stochastic representation.

A. Slater projections are an overcomplete operator basis

The Slater projections (12) form a complete basis in the space of density operators. Indeed, we can select an orthonormal basis $\boldsymbol{\varphi}_k$ in the one-body Hilbert space H. Then the N-particle states $|\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}\rangle = |\boldsymbol{\varphi}_{k_1} \cdots \boldsymbol{\varphi}_{k_N}\rangle$, labeled by the integer vector index $\boldsymbol{k} = (k_1, \ldots, k_N)$, form a basis in the N-particle Fock subspace [21], with a resolution of unity,

$$P_N = \frac{1}{N!} \sum_{\boldsymbol{k}} |\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}\rangle\langle\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}|, \tag{13}$$

where P_N is the projection of the Fock space onto the N-particle subspace. Now we consider the Slater projection $|\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}|$ for a general set of orbitals $\vec{\boldsymbol{\phi}}^{\,(\alpha)}$. We employ the resolution of unity (13):

$$|\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}| = P_N |\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}| P_N = \sum_{\boldsymbol{k},\boldsymbol{k}'} C_{\boldsymbol{k},\boldsymbol{k}'} |\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}\rangle\langle\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k}')}|. \tag{14}$$

Therefore, the projections $|\vec{\boldsymbol{\phi}}^{\,(1)}\rangle\langle\vec{\boldsymbol{\phi}}^{\,(2)}|$ are not linearly independent of each other, and the basis (12) is overcomplete.

B. Slater projections lead to the quasiprobability representation in generalized phase space

The N-particle density operator $\widehat{\rho}_N$ can be expanded over the basis (12) using the resolution of unity (13):

$$\widehat{\rho}_N = P_N \widehat{\rho}_N P_N = \frac{1}{N!^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} \langle\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}|\widehat{\rho}_N|\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k}')}\rangle |\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k})}\rangle\langle\vec{\boldsymbol{\varphi}}_{(\boldsymbol{k}')}|. \tag{15}$$

This means that we can always represent the density operator $\widehat{\rho}_N$ as (11). The representation (11) is interpreted in the following way: The space of vector variables $(\vec{\boldsymbol{\phi}}^{\,(1)}, \vec{\boldsymbol{\phi}}^{\,(2)*}, \vec{\boldsymbol{\phi}}^{\,(1)*}, \vec{\boldsymbol{\phi}}^{\,(2)})$ is called the generalized phase space, and the functional $\mathcal{P}$ is called the quasiprobability

distribution functional in this generalized phase space. In the following, we omit the adjective "generalized" whenever it does not lead to ambiguity. The list of arguments of $\mathcal{P}$ is too long in Eq. (11). Therefore, we introduce the vector $z = (\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*})$ of dimension $2N\mathcal{N}$. We say that $\widehat{\rho}_N$ corresponds to $\mathcal{P}$ in the phase-space representation,

$$\widehat{\rho}_N \longleftrightarrow \mathcal{P}(z,z^*), \tag{16}$$

whenever Eq. (11) holds. Hereinafter, for brevity we refer to Eq. (11) as the "Slater-projection representation."

C. Slater-projection quasiprobabilities can be chosen real positive

We employ the overcompleteness property of (12) to choose the expansion coefficient $\mathcal{P}$ to be real and positive. Having done that, we can interpret $\mathcal{P}$ as a true probability distribution in phase space. The standard trick to accomplish this is to separate the phase of $\mathcal{P}$ [8,19,22]:

$$\mathcal{P}(z,z^*) = |\mathcal{P}(z,z^*)|e^{i\xi(z,z^*)}. \tag{17}$$

Then we can always absorb the phase ξ into $|\overrightarrow{\boldsymbol{\phi}}^{(1)}\rangle\langle\overrightarrow{\boldsymbol{\phi}}^{(2)}|$,

$$\widehat{\rho}_N = \int dz dz^* |\mathcal{P}(z,z^*)| \left|\boldsymbol{\phi}_1^{(1)\prime}\cdots\boldsymbol{\phi}_N^{(1)\prime}\right\rangle\left\langle\boldsymbol{\phi}_1^{(2)\prime}\cdots\boldsymbol{\phi}_N^{(2)\prime}\right|, \tag{18}$$

where $\boldsymbol{\phi}_l^{(1)\prime} = \boldsymbol{\phi}_l^{(1)} e^{i\xi(z,z^*)/2N}$ and $\boldsymbol{\phi}_l^{(2)\prime} = \boldsymbol{\phi}_l^{(2)} e^{-i\xi(z,z^*)/2N}$. If we change the variables as $\boldsymbol{\phi}_l^{(\alpha)} \to \boldsymbol{\phi}_l^{(\alpha)\prime}$ and compute the Jacobian determinant, we can return to the form (11), where the $\mathcal{P}$ is now real and positive. However, from the point of view of the stochastic simulations one may stop at (18): We sample the initial conditions $\boldsymbol{\phi}_l^{(\alpha)}$ with the quasiprobability distribution $|\mathcal{P}(z,z^*)|$, and each time we multiply the sampled wave functions by the phase factor $e^{\pm i\xi(z,z^*)/2N}$. Note that since, in general, $\xi(z,z^*)$ depends on $\boldsymbol{\phi}_l^{(\alpha)}$, we cannot omit this phase factor.

All these features, the completeness property [Eq. (13)], the representability of density operator [Eq. (11)], and the existence of positive quasiprobabilities [Eq. (18)], make the stochastic TDHF method (and in fact all the stochastic wave-function methods [9]) similar to the generalized phase-space representations [12,14,15]. This was already observed in [12], and for the case of bosonic systems it was elaborated to some extent in [9]. However, such observations were never elaborated for the systems of fermions. In the following, we fill this gap.

D. Action of number-conserving operators on the Slater-projection basis

Suppose that we act on the Slater state by a normally-ordered number-conserving operator,

$$L = \widehat{a}_{r_1}^\dagger \cdots \widehat{a}_{r_m}^\dagger \widehat{a}_{s_m} \cdots \widehat{a}_{s_1} |\boldsymbol{\phi}_1 \cdots \boldsymbol{\phi}_N\rangle, \tag{19}$$

where $m \leqslant N$. For the purpose of the following, let us represent L as action of differential operator upon the Slater state. In order to accomplish this, we find the result of sequential actions of $\widehat{a}_{s_1}, \widehat{a}_{s_2}, \ldots, \widehat{a}_{s_m}$ upon the Slater state in (19). Using the definition of the Slater state (5), we evaluate the action of $\widehat{a}_{s_1}$,

$$L = \widehat{a}_{r_1}^\dagger \cdots \widehat{a}_{r_m}^\dagger \widehat{a}_{s_m} \cdots \widehat{a}_{s_2} \sum_{l_1=1}^{N} (-1)^{l_1-1} \left\{ \prod_{k=1}^{l_1-1} \left[\sum_{q=1}^{\mathcal{N}} \phi_{kq} \widehat{a}_q^\dagger \right] \right\} \times \phi_{l_1 s_1} \left\{ \prod_{k=l_1+1}^{N} \left[\sum_{q=1}^{\mathcal{N}} \phi_{kq} \widehat{a}_q^\dagger \right] \right\} |0\rangle, \tag{20}$$

where the products are equal to unity if the lower limit is greater that the higher limit. Now we denote

$$Q_a^b = \begin{cases} \prod_{k=a}^{b} \left[\sum_{q=1}^{\mathcal{N}} \phi_{kq} \widehat{a}_q^\dagger \right] & \text{for } a \leqslant b, \\ 1 & \text{for } a > b, \end{cases} \tag{21}$$

and evaluate the action of $\widehat{a}_{s_2}$ in (20),

$$L = \widehat{a}_{r_1}^\dagger \cdots \widehat{a}_{r_m}^\dagger \widehat{a}_{s_m} \cdots \widehat{a}_{s_3} \times \left[\sum_{l_2<l_1} (-1)^{l_1-1+l_2-1} Q_1^{l_2-1} \phi_{l_2 s_2} Q_{l_2+1}^{l_1-1} \phi_{l_1 s_1} Q_{l_1+1}^{N} |0\rangle - \sum_{l_2>l_1} (-1)^{l_1-1+l_2-1} Q_1^{l_1-1} \phi_{l_1 s_1} Q_{l_1+1}^{l_2-1} \phi_{l_2 s_2} Q_{l_2+1}^{N} |0\rangle \right]. \tag{22}$$

If we inspect this expression, we observe that the action of each subsequent $\widehat{a}_{s_j}$ introduces summation over a new index l_j, which runs in the range $1,\ldots,N$. The value l_j means that $\widehat{a}_{s_j}$ has crossed the creation operators $(l_j - 1)$ times before annihilating with $\widehat{a}_{s_j}^\dagger$. Therefore, all the summands have the common prefactor $(-1)^{\sum_{j=1}^{m} l_j - m}$. However, in this summation, when l_j crosses l_i with $j > i$, this corresponds to the situation when $\widehat{a}_{s_j}$ crosses the factor $\phi_{l_i s_i}$, and the corresponding $\widehat{a}_{s_i}^\dagger$ is absent (since it is already has been annihilated by $\widehat{a}_{s_i}$). Due to the anticommutation relations (2), this means that, when l_j crosses l_i with $j > i$, the corresponding summand acquires the additional factor (-1). That is, the resulting additional factor for each summand is $(-1)^{|P|}$, where $|P|$ is the number of transpositions in the sequence $l_1,\ldots,l_m$, if we consider this sequence as a permutation P of the sequence which is sorted in descending order. Taking into account these considerations, we can write the result of the action of all the $\widehat{a}_{s_j}$:

$$L = \widehat{a}_{r_1}^\dagger \cdots \widehat{a}_{r_m}^\dagger \sum_{l_1>\cdots>l_m} (-1)^{\sum_{j=1}^{m} l_j - m} \sum_{P} (-1)^{|P|} \times Q_1^{l_m-1} \phi_{l_m s_{P_m}} \left\{ \prod_{j=m}^{2} Q_{l_j+1}^{l_{j-1}-1} \phi_{l_{j-1} s_{P_{j-1}}} \right\} Q_{l_1+1}^{N} |0\rangle. \tag{23}$$

Here, in the second line the multiplication in the product is performed in the reverse order from m to 2. Now, we transform this expression so as to restore the form of the Slater state on the right of Eq. (23). We exchange the positions of the factors $\widehat{a}_{r_j}^\dagger$ and $\phi_{l_j s_{P_j}}$, starting from $j = m$ and ending at $j = 1$. Such reordering will cancel the common prefactor $(-1)^{\sum_{j=1}^{m} l_j - m}$,

and we arrive at the relation

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}|\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N\rangle\\&\quad=\sum_{l_1>\cdots>l_m}\sum_{P}(-1)^{|P|}\phi_{l_1 s_{P_1}}\cdots\phi_{l_m s_{P_m}}\\&\qquad\times\frac{\partial}{\partial\phi_{l_1 r_1}}\cdots\frac{\partial}{\partial\phi_{l_m r_m}}|\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N\rangle,\end{aligned}\tag{24}$$

where the Wirtinger derivatives with respect to complex variables are defined as [23]

$$\frac{\partial}{\partial\phi_{lr}}=\frac{1}{2}\left(\frac{\partial}{\partial x_{lr}}-i\frac{\partial}{\partial y_{lr}}\right),\tag{25}$$

$$\frac{\partial}{\partial\phi^{*}_{lr}}=\frac{1}{2}\left(\frac{\partial}{\partial x_{lr}}+i\frac{\partial}{\partial y_{lr}}\right).\tag{26}$$

Here x_{lr} and y_{lr} are the real and the imaginary parts of ϕ_{lr}. By applying Hermitian conjugation and changing the variables $r\leftrightarrow s$, we obtain a similar relation for the bra state:

$$\begin{aligned}&\langle\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N|\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\\&\quad=\sum_{l_1>\cdots>l_m}\sum_{P}(-1)^{|P|}\phi^{*}_{l_1 r_{P_1}}\cdots\phi^{*}_{l_m r_{P_m}}\\&\qquad\times\frac{\partial}{\partial\phi^{*}_{l_1 s_1}}\cdots\frac{\partial}{\partial\phi^{*}_{l_m s_m}}\langle\boldsymbol{\phi}_1\cdots\boldsymbol{\phi}_N|.\end{aligned}\tag{27}$$

E. Expected values in Slater-projection representation

Let us discuss how the expected values of the observables are represented in the Slater-projection representation. Given a quantum observable $\widehat{O}$, its expected value for a quantum system in state $\widehat{\rho}_N$ is

$$\langle\widehat{O}\rangle=\mathrm{Tr}\widehat{O}\widehat{\rho}_N.\tag{28}$$

Substituting here the expansion (11), we represent the quantum average as a classical expectation of the c-number function $\mathcal{O}(z)$ in the phase space,

$$\langle\widehat{O}\rangle=\int dzdz^{*}\mathcal{O}(z)\mathcal{P}(z,z^{*}),\tag{29}$$

where the c-number function $\mathcal{O}$ is found to be

$$\mathcal{O}(z)=\mathrm{Tr}\widehat{O}\widehat{\Lambda}(z).\tag{30}$$

Taking into account Eqs. (29) and (30), we may say that the observable $\hat{O}$ corresponds to the c-number function $\mathcal{O}$ in the phase-space representation,

$$\widehat{O}\longleftrightarrow\mathcal{O}(z).\tag{31}$$

Suppose that we are given a normally ordered number-conserving observable

$$\widehat{O}_{\mathbf{r},\mathbf{s}}=\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}.\tag{32}$$

In this case, we can use the result (24) to evaluate the expression for $\widehat{O}_{\mathbf{r},\mathbf{s}}\widehat{\Lambda}$ in the definition of $\mathcal{O}$ [Eq. (30)],

$$\begin{aligned}\mathcal{O}_{\mathbf{r},\mathbf{s}}(z)=\mathrm{Tr}\widehat{O}_{\mathbf{r},\mathbf{s}}\widehat{\Lambda}(z)&=\sum_{l_1>\cdots>l_m}\sum_{P}(-1)^{|P|}\phi^{(1)}_{l_{P_1}s_1}\cdots\phi^{(1)}_{l_{P_m}s_m}\\&\times\frac{\partial}{\partial\phi^{(1)}_{l_1 r_1}}\cdots\frac{\partial}{\partial\phi^{(1)}_{l_m r_m}}\det M,\end{aligned}\tag{33}$$

where we have reordered the terms $\phi^{(1)}_{l_j s_{P_j}}$; M is the overlap matrix

$$M=\begin{bmatrix}\langle\boldsymbol{\phi}^{(2)}_1|\boldsymbol{\phi}^{(1)}_1\rangle&\cdots&\langle\boldsymbol{\phi}^{(2)}_1|\boldsymbol{\phi}^{(1)}_N\rangle\\\cdots&\cdots&\cdots\\\langle\boldsymbol{\phi}^{(2)}_N|\boldsymbol{\phi}^{(1)}_1\rangle&\cdots&\langle\boldsymbol{\phi}^{(2)}_N|\boldsymbol{\phi}^{(1)}_N\rangle\end{bmatrix}.\tag{34}$$

Note that the action of the derivative $\partial/\partial\phi^{(1)}_{l_j r_j}$ with the subsequent multiplication by $\phi^{(1)}_{l_{P_j}s_j}$ amounts to the replacement of the l_jth column $(\langle\boldsymbol{\phi}^{(2)}_1|\boldsymbol{\phi}^{(1)}_{l_j}\rangle\cdots\langle\boldsymbol{\phi}^{(2)}_N|\boldsymbol{\phi}^{(1)}_{l_j}\rangle)^{T}$ with $(\phi^{(2)*}_{1r_j}\phi^{(1)}_{l_{P_j}s_j}\cdots\phi^{(2)*}_{Nr_j}\phi^{(1)}_{l_{P_j}s_j})^{T}$ in the determinant $\det M$. To compute this modified determinant, which is denoted as $\det M^{(1)}$, we introduce the collection of matrix column indices $\boldsymbol{p}=(l_m,l_{m-1},\ldots,l_1)$. We also introduce the complementary collection $\bar{\boldsymbol{p}}=(\bar{p}_1\cdots\bar{p}_{N-m})$, which is obtained from $(1,\ldots,N)$ by discarding all the indices entering into $\boldsymbol{p}$. The modified matrix $M^{(1)}$ is defined as $M^{(1)}_{i\bar{p}_j}=\langle\boldsymbol{\phi}^{(2)}_i|\boldsymbol{\phi}^{(1)}_{\bar{p}_j}\rangle$ and $M^{(1)}_{ip_j}=\phi^{(2)*}_{ir_{\sigma j}}\phi^{(1)}_{p_{\sigma P_{\sigma j}}s_{\sigma j}}$, where σ is the inversion of order of the sequence $(1,\ldots,m)$. Note that since $|\sigma P\sigma|=|P|$ and the summation in Eq. (33) is over the set of all the permutations, we redefine $M^{(1)}_{ip_j}=\phi^{(2)*}_{ir_{\sigma j}}\phi^{(1)}_{p_{P_j}s_{\sigma j}}$. Equation (33) assumes the form

$$\mathcal{O}_{\mathbf{r},\mathbf{s}}(z)=\sum_{p_1<\cdots<p_m}\sum_{P}(-1)^{|P|}\det M^{(1)}.\tag{35}$$

Now we employ Laplace's theorem on cofactor expansion of determinant along the columns $\boldsymbol{p}$ [24],

$$\begin{aligned}\det M^{(1)}=(-1)^{\sum_{j=1}^{m}p_j}&\sum_{q_1<\cdots<q_m}(-1)^{\sum_{j=1}^{m}q_j}\\&\times\det M^{(1)}(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})\det M^{(1)}(\boldsymbol{q},\boldsymbol{p}),\end{aligned}\tag{36}$$

for $p_1<\cdots<p_m$. Here we have introduced the collection of rows $\boldsymbol{q}=(q_1\cdots q_m)$. The matrix $M^{(1)}(\boldsymbol{q},\boldsymbol{p})$ is defined as $[M^{(1)}(\boldsymbol{q},\boldsymbol{p})]_{ij}=M^{(1)}_{q_i p_j}$. Substituting (36) into Eq. (35), and using the fact that $M^{(1)}(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})=M(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})$, we obtain the phase-space correspondence for the observables:

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\\&\longleftrightarrow\sum_{p_1<\cdots<p_m}\sum_{q_1<\cdots<q_m}(-1)^{\sum_{j=1}^{m}(p_j+q_j)}\\&\qquad\times\det M(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})\sum_{P,Q}(-1)^{|P|+|Q|}\\&\qquad\times\phi^{(2)*}_{q_{Q_1}r_{\sigma 1}}\cdots\phi^{(2)*}_{q_{Q_m}r_{\sigma m}}\phi^{(1)}_{p_{P_1}s_{\sigma 1}}\cdots\phi^{(1)}_{p_{P_m}s_{\sigma m}}.\end{aligned}\tag{37}$$

Using the theorem for the minor of the inverse [25],

$$\det M^{-1}(\boldsymbol{q},\boldsymbol{p})=(-1)^{\sum_{j=1}^{m}(\bar{p}_j+\bar{q}_j)}\frac{\det M(\bar{\boldsymbol{q}},\bar{\boldsymbol{p}})}{\det M},\tag{38}$$

for $p_1<\cdots<p_m$ and for $q_1<\cdots<q_m$, we can simplify the expression (37):

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\\&\longleftrightarrow\det M\sum_{p_1\cdots p_m}\sum_{q_1\cdots q_m}\det M^{-1}(\boldsymbol{q},\boldsymbol{p})\\&\qquad\times\phi^{(2)*}_{q_1 r_{\sigma 1}}\cdots\phi^{(2)*}_{q_m r_{\sigma m}}\phi^{(1)}_{p_1 s_{\sigma 1}}\cdots\phi^{(1)}_{p_m s_{\sigma m}}.\end{aligned}\tag{39}$$

In fact, here we can eliminate σ's by renumbering p_j and q_j and by simultaneously permuting the columns and the rows in $\det M^{-1}(\boldsymbol{q},\boldsymbol{p})$:

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\\&\quad\longleftrightarrow \det M\sum_{p_1\cdots p_m}\sum_{q_1\cdots q_m}\det M^{-1}(\boldsymbol{q},\boldsymbol{p})\\&\qquad\times\phi^{(2)*}_{q_1r_1}\cdots\phi^{(2)*}_{q_mr_m}\phi^{(1)}_{p_1s_1}\cdots\phi^{(1)}_{p_ms_m}.\end{aligned}\tag{40}$$

For $m=1$ and $m=2$ our expression (40) coincides with the results obtained earlier in [26].

IV. QUASIPROBABILITY MASTER EQUATION

A. Star-product operator correspondences

Our ultimate goal is to find the representation of the quantum time evolution (3) in the phase space. At every time moment t, the density operator $\widehat{\rho}_N(t)$ can be represented by some quasiprobability $\mathcal{P}(z,z^*,t)$. Thus, we may ask the following question: What is the quasiprobability master equation (QME) which governs the time evolution of $\mathcal{P}(z,z^*,t)$? To answer this question, we inspect the right-hand side of Eq. (3), and we see that it is a sum of left-product terms $\widehat{a}^{\dagger}_{k_1}\cdots\widehat{a}^{\dagger}_{k_m}\widehat{a}_{k'_m}\cdots\widehat{a}_{k'_1}\widehat{\rho}_N$ and of right-product terms $\widehat{\rho}_N\widehat{a}^{\dagger}_{k_1}\cdots\widehat{a}^{\dagger}_{k_m}\widehat{a}_{k'_m}\cdots\widehat{a}_{k'_1}$. Therefore, one possibility to construct the QME is to find the phase-space correspondences for such products, and that is what we are going to do now.

Using the expansion (11), we obtain for the left-product term

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\widehat{\rho}_N\\&\quad=\int dzdz^*\mathcal{P}(z,z^*)\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}|\overrightarrow{\boldsymbol{\phi}}^{(1)}\rangle\langle\overrightarrow{\boldsymbol{\phi}}^{(2)}|\\&\quad=\int dzdz^*\mathcal{P}(z,z^*)\mathcal{S}[r_1\cdots r_m;\,s_m\cdots s_1]|\overrightarrow{\boldsymbol{\phi}}^{(1)}\rangle\langle\overrightarrow{\boldsymbol{\phi}}^{(2)}|,\end{aligned}\tag{41}$$

where $\mathcal{S}[r_1\cdots r_m;\,s_m\cdots s_1]$ is the differential operator acting on the Slater state at the right-hand side of relation (24). Note that in the first equality in Eq. (41) we exchange the operator and the improper integral, which is allowed since in the case of a finite-lattice system with finite number of particles, the action of operator is a sum of a finite number of matrix elements. It is seen that if we could integrate by parts without the boundary terms, then we would immediately obtain the phase-space correspondence:

$$\begin{aligned}&\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\widehat{\rho}_N\longleftrightarrow(-1)^m\sum_{l_1>\cdots>l_m}\sum_{P}(-1)^{|P|}\\&\quad\times\frac{\partial}{\partial\phi^{(1)}_{l_1r_1}}\cdots\frac{\partial}{\partial\phi^{(1)}_{l_mr_m}}\left\{\phi^{(1)}_{l_1s_{P_1}}\cdots\phi^{(1)}_{l_ms_{P_m}}\mathcal{P}\right\}.\end{aligned}\tag{42}$$

Reiterating the same treatment for the right-product term, we would get

$$\begin{aligned}&\widehat{\rho}_N\widehat{a}^{\dagger}_{r_1}\cdots\widehat{a}^{\dagger}_{r_m}\widehat{a}_{s_m}\cdots\widehat{a}_{s_1}\\&\quad\longleftrightarrow(-1)^m\sum_{l_1>\cdots>l_m}\sum_{P}(-1)^{|P|}\\&\qquad\times\frac{\partial}{\partial\phi^{(2)*}_{l_1s_1}}\cdots\frac{\partial}{\partial\phi^{(2)*}_{l_ms_m}}\left\{\phi^{(2)*}_{l_1r_{P_1}}\cdots\phi^{(2)*}_{l_mr_{P_m}}\mathcal{P}\right\}.\end{aligned}\tag{43}$$

In the following, the phase-space correspondences (42) and (43) will be called the "operator correspondences of the left-star-product type" and "operator correspondences of the right-star-product type" correspondingly [9], since they bear resemblance to the star product in the deformation quantization [27].

B. The space of admissible quasiprobability distributions

The derivation of these two phase-space correspondences, Eqs. (42) and (43), imposes a requirement on the quasiprobabilities $\mathcal{P}$: They should be such that the boundary term, which arises during the integration by parts, is vanishing. Therefore, we assume that we have chosen a certain space D of quasiprobability distributions which satisfy this requirement. We call D the "space of admissible quasiprobability distributions." To fulfill the requirement of vanishing boundary terms, it is *sufficient* to define D as the space of all such quasiprobability distributions $\mathcal{P}$ that (i) there exists $\widehat{\rho}_N$ for which the correspondence (16) is well defined and (ii) $\mathcal{P}$ is a rapidly decreasing function. We say that the quasiprobability distribution $\mathcal{P}$ is a rapidly decreasing function if the tails of $\mathcal{P}$ and of all its derivatives eventually fall off faster than any inverse power law. In mathematical formal terms, for $\mathcal{P}$ to be rapidly decreasing, we require that for any (mixed) partial derivative

$$f=\prod_{i=1}^{a}\frac{\partial}{\partial\phi^{(\alpha_i)}_{k_ir_i}}\prod_{j=1}^{b}\frac{\partial}{\partial\phi^{(\beta_j)*}_{l_js_j}}\mathcal{P},\tag{44}$$

for any monomial

$$g=\prod_{i=1}^{c}\phi^{(\gamma_i)}_{p_iu_i}\prod_{j=1}^{d}\phi^{(\delta_j)*}_{m_jv_j},\tag{45}$$

and for arbitrarily small fixed $\epsilon>0$, there exists such a constant R that, for every $\overrightarrow{\boldsymbol{\phi}}^{(1)}$, $\overrightarrow{\boldsymbol{\phi}}^{(2)}$ with $\|\overrightarrow{\boldsymbol{\phi}}^{(1)}\|\geqslant R$ and $\|\overrightarrow{\boldsymbol{\phi}}^{(2)}\|\geqslant R$, we have $|fg|<\epsilon$.

C. Formal quasiprobability master equation

Now we are ready to derive our first QME in the Slater-projection representation. We proceed by finding the phase-space correspondence for each term of the quantum Liouville equation (3).

To find the representation for the time-derivative term $\partial_t\widehat{\rho}_N(t)$, we can write

$$\frac{\partial}{\partial t}\widehat{\rho}_N(t)=\int dzdz^*\frac{\partial}{\partial t}\mathcal{P}(z,z^*,t)|\overrightarrow{\boldsymbol{\phi}}^{(1)}\rangle\langle\overrightarrow{\boldsymbol{\phi}}^{(2)}|.\tag{46}$$

From this relation, it can be deduced that one possible correspondence is

$$\frac{\partial}{\partial t}\widehat{\rho}_N\longleftrightarrow\frac{\partial}{\partial t}\mathcal{P}.\tag{47}$$

Here care must be taken. In Eq. (46) we have exchanged the time derivative and the improper integral. Therefore, as is known from the calculus [28], for the correspondence (47) to be valid at a time moment τ, there should exist a neighborhood $U(\tau,\epsilon)=[\tau-\epsilon,\tau+\epsilon]$ such that the improper integral at the right-hand side of Eq. (46) is uniformly converging for all $t\in U(\tau,\epsilon)$. The sufficient condition for this is that there exists a rapidly decreasing function g and a constant R such that

$|\partial_t \mathcal{P}(t)| < g$ for all $\|\overrightarrow{\boldsymbol{\phi}}^{(1)}\| \geqslant R$ and $\|\overrightarrow{\boldsymbol{\phi}}^{(2)}\| \geqslant R$ and for all $t \in U(\tau,\epsilon)$. For brevity, we refer to this sufficient condition as one where the function $\partial_t \mathcal{P}(t)$ should have "uniformly dominated tails."

Now, referring to the definition of $\widehat{H}$ [Eq. (1)] and applying the rules (42) and (43) in the commutator $[\widehat{H}, \hat{\rho}_N]/i\hbar$, we find the QME which is a phase-space counterpart of the quantum Liouville equation (3):

$$\frac{\partial}{\partial t}\mathcal{P} = -\sum_{lr}\frac{\partial}{\partial \phi^{(1)}_{lr}}\left\{\frac{1}{i\hbar}\langle r|\widehat{T}|\boldsymbol{\phi}^{(1)}_l\rangle\mathcal{P}\right\} + \frac{1}{4}\sum_{lr}\sum_{ms}\frac{\partial^2}{\partial\phi^{(1)}_{lr}\partial\phi^{(1)}_{ms}}\left\{\frac{1}{i\hbar}\left(r,s|\widehat{V}^{(A)}|\boldsymbol{\phi}^{(1)}_l,\boldsymbol{\phi}^{(1)}_m\right)\mathcal{P}\right\} + \left[-\sum_{lr}\frac{\partial}{\partial\phi^{(2)}_{lr}}\left\{\frac{1}{i\hbar}\langle r|\widehat{T}|\boldsymbol{\phi}^{(2)}_l\rangle\mathcal{P}\right\} + \frac{1}{4}\sum_{lr}\sum_{ms}\frac{\partial^2}{\partial\phi^{(2)}_{lr}\partial\phi^{(2)}_{ms}}\left\{\frac{1}{i\hbar}\left(r,s|\widehat{V}^{(A)}|\boldsymbol{\phi}^{(2)}_l,\boldsymbol{\phi}^{(2)}_m\right)\mathcal{P}\right\}\right]^*. \tag{48}$$

Here $V^{(A)}_{rsuv} = (V_{rsuv} - V_{rsvu})/2$.

We call the QME (48) the formal quasiprobability master equation, because it is obtained by the formal application of the rules (42), (43), and (47). However, let us recall that we can be sure that this QME is well-defined, and the time dependence of the expected values is the same as that predicted by the quantum Liouville equation (3), only if the following condition is satisfied: Taking any $\mathcal{P} \in D$ as an initial condition for Eq. (48), there exists a solution $\mathcal{P}(t)$ for all times t, and this solution is such that at all times t, $\mathcal{P}(t)$ belongs to D, and $\partial_t\mathcal{P}(t)$ has uniformly dominated tails. We discuss these conditions in Sec. VII. In the next section, we address the question of the stochastic interpretation of the QME (48).

D. Fokker-Planck equation in complex variables

We observe that the QME (48) has the form similar to that of Fokker-Planck equation, with the complication that the variables and the coefficients are complex. To solve this complication, we employ the general form of Fokker-Planck equation in complex variables, which was derived in Appendix B of Ref. [9]. Suppose that we have two real vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ of equal dimension $\mathcal{M}$ (in our case $\mathcal{M} = 2N\mathcal{N}$). We combine them into a complex vector $\boldsymbol{z} = \boldsymbol{x} + i\boldsymbol{y}$ and consider the pair $(\boldsymbol{z},\boldsymbol{z}^*)$ as independent variables, which is possible due to the following property of the Wirtinger derivatives: $\partial z_i/\partial z_j^* = \partial z_i^*/\partial z_j = 0$. We interpret the pair $(\boldsymbol{z},\boldsymbol{z}^*)$ as a single vector $\underline{z} = (\boldsymbol{z},\boldsymbol{z}^*)$ with components $\underline{z}_{\alpha j} = z_j$ for $\alpha = 1$ and $\underline{z}_{\alpha j} = z_j^*$ for $\alpha = 2$. Therefore, the vector $\underline{z}$ is indexed by a compound index αj, where the first greek index designates whether to choose $\boldsymbol{z}$ or its complex conjugate, and the second latin index indicates the component of $\boldsymbol{z}$ (or $\boldsymbol{z}^*$). The matrices $\underline{\underline{M}}$, which act on such vectors, have the block structure

$$\underline{\underline{M}} = \begin{bmatrix} P & Q \\ Q^* & P^* \end{bmatrix}, \tag{49}$$

where P and Q are arbitrary complex $\mathcal{M}\times\mathcal{M}$ matrices. The elements $\underline{\underline{M}}_{\alpha\beta jk}$ of the matrix $\underline{\underline{M}}$ are indexed by the two compound indices αj and βk, where (α,β) refers to the block submatrix, and (j,k) refers to the element within the selected block submatrix. Now, suppose that we have a general complex stochastic Ito process,

$$dz_j = A_j dt + \sum_{k=1}^{2\mathcal{M}} B_{jk} dW_k, \tag{50}$$

where $d\boldsymbol{z}$ is an increment of the vector $\boldsymbol{z}$; $\boldsymbol{A}$ is an arbitrary complex drift vector; B is an arbitrary complex $\mathcal{N}\times 2\mathcal{N}$ noise matrix; the real Wiener increments dW_k obey the standard conditions $\mathrm{E}[dW_k] = 0$ and $\mathrm{E}[dW_k dW_j] = \delta_{kj}dt$. It is shown in Appendix B of Ref. [9] that the joint probability distribution $\mathcal{P}(\underline{z}) \equiv \mathcal{P}(\boldsymbol{z},\boldsymbol{z}^*) \equiv \mathcal{P}(\boldsymbol{x},\boldsymbol{y})$ evolves in time according to the Fokker-Planck equation

$$\frac{\partial}{\partial t}\mathcal{P} = -\sum_{\alpha j}\frac{\partial}{\partial \underline{z}_{\alpha j}}\{\underline{A}_{\alpha j}\mathcal{P}\} + \frac{1}{2}\sum_{\alpha j}\sum_{\beta k}\frac{\partial^2}{\partial \underline{z}_{\alpha j}\partial \underline{z}^*_{\beta k}}\{\underline{\underline{D}}_{\alpha\beta jk}\mathcal{P}\}, \tag{51}$$

where $\underline{A} = (\boldsymbol{A},\boldsymbol{A}^*)$; $\underline{\underline{D}}$ is a diffusion matrix,

$$\underline{\underline{D}} = \begin{bmatrix} BB^\dagger & BB^T \\ (BB^T)^* & (BB^\dagger)^* \end{bmatrix} = \begin{bmatrix} B \\ B^* \end{bmatrix}[B^\dagger \quad (B^*)^\dagger]. \tag{52}$$

From this equation, we see that $\underline{\underline{D}}$ is a Hermitian and positive-(semi-)definite matrix.

Now, if we compare the formal QME (48) with the general form of Fokker-Planck equation (51), we see that the QME (48) has the following deficiencies: (i) The drift terms lack their complex conjugates; (ii) the diffusion matrices are not Hermitian. Therefore, the QME (48) cannot be interpreted stochastically. In the following sections, we describe how to fix these deficiencies using the nonuniqueness of the quasiprobability distributions and their master equations.

E. Nonuniqueness of the quasiprobability distribution

As mentioned in Sec. III C, the quasiprobability $\mathcal{P}$ in the phase-space correspondence (16) is not unique, since the basis (12) is overcomplete. It is important to characterize this nonuniqueness, since it implies that the phase-space representation of the quantum evolution (3) is also not unique; i.e., there exist different QMEs, and these QMEs may have different efficiency with respect to Monte Carlo simulation. To obtain the characterization of this nonuniqueness, in the following we investigate the inner-product structure which is generated by the expansion (11). A preliminary treatment of this problem (in the context of a bosonic system) was given in our preceding work [9]. Here we refine our treatment.

Let us select a certain orthonormal basis φ_r, $r = 1,\ldots,\mathcal{N}$, in the one-body Hilbert space H. Consider the matrix elements

$$\Lambda_{\boldsymbol{k},\boldsymbol{k}'}(\boldsymbol{z}) = \langle \boldsymbol{k}|\widehat{\Lambda}(\boldsymbol{z})|\boldsymbol{k}'\rangle, \tag{53}$$

where the N-particle states $|\boldsymbol{k}\rangle = |\varphi_{k_1}\cdots\varphi_{k_N}\rangle$ and $|\boldsymbol{k}'\rangle$ are labeled by the integer vector indices $\boldsymbol{k} = (k_1, \ldots, k_N)$ and $\boldsymbol{k}'$. The matrix elements $\Lambda_{\boldsymbol{k},\boldsymbol{k}'}(\boldsymbol{z})$ are polynomials of degree $2N$ of the variables $\phi^{(1)}_{lr}$ and $\phi^{(2)*}_{lr}$, $l = 1, \ldots, N$, $r = 1, \ldots, \mathcal{N}$. Let us denote by S the space which is spanned by the polynomials $\Lambda_{\boldsymbol{k},\boldsymbol{k}'}(\boldsymbol{z})$. Comparing the definition of the phase-space representation of observable Eq. (30) with the matrix element Eq. (53), we see that actually the matrix element $\Lambda_{\boldsymbol{k},\boldsymbol{k}'}$ is a phase-space representation of the (non-Hermitian) observable $|\boldsymbol{k}'\rangle\langle\boldsymbol{k}|$. Since any N-particle observable can be expanded over the dyadics $|\boldsymbol{k}'\rangle\langle\boldsymbol{k}|$, we conclude that S is the space of all the c-number functions $\mathcal{O}(\boldsymbol{z})$ which correspond to a certain (Hermitian or non-Hermitian) observable operator $\widehat{O}$. Then the density-operator expansion (11) can be represented as the inner product

$$\langle\boldsymbol{k}|\widehat{\rho}_N|\boldsymbol{k}'\rangle = \langle\Lambda^*_{\boldsymbol{k},\boldsymbol{k}'}|\mathcal{P}\rangle_{SD} \tag{54}$$

between the elements of the spaces S and D. Since the basis $\widehat{\Lambda}$ [Eq. (12)] is overcomplete, there is a nontrivial subspace Z of D such that every quasiprobability $\mathcal{Z} \in Z$ is orthogonal to every $\mathcal{O}^* \in S^*$: $\langle\mathcal{O}^*|\mathcal{Z}\rangle_{SD} = 0$. The quasiprobabilities $\mathcal{P}$ and $\mathcal{P} + \mathcal{Z}$ always correspond to the same $\widehat{\rho}_N$, and vice versa: If for some $\mathcal{P}$ the quasiprobabilities $\mathcal{P}$ and $\mathcal{P} + \mathcal{Z}$ correspond to the same $\widehat{\rho}_N$, then $\mathcal{Z} \in Z$. Therefore, we conclude that all the nonuniqueness is contained in the space Z. The phase-space correspondence (16) generates the equivalence relation between the quasiprobability distributions,

$$\mathcal{P} \sim \mathcal{P} + \mathcal{Z}, \tag{55}$$

and the equivalence classes are in one-to-one correspondence with the elements $\mathcal{R} \in R$ of the quotient space $R = D/Z$. We call Z the zero-representation space, since we have $\mathcal{Z} \sim 0$ for every $\mathcal{Z} \in Z$.

In principle, we can find the space Z for the basis $\widehat{\Lambda}$ [Eq. (12)], e.g., see Sec. III B of Ref. [9]. However, that is not what we need. We need to fix the drift and the diffusion terms of the formal QME (48). Therefore, we need the possibility to add the terms of the form $\lambda^T\mathcal{P}$ to the right-hand side of Eq. (48), where λ^T is a certain linear (differential) operator. The necessary and sufficient condition for such a possibility is that $\lambda^T\mathcal{P} \in Z$. In other words, we need to characterize the linear operators $\lambda^T : D \to Z$.

According to the star-product correspondences (42) and (43), the right-hand side of QME is always a differential operator with polynomial coefficients. We denote the space of such operators as L. In order to fix the drift and the diffusion terms, the operators λ^T should belong to the space L. We assume that the space of admissible quasiprobability distributions D is chosen such that for each $\alpha \in L$ there exists an adjoint operator $\alpha^\dagger$. More precisely, we assume that (i) there exists a space S' of functions in the phase space, with a well-defined inner product $\langle\cdot|\cdot\rangle_{S'D}$ between the elements of S' and D; (ii) for any $\alpha \in L$ there exists a linear operator $\alpha^\dagger : S \to S'$ such that

$$\langle\mathcal{O}^*|\alpha\mathcal{P}\rangle_{SD} = \langle(\alpha^T\mathcal{O})^*|\mathcal{P}\rangle_{S'D}, \tag{56}$$

where $\alpha^T \equiv (\alpha^\dagger)^*$. This assumption greatly simplifies the treatment. Indeed, consider the subspace A^T of L, which is defined to consists of operators $\lambda^T : D \to Z$. Then, according to the definition of adjoint operator (56), we have

$$\langle(\lambda\mathcal{O})^*|\mathcal{P}\rangle_{S'D} = \langle\mathcal{O}^*|\lambda^T\mathcal{P}\rangle_{SD} = 0 \tag{57}$$

for every $\mathcal{O} \in S$ and for every $\mathcal{P} \in D$. This means that the image $\mathrm{im}\lambda^*$ should be orthogonal to D. However, if the space D is reach enough (as it is in our case), this means that $\mathrm{im}\lambda^* = 0$. In other words, $S \subset \ker\lambda$, and $\lambda\Lambda_{\boldsymbol{k},\boldsymbol{k}'} = 0$. We call such operators λ the annihilators of the basis $\widehat{\Lambda}$. Now we have attained the characterization of the nonuniqueness of the QME: For any annihilator λ, formally we can add the term $\lambda^T\mathcal{P}$ to the right-hand side of the QME (48) since $\lambda^T\mathcal{P} \sim 0$. Note that for any linear operator $d : D \to D$ we also have

$$\lambda^T d\mathcal{P} \sim 0. \tag{58}$$

The terms like (58) define the additive group of (formal) automorphisms of the QME. In the literature on the generalized phase-space methods [29], this group is called the group of gauge transformations; the terms (58) are called gauge terms, and d is called gauge parameter.

In order to fix the drift and diffusion terms, we are interested in the annihilators which are the first- and the second-order differential operators. For the Slater projections (12), we describe such annihilators in the next section.

F. Annihilators of the Slater projections

In our case of the Slater projections (12), we can easily identify the following types of annihilators. The annihilators of the first type correspond to the analyticity of the basis $\hat{\Lambda}$,

$$\frac{\partial}{\partial\phi^{(1)*}_{lr}}\hat{\Lambda}(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{59}$$

$$\frac{\partial}{\partial\phi^{(2)}_{lr}}\hat{\Lambda}(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{60}$$

where $l = 1, \ldots, N$ and $r = 1, \ldots, \mathcal{N}$. We call them the "analyticity annihilators." To find the other types of annihilators, we employ a differential property of the Slater determinant states,

$$|\boldsymbol{\phi}_1\cdots\boldsymbol{\psi}_l\cdots\boldsymbol{\phi}_N\rangle = \sum_r \psi_{lr}\frac{\partial}{\partial\phi_{lr}}|\overrightarrow{\boldsymbol{\phi}}\rangle, \tag{61}$$

where $l = 1, \ldots, N$. On the left-hand side of this equation, the arbitrary orbital $\boldsymbol{\psi}_l$ replaces the original orbital $\boldsymbol{\phi}_l$. Taking into account this property, and also the facts that (i) the basis $\hat{\Lambda}$ is a homogeneous function of degree 1 in each orbital $\boldsymbol{\phi}_l$, and (ii) the Slater determinant is zero if there are identical orbitals, we obtain the annihilators of the second type,

$$\left[\sum_r \phi^{(1)}_{pr}\frac{\partial}{\partial\phi^{(1)}_{lr}} - \delta_{lp}\right]\hat{\Lambda}(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{62}$$

$$\left[\sum_r \phi^{(2)*}_{pr}\frac{\partial}{\partial\phi^{(2)*}_{lr}} - \delta_{lp}\right]\hat{\Lambda}(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{63}$$

where δ_{lp} is the Kronecker δ. We call them the "homogeneity annihilators." In the same way, we find the third type of

annihilators,

$$\sum_{rs} J_{rs} \frac{\partial^2}{\partial \phi_{lr}^{(1)} \partial \phi_{ms}^{(1)}} \hat{\Lambda}(\vec{\boldsymbol{\phi}}^{(1)}, \vec{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{64}$$

$$\sum_{rs} J_{rs} \frac{\partial^2}{\partial \phi_{lr}^{(2)*} \partial \phi_{ms}^{(2)*}} \hat{\Lambda}(\vec{\boldsymbol{\phi}}^{(1)}, \vec{\boldsymbol{\phi}}^{(2)*}) = 0, \tag{65}$$

where l, m are arbitrary in the interval $[1, N]$ and J is a complex symmetric $\mathcal{N} \times \mathcal{N}$ matrix: $J_{rs} = J_{sr}$, but otherwise J is arbitrary. We call these annihilators the "antisymmetry annihilators."

The expressions for the annihilator operators λ are given by the differential operators on the left-hand side of Eqs. (59) and (60) and Eqs. (62)–(65).

G. Using the basis analyticity to perform the stochastic unraveling of the quasiprobability master equation

As it is demonstrated in Sec. IV C, after application of the star-product operator correspondences (42) and (43), the quantum Liouville equation (3) is mapped onto the QME (48), which has the following form:

$$\frac{\partial}{\partial t}\mathcal{P} = -\sum_j \frac{\partial}{\partial z_j}\{A_j \mathcal{P}\} + \frac{1}{2}\sum_{jk} \frac{\partial^2}{\partial z_j \partial z_k}\{D_{jk}\mathcal{P}\}. \tag{66}$$

Note that the matrix D can always be chosen symmetric due to the symmetry property of the mixed partial derivatives. Here, since the vector $z = (\vec{\boldsymbol{\phi}}^{(1)}, \vec{\boldsymbol{\phi}}^{(2)*})$ has a block structure, the drift vector $\boldsymbol{A}$ and the diffusion matrix D can also be written in the block form. For the drift vector we have

$$\boldsymbol{A} = (\vec{\boldsymbol{A}}^{(1)}, \vec{\boldsymbol{A}}^{(2)*}), \tag{67}$$

where $\vec{\boldsymbol{A}}^{(\alpha)} = (\boldsymbol{A}_1^{(\alpha)}, \ldots, \boldsymbol{A}_N^{(\alpha)})$, and, according to Eq. (48),

$$\left|\boldsymbol{A}_l^{(\alpha)}\right\rangle = \frac{1}{i\hbar}\widehat{T}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle. \tag{68}$$

Therefore, the indices j and k in Eq. (66) are compound: $j = (\alpha l r)$, where $\alpha = 1, \ldots, 2$ is a type of orbital (from bra or from ket state), $l = 1, \ldots, N$ is the index of orbital, and $r = 1, \ldots, \mathcal{N}$ is the component index.

For the diffusion matrix we have the block structure

$$D = \begin{bmatrix} \bar{D}^{(11)} & \bar{D}^{(12)} \\ \bar{D}^{(21)} & \bar{D}^{(22)} \end{bmatrix}. \tag{69}$$

Here, according to Eq. (48), $\bar{D}^{(12)} = \bar{D}^{(21)} = 0$, and the elements of the matrices $\bar{D}^{(\alpha\alpha)}$ are

$$\langle r|\bar{D}_{lm}^{(11)}|s\rangle \equiv \bar{D}_{lmrs}^{(11)} = \frac{1}{2i\hbar}\left(r,s|\widehat{V}^{(A)}|\boldsymbol{\phi}_l^{(1)},\boldsymbol{\phi}_m^{(1)}\right), \tag{70}$$

$$\langle r|\bar{D}_{lm}^{(22)}|s\rangle \equiv \bar{D}_{lmrs}^{(22)} = \left[\frac{1}{2i\hbar}\left(r,s|\widehat{V}^{(A)}|\boldsymbol{\phi}_l^{(2)},\boldsymbol{\phi}_m^{(2)}\right)\right]^*. \tag{71}$$

Since D is symmetric, we have $\bar{D}_{lmrs}^{(\alpha\beta)} = \bar{D}_{mlsr}^{(\beta\alpha)}$.

If we compare Eq. (66) with the general form of Fokker-Planck equation (51), we see that this equation lacks the complex conjugates of the drifts,

$$-\sum_j \frac{\partial}{\partial z_j^*}\{A_j^* \mathcal{P}\}. \tag{72}$$

Moreover, for the condition that the diffusion matrix be Hermitian, the QME (66) lacks the second-order derivative terms

$$\sum_{j,k} \frac{\partial}{\partial z_j^*}\left[\frac{\partial}{\partial z_k}\{G_{jk}\mathcal{P}\} + \frac{1}{2}\frac{\partial}{\partial z_k^*}\{D_{jk}^*\mathcal{P}\}\right], \tag{73}$$

where G is currently an arbitrary Hermitian matrix, which will be found later from the requirement of positivity of diffusion.

Our operator basis is an analytic function due to the annihilators (59) and (60), which in the notation of the current section look like

$$\frac{\partial}{\partial z_j^*}\hat{\Lambda}(z) = 0. \tag{74}$$

According to Eq. (58), we conclude that we can add the term

$$0 \sim \frac{\partial}{\partial z_j^*} d\mathcal{P} \tag{75}$$

to the right-hand side of the QME (66). Now, inspecting the lacking terms (72) and (73), we observe that they have just the form of Eq. (75), and we can freely add them at the right-hand side of the QME (66). Having added them, the drift terms become correct, and the diffusion matrix becomes Hermitian. The last problem is to make the diffusion matrix positive-(semi-)definite. In order to solve it, we inspect the block structure of the diffusion matrix (52) and, upon comparison with the second-order derivative terms in Eqs. (66) and (73), we observe that it is enough to find such a matrix B that

$$D = BB^T. \tag{76}$$

Such a decomposition of D always exists for a symmetric matrix, since we always can perform the Takagi factorization [25], which is a special case of the decomposition (76). Having found B, we just set $G = (BB^\dagger)^*$ in Eq. (73), and immediately obtain that the QME (66) is unraveled by the complex stochastic Ito process (50).

In general, the noise matrix can be written in the block form

$$B = \begin{bmatrix} \bar{B}^{(11)} & \bar{B}^{(12)} \\ \bar{B}^{(21)} & \bar{B}^{(22)} \end{bmatrix}, \tag{77}$$

where the elements of $\bar{B}^{(\alpha\beta)}$ are

$$\langle r|\bar{B}_l^{(\alpha\beta)}|\omega\rangle = \bar{B}_{lr,\omega}^{(\alpha\beta)}, \tag{78}$$

and $|\omega\rangle$ is a certain basis in the space of Wiener increments. Therefore, in Eq. (50) the index k is compound: $k = (\beta\omega)$. The decomposition (76) assumes the general block form

$$\bar{D}_{lm}^{(\alpha\beta)} = \sum_{\gamma=1}^{2} \bar{B}_l^{(\alpha\gamma)} \bar{B}_m^{(\beta\gamma)T}. \tag{79}$$

The explicit expression for the matrix B is found in the next section.

H. Factorization of diffusion matrix

As it was said after Eq. (69), the matrix D is block diagonal

$$D = \begin{bmatrix} D^{(11)} & 0 \\ 0 & [D^{(22)}]^* \end{bmatrix}, \tag{80}$$

where we have introduced the matrices $D^{(\alpha\alpha)}$ with components

$$\langle r|D^{(\alpha\alpha)}_{lm}|s\rangle = D^{(\alpha\alpha)}_{lrms} = \frac{1}{2i\hbar}\big(r,s|\widehat{V}^{(A)}|\boldsymbol{\phi}^{(\alpha)}_l,\boldsymbol{\phi}^{(\alpha)}_m\big). \tag{81}$$

Due to the block-diagonal structure, it is enough to factorize $D^{(\alpha\alpha)} = B^{(\alpha\alpha)}B^{(\alpha\alpha)T}$ for each α individually. Whereas one can attempt to perform the (probably numerical) Takagi factorization [25] of $D^{(\alpha\alpha)}$ as it is given by Eq. (81), currently in the literature another approach is used. First, the interaction potential V_{rsuv} is factorized as [3,5]

$$V_{rsuv} = \sum_\gamma \hbar\omega_\gamma O^{(\gamma)}_{ru} O^{(\gamma)}_{sv}, \tag{82}$$

where ω_γ are real coefficients, and $O^{(\gamma)}_{ru}$ are matrix elements $\langle r|\widehat{O}^{(\gamma)}|u\rangle$ of a certain one-body Hermitian operators $\widehat{O}^{(\gamma)}$. Then, for the antisymmetrized interaction potential $V^{(A)}_{rsuv}$ we have

$$V^{(A)}_{rsuv} = \frac{1}{2}\sum_\gamma \hbar\omega_\gamma\big(O^{(\gamma)}_{ru}O^{(\gamma)}_{sv} - O^{(\gamma)}_{rv}O^{(\gamma)}_{su}\big). \tag{83}$$

If we substitute this expression for $V^{(A)}_{rsuv}$ into Eq. (81), we obtain

$$D^{(\alpha\alpha)}_{lrms} = \frac{1}{2}\sum_\gamma\big\{B^{(\alpha\alpha)}_{lr,\gamma}[B^{(\alpha\alpha)T}]_{\gamma,ms} - B^{(\alpha\alpha)}_{mr,\gamma}[B^{(\alpha\alpha)T}]_{\gamma,ls}\big\}, \tag{84}$$

where

$$B^{(\alpha\alpha)}_{lr,\gamma} = \sqrt{\frac{\omega_\gamma}{2i}}\langle r|\widehat{O}^{(\gamma)}|\boldsymbol{\phi}^{(\alpha)}_l\rangle. \tag{85}$$

In order to factorize the matrix $D^{(\alpha\alpha)}$, we need to get rid of the antisymmetrization with respect to l, m in Eq. (84). This is accomplished by employing the antisymmetry annihilators (64) and (65): To the right-hand side of the QME (48) we add the term

$$0 \sim \frac{1}{2}\sum_{lm}\sum_{rs}\frac{\partial^2}{\partial\phi^{(1)}_{lr}\partial\phi^{(1)}_{ms}}\big\{J^{(11)}_{lrms}\mathcal{P}\big\} + \left[\frac{1}{2}\sum_{lm}\sum_{rs}\frac{\partial^2}{\partial\phi^{(2)}_{lr}\partial\phi^{(2)}_{ms}}\big\{J^{(22)}_{lrms}\mathcal{P}\big\}\right]^*, \tag{86}$$

where the symmetric matrix $J^{(\alpha\alpha)}$ is

$$J^{(\alpha\alpha)}_{lrms} = J^{(\alpha\alpha)}_{lsmr} = \frac{1}{2}\sum_\gamma\big\{B^{(\alpha\alpha)}_{lr,\gamma}[B^{(\alpha\alpha)T}]_{\gamma,ms} + B^{(\alpha\alpha)}_{mr,\gamma}[B^{(\alpha\alpha)T}]_{\gamma,ls}\big\}. \tag{87}$$

After performing this addition, we get a new QME, where the diffusion matrix is now

$$D' = \begin{bmatrix} D^{(11)\prime} & 0 \\ 0 & [D^{(22)\prime}]^* \end{bmatrix}, \tag{88}$$

with

$$D^{(\alpha\alpha)\prime}_{lrms} = \sum_\gamma B^{(\alpha\alpha)}_{lr,\gamma}[B^{(\alpha\alpha)T}]_{\gamma,ms} = \frac{1}{2i\hbar}\big(r,s|\widehat{V}|\boldsymbol{\phi}^{(\alpha)}_l,\boldsymbol{\phi}^{(\alpha)}_m\big). \tag{89}$$

Comparing this expression with the factorization condition (76), we conclude that the stochastic unraveling is complete, and the stochastic process is

$$d\big|\boldsymbol{\phi}^{(\alpha)}_l\big\rangle = \frac{1}{i\hbar}\widehat{T}\big|\boldsymbol{\phi}^{(\alpha)}_l\big\rangle dt + \frac{1}{\sqrt{2i}}\sum_\gamma\sqrt{\omega_\gamma}\widehat{O}^{(\gamma)}\big|\boldsymbol{\phi}^{(\alpha)}_l\big\rangle dW^{(\alpha)}_\gamma, \tag{90}$$

where $l = 1,\ldots,N$; the real Wiener increments $dW^{(\alpha)}_\gamma$ obey the standard conditions: $\mathrm{E}[dW^{(\alpha)}_\gamma] = 0$, $\mathrm{E}[dW^{(\alpha)}_\gamma dW^{(\beta)}_{\gamma'}] = \delta_{\alpha\beta}\delta_{\gamma\gamma'}dt$.

V. EQUIVALENT TRANSFORMATIONS OF QUASIPROBABILITY MASTER EQUATIONS

In the previous sections, we have performed the (formally) equivalent transformation of the QME (48) into a Fokker-Planck equation. In order to accomplish this, we have employed the analyticity (59) and (60) and the antisymmetry (64) and (65) annihilators, whose parameters are uniquely defined by the drift and the diffusion terms of the initial QME (48). However, the existence of the homogeneity annihilators (64) and (65) provides us with additional degrees of freedom, and as a consequence the Fokker-Planck equation is not unique [9]. This means that there are such transformations of the drift and diffusion terms in Eq. (66),

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{A}^\Delta, \tag{91}$$

$$D \to D' = D + D^\Delta, \tag{92}$$

that the QME (formally) remains equivalent to itself. In this section, we describe the equivalent transformations of the Fokker-Planck equations.

Note that the annihilators (59) and (60), (62) and (63), and (64) and (65), assume the most symmetrical form in terms of the variables $(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)*})$. On the other side, the stochastic equations (90) assume the most symmetrical form in terms of the variables $(\overrightarrow{\boldsymbol{\phi}}^{(1)}, \overrightarrow{\boldsymbol{\phi}}^{(2)})$. Therefore, to maintain the conciseness of the expressions for SDEs and for their equivalent transformations, we introduce the overline notation $\bar{\boldsymbol{\phi}}^{(\alpha)}_l$: $\bar{\boldsymbol{\phi}}^{(1)}_l = \boldsymbol{\phi}^{(1)}_l$ and $\bar{\boldsymbol{\phi}}^{(2)}_l = \boldsymbol{\phi}^{(2)*}_l$.

A. Homogeneity annihilators

Suppose that we have a table of linear operators $d^{(\alpha)}_{lp}: D \to D$ for $l,p = 1,\ldots,N$. Then if we act on $d^{(\alpha)}_{lp}\mathcal{P}$ by the transposes of homogeneity annihilators (62) and (63), we conclude that we can add the term

$$0 \sim \sum_{\alpha l} d^{(\alpha)}_{ll}\mathcal{P} + \sum_{\alpha lr}\frac{\partial}{\partial\bar{\phi}^{(\alpha)}_{lr}}\left\{\sum_p \bar{\phi}^{(\alpha)}_{pr}d^{(\alpha)}_{lp}\mathcal{P}\right\} \tag{93}$$

to the right-hand side of the QME (66). In the following, we consider several specific forms of $d^{(\alpha)}_{lp}$.

1. Scalar gauge function

The first case is when the gauge operator $d^{(\alpha)}_{lp}$ is a scalar function,

$$d^{(\alpha)}_{lp} = \bar{\omega}^{(\alpha)}_{lp}(\boldsymbol{z},\boldsymbol{z}^*), \tag{94}$$

where $\omega_{lp}^{(\alpha)}(z,z^*)$ is a table of $2\times N\times N$ arbitrary complex functions; the symbol $\bar{\omega}_{lp}^{(\alpha)}$ is interpreted as $\bar{\omega}_{lp}^{(1)}=\omega_{lp}^{(1)}$ and $\bar{\omega}_{lp}^{(2)}=\omega_{lp}^{(2)*}$. Then, from Eq. (93) we conclude that we can add the term

$$0\sim\sum_{\alpha l}\bar{\omega}_{ll}^{(\alpha)}\mathcal{P}-\sum_{\alpha lr}\frac{\partial}{\partial\bar{\phi}_{lr}^{(\alpha)}}\left\{-\sum_{p}\bar{\phi}_{pr}^{(\alpha)}\bar{\omega}_{lp}^{(\alpha)}\mathcal{P}\right\} \tag{95}$$

to the QME. This relation means that we can absorb (remove) the part of the drift vector

$$-\left|A_l^{\Delta(\alpha)}\right\rangle=\sum_{p}\left|\boldsymbol{\phi}_p^{(\alpha)}\right\rangle\omega_{lp}^{(\alpha)}(z,z^*) \tag{96}$$

into the potential,

$$V^{\Delta}(z,z^*)=\sum_{\alpha l}\bar{\omega}_{ll}^{(\alpha)}(z,z^*). \tag{97}$$

In particular, if $\omega^{(\alpha)}$ are traceless matrices, then no potential term will appear. If we unravel the QME into the Fokker-Planck equation, then the appearance of the potential term $V^{\Delta}(z,z^*)\mathcal{P}$ means that our stochastic process becomes weighted, and the QME should be interpreted according to the Feynman-Kac formula [9,30].

2. *First-order differential gauge operator*

Now we consider the case when the gauge parameter $d_{lm}^{(\alpha)}$ in (93) is a first-order differential operator,

$$d_{lp}^{(\alpha)}=-\sum_{\beta ms}\frac{\partial}{\partial\bar{\phi}_{ms}^{(\beta)}}\bar{g}_{\alpha lmp,s}^{(\beta)}(z,z^*), \tag{98}$$

where $g_{\alpha lmp,s}^{(\beta)}(z,z^*)$ is a table of $2\times 2\times N\times N\times N\times\mathcal{N}$ arbitrary complex functions. Upon substituting this expression for $d_{lp}^{(\alpha)}$ into Eq. (93), and after making a few algebraic rearrangements, we obtain the gauge term

$$\begin{aligned}0\sim&-\sum_{\alpha lr}\frac{\partial}{\partial\bar{\phi}_{lr}^{(\alpha)}}\left\{\sum_{p}\left[\sum_{\beta}\bar{g}_{\beta plp,r}^{(\alpha)}-\bar{g}_{\alpha lpp,r}^{(\alpha)}\right]\mathcal{P}\right\}\\&+\frac{1}{2}\sum_{\alpha lr}\sum_{\beta ms}\frac{\partial^2}{\partial\bar{\phi}_{lr}^{(\alpha)}\partial\bar{\phi}_{ms}^{(\beta)}}\\&\times\left\{-\sum_{p}\left[\bar{\phi}_{pr}^{(\alpha)}\bar{g}_{\alpha lmp,s}^{(\beta)}+\bar{g}_{\beta mlp,r}^{(\alpha)}\bar{\phi}_{ps}^{(\beta)}\right]\mathcal{P}\right\}.\end{aligned} \tag{99}$$

This relation means that we can absorb (remove) the part of the diffusion matrix

$$-D_{lm}^{\Delta(\alpha\beta)}=\sum_{p}\left[\left|\bar{\boldsymbol{\phi}}_p^{(\alpha)}\right\rangle\left\langle\bar{\boldsymbol{g}}_{\alpha lmp}^{(\beta)*}\right|+\left|\bar{\boldsymbol{g}}_{\beta mlp}^{(\alpha)}\right\rangle\left\langle\bar{\boldsymbol{\phi}}_p^{(\beta)*}\right|\right] \tag{100}$$

into the drift vector

$$\left|A_l^{\Delta(\alpha)}\right\rangle=\sum_{\beta p}\left|\boldsymbol{g}_{\beta plp}^{(\alpha)}\right\rangle-\sum_{p}\left|\boldsymbol{g}_{\alpha lpp}^{(\alpha)}\right\rangle. \tag{101}$$

Here the bra-ket notation is defined as $\langle r|\boldsymbol{g}_{\alpha lmp}^{(\beta)}\rangle=g_{\alpha lmp,r}^{(\beta)}$. Note that when we pass from the QME terms (98)–(100) to the SDE term (101), we remove the overlines.

B. Factorization of the modified diffusion matrix

Once we apply the gauge transformations (100) and (101), we need to factorize the modified diffusion matrix

$$D'=D+D^{\Delta}, \tag{102}$$

where it is assumed that we start from some diffusion matrix D (69), which is factorized according to (79) by a certain known noise matrix (77). Here we describe one particular case where the factorization can be carried out explicitly. This case is important since all the currently known stochastic TDHF methods in the literature are special instances of it. Suppose that the gauge function $g_{\alpha lmp,s}^{(\beta)}$ has the form

$$\left|\bar{\boldsymbol{g}}_{\alpha lmp}^{(\beta)}\right\rangle=\sum_{\gamma}\bar{B}_m^{(\beta\gamma)}\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle-\frac{1}{2}\sum_{q}\left|\bar{\boldsymbol{\phi}}_q^{(\beta)}\right\rangle\sum_{\gamma}\left\langle\bar{\boldsymbol{\lambda}}_{\beta mq}^{(\gamma)*}\right|\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle, \tag{103}$$

where $\lambda_{\alpha lp,\omega}^{(\gamma)}(z,z^*)=\langle\omega|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\rangle$ is a table of $2\times 2\times N\times N\times\mathcal{N}_\omega$ arbitrary complex functions; $\mathcal{N}_\omega$ is a dimension of the space of Wiener increments. Then, the modified diffusion matrix (102) is factorized by the modified noise matrix

$$\bar{B}_l'^{(\alpha\beta)}=\bar{B}_l^{(\alpha\beta)}-\sum_{p}\left|\bar{\boldsymbol{\phi}}_p^{(\alpha)}\right\rangle\left\langle\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\beta)*}\right|. \tag{104}$$

This fact can be verified by direct algebraic calculation. Now let us evaluate the drift addition $\boldsymbol{A}_l^{\Delta(\alpha)}$ by substituting into Eq. (101) the expression for the gauge function (103):

$$\begin{aligned}\left|\bar{\boldsymbol{A}}_l^{\Delta(\alpha)}\right\rangle=&\sum_{\gamma p}\left\{\bar{B}_l^{(\alpha\gamma)}\sum_{\beta}\left|\bar{\boldsymbol{\lambda}}_{\beta pp}^{(\gamma)}\right\rangle-\bar{B}_p^{(\alpha\gamma)}\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle\right\}\\&+\frac{1}{2}\sum_{q}\left|\bar{\boldsymbol{\phi}}_q^{(\alpha)}\right\rangle\sum_{\gamma p}\left\{-\left\langle\bar{\boldsymbol{\lambda}}_{\alpha lq}^{(\gamma)*}\right|\sum_{\beta}\left|\bar{\boldsymbol{\lambda}}_{\beta pp}^{(\gamma)}\right\rangle\right.\\&\left.+\left\langle\bar{\boldsymbol{\lambda}}_{\alpha pq}^{(\gamma)*}\right|\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle\right\}.\end{aligned} \tag{105}$$

Note that the second term on the right-hand side of this equation has the form of scalar-gauge drift addition Eq. (96). Therefore, after absorbing this term into the potential term (97), we obtain that the gauge function (103) is equivalent to the simultaneous transformation of the noise matrix (104) of the drift vector

$$\left|\bar{\boldsymbol{A}}_l'^{(\alpha)}\right\rangle=\left|\bar{\boldsymbol{A}}_l^{(\alpha)}\right\rangle+\sum_{\gamma p}\left\{\bar{B}_l^{(\alpha\gamma)}\sum_{\beta}\left|\bar{\boldsymbol{\lambda}}_{\beta pp}^{(\gamma)}\right\rangle-\bar{B}_p^{(\alpha\gamma)}\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle\right\} \tag{106}$$

and of the potential term

$$V'=V+\frac{1}{2}\sum_{\alpha\gamma lp}\left\{-\left\langle\bar{\boldsymbol{\lambda}}_{\alpha ll}^{(\gamma)*}\right|\sum_{\beta}\left|\bar{\boldsymbol{\lambda}}_{\beta pp}^{(\gamma)}\right\rangle+\left\langle\bar{\boldsymbol{\lambda}}_{\alpha pl}^{(\gamma)*}\right|\left|\bar{\boldsymbol{\lambda}}_{\alpha lp}^{(\gamma)}\right\rangle\right\}. \tag{107}$$

Now we interpret the potential term according to the Feynman-Kac formula and introduce the expansion of the density

operator $\hat{\rho}_N$,

$$\widehat{\rho}_N = \int d\Omega d\Omega^* dz dz^* \mathcal{P}(\Omega,\Omega^*,z,z^*)\widehat{\Lambda}(\Omega,z), \tag{108}$$

over the weighted Slater projections,

$$\widehat{\Lambda}(\Omega,z) = \exp(\Omega)|\overrightarrow{\boldsymbol{\phi}}^{(1)}\rangle\langle\overrightarrow{\boldsymbol{\phi}}^{(2)}|. \tag{109}$$

If we start from the QME with the diffusion matrix (89) [with the noise matrix (85)] and apply the gauge (103), we obtain the family of stochastic equations for the weighted Slater projections,

$$\begin{aligned}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle = {}& \frac{1}{i\hbar}\widehat{T}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle dt + \frac{1}{\sqrt{2i}}\sum_\gamma \sqrt{\omega_\gamma}\widehat{O}^{(\gamma)} \\ & \times \sum_p \left\{ \left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle \sum_\beta \lambda^{(\alpha)}_{\beta pp,\gamma} - \left|\boldsymbol{\phi}_p^{(\alpha)}\right\rangle \lambda^{(\alpha)}_{\alpha lp,\gamma} \right\} dt \\ & + \sum_\gamma \left(\sqrt{\frac{\omega_\gamma}{2i}}\widehat{O}^{(\gamma)}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle - \sum_p \left|\boldsymbol{\phi}_p^{(\alpha)}\right\rangle \lambda^{(\alpha)}_{\alpha lp,\gamma} \right) dW_\gamma^{(\alpha)} \\ & - \sum_p \left|\boldsymbol{\phi}_p^{(\alpha)}\right\rangle \sum_\gamma \lambda^{(\bar{\alpha})*}_{\alpha lp,\gamma} dW_\gamma^{(\bar{\alpha})}, \end{aligned} \tag{110}$$

$$d\Omega = \frac{1}{2}\sum_{\alpha\gamma lp} \left\{ -\bar{\lambda}^{(\gamma)}_{\alpha ll,\gamma} \sum_\beta \bar{\lambda}^{(\gamma)}_{\beta pp,\gamma} + \bar{\lambda}^{(\gamma)}_{\alpha pl,\gamma}\bar{\lambda}^{(\gamma)}_{\alpha lp,\gamma} \right\} dt, \tag{111}$$

where $\lambda^{(\beta)}_{\alpha lp,\gamma}(\Omega,\Omega^*,z,z^*) = \langle\gamma|\bar{\boldsymbol{\lambda}}^{(\beta)}_{\alpha lp}\rangle$ is a table of $2\times 2\times N\times N\times \mathcal{N}_\omega$ arbitrary functions in the weighted phase space; the value of the index $\bar{\alpha}$ is opposite to that of α: $\bar{1}=2$ and $\bar{2}=1$. The right-hand side of the equation for Ω (111) is equal to the potential addition (107).

1. Projective transformations of the diffusion matrix

All the currently known-in-literature stochastic TDHF methods [3–7] can be obtained within a specific form of $\bar{\boldsymbol{\lambda}}^{(\gamma)}_{\alpha lp}$ in Eq. (103),

$$\left|\bar{\boldsymbol{\lambda}}^{(\gamma)}_{\alpha lp}\right\rangle = \delta_{\alpha\gamma}\bar{B}^{(\alpha\alpha)T}_l\left|\bar{\boldsymbol{\kappa}}^{(\alpha)}_{lp}\right\rangle, \tag{112}$$

where $\kappa^{(\alpha)}_{lp,r}(\Omega,\Omega^*,z,z^*) = \langle r|\boldsymbol{\kappa}^{(\alpha)}_{lp}\rangle$ is a table of $2\times N\times N\times \mathcal{N}$ arbitrary functions; $\bar{B}^{(11)}_l = B^{(11)}_l$, $\bar{B}^{(22)}_l = B^{(22)*}_l$, and $B^{(\alpha\alpha)}_l$ is defined according to Eq. (85). Substituting the expression for $\bar{\boldsymbol{\lambda}}^{(\gamma)}_{\alpha lp}$ Eq. (112) into the gauge transformations (104)–(106)–(107), we obtain that the modified diffusion matrix assumes the form

$$\bar{D}'^{(\alpha\alpha)}_{lm} = \left(I - \bar{p}^{(\alpha)}_l\right)\bar{D}^{(\alpha\alpha)}_{lm}\left(I - \bar{p}^{(\alpha)T}_m\right), \tag{113}$$

where the projections p_l are defined as

$$p^{(\alpha)}_l = \sum_q \left|\boldsymbol{\phi}^{(\alpha)}_q\right\rangle\left\langle\boldsymbol{\kappa}^{(\alpha)*}_{lq}\right|. \tag{114}$$

The modified diffusion matrix (113) is factorized by the modified noise matrix

$$\bar{B}'^{(\alpha\alpha)}_l = \left(I - \bar{p}^{(\alpha)}_l\right)\bar{B}^{(\alpha\alpha)}_l. \tag{115}$$

The drift term is transformed as

$$\left|\bar{\boldsymbol{A}}'^{(\alpha)}_l\right\rangle = \left|\bar{\boldsymbol{A}}^{(\alpha)}_l\right\rangle + \sum_p \left(\bar{D}^{(\alpha\alpha)}_{lp}\left|\bar{\boldsymbol{\kappa}}^{(\alpha)}_{pp}\right\rangle - \bar{D}^{(\alpha\alpha)}_{pl}\left|\bar{\boldsymbol{\kappa}}^{(\alpha)}_{lp}\right\rangle\right), \tag{116}$$

and the potential term is transformed as

$$\begin{aligned} V' = V + \frac{1}{2}\sum_{\alpha lp} & \left(\left\langle\bar{\boldsymbol{\kappa}}^{(\alpha)*}_{pl}\right|\bar{D}^{(\alpha\alpha)}_{pl}\left|\bar{\boldsymbol{\kappa}}^{(\alpha)}_{lp}\right\rangle \right. \\ & \left. - \left\langle\bar{\boldsymbol{\kappa}}^{(\alpha)*}_{ll}\right|\bar{D}^{(\alpha\alpha)}_{lp}\left|\bar{\boldsymbol{\kappa}}^{(\alpha)}_{pp}\right\rangle\right). \end{aligned} \tag{117}$$

We obtain the following family of stochastic equations:

$$\begin{aligned}\left\langle r\left|\boldsymbol{\phi}^{(\alpha)}_l\right.\right\rangle = {}& \frac{1}{i\hbar}\langle r|\widehat{T}\left|\boldsymbol{\phi}^{(\alpha)}_l\right\rangle dt + \frac{1}{2i\hbar}\sum_{p\neq l}\left\{\left(r,\boldsymbol{\kappa}^{(\alpha)*}_{pp}|\widehat{V}|\boldsymbol{\phi}^{(\alpha)}_l,\boldsymbol{\phi}^{(\alpha)}_p\right)\right. \\ & \left. - \left(r,\boldsymbol{\kappa}^{(\alpha)*}_{lp}|\widehat{V}|\boldsymbol{\phi}^{(\alpha)}_p,\boldsymbol{\phi}^{(\alpha)}_l\right)\right\}dt \\ & + \sum_\gamma \sqrt{\frac{\omega_\gamma}{2i}}\langle r|\left(1 - \sum_p \left|\boldsymbol{\phi}^{(\alpha)}_p\right\rangle\left\langle\boldsymbol{\kappa}^{(\alpha)*}_{lp}\right|\right) \\ & \times \widehat{O}^{(\gamma)}\left|\boldsymbol{\phi}^{(\alpha)}_l\right\rangle dW^{(\alpha)}_\gamma, \end{aligned} \tag{118}$$

$$\begin{aligned} V^{(\alpha)} = {}& \frac{1}{4i\hbar}\sum_{lp}\left\{\left(\boldsymbol{\kappa}^{(\alpha)*}_{pl},\boldsymbol{\kappa}^{(\alpha)*}_{lp}|\widehat{V}|\boldsymbol{\phi}^{(\alpha)}_p,\boldsymbol{\phi}^{(\alpha)}_l\right)\right. \\ & \left. - \left(\boldsymbol{\kappa}^{(\alpha)*}_{ll},\boldsymbol{\kappa}^{(\alpha)*}_{pp}|\widehat{V}|\boldsymbol{\phi}^{(\alpha)}_l,\boldsymbol{\phi}^{(\alpha)}_p\right)\right\}, \end{aligned} \tag{119}$$

$$d\Omega = dt\sum_\alpha \bar{V}^{(\alpha)}. \tag{120}$$

VI. EXAMPLES

In this section, we illustrate how to use the equivalent transformations of QMEs in order to satisfy various constraints. We begin this section by rederiving all the currently known-in-literature stochastic Hartree-Fock methods, and we conclude this section by presenting one method which is a Fermi counterpart of the simple scheme of Carusotto *et al.* [8] for bosons. The validity of these methods, their convergence towards exact quantum dynamics, is discussed in Sec. VII

A. Stochastic mean-field method of Juillet and Chomaz [3]

As it was discussed in [8,9], the magnitude of the diffusion matrix determines the growth rate of the spread of stochastic trajectories in the phase space. The more is the spread of the trajectories, the more is the variance of the simulation results. Therefore, we want to minimize the magnitude of the diffusion matrix. We look for such a gauge function $g^{(\beta)}_{\alpha lmp,r}$ in the transform (100) and (101) that the Hilbert-Schmidt norm of the modified diffusion matrix (100) is minimal,

$$g^{(\beta)}_{\alpha lmp,r} = \arg\min \mathrm{Tr}D'D'^\dagger, \tag{121}$$

where

$$\mathrm{Tr}D'D'^\dagger = \sum_{\alpha\beta lmrs}\left|D'^{(\alpha\beta)}_{lmrs}\right|^2. \tag{122}$$

In order to find $g^{(\beta)}_{\alpha lmp,r}$, we need to solve the equation

$$\frac{\partial}{\partial\bar{g}^{(\beta)}_{\alpha lmp,r}}\mathrm{Tr}D'D'^\dagger = 0. \tag{123}$$

If we insert into this equation the definition of D' [Eqs. (92) and (100)] and perform the differentiation, we obtain

$$\langle \bar{\boldsymbol{\phi}}_p^{(\alpha)} | \bar{D}'^{(\alpha\beta)}_{lm} = 0 \tag{124}$$

for any p, l, and m in the range $1, \ldots, N$. For $\alpha \neq \beta$, we have a homogeneous equation on $g^{(\beta)}_{\alpha lmp,r}$. Therefore, in this case we can set $g^{(\beta)}_{\alpha lmp,r} = 0$. To satisfy Eq. (124) in the case $\alpha = \beta$, it is enough to apply the projective transform (113), in which the projection $\bar{p}_l^{(\alpha)} \equiv \bar{p}^{(\alpha)}$ is chosen such that

$$\langle \bar{\boldsymbol{\phi}}_p^{(\alpha)} | (I - \bar{p}^{(\alpha)}) = 0. \tag{125}$$

That is, $\bar{p}^{(\alpha)\dagger}$ should be chosen as a projection onto the subspace which is spanned by all $\bar{\boldsymbol{\phi}}_p^{(\alpha)}$ for $p = 1, \ldots, N$,

$$\bar{p}^{(\alpha)} = \sum_q |\bar{\boldsymbol{\phi}}_q^{(\alpha)}\rangle\langle \bar{\boldsymbol{\psi}}_q^{(\alpha)}|, \tag{126}$$

where $\boldsymbol{\psi}_q^{(\alpha)}$ is a biorthogonal basis for $\boldsymbol{\phi}_q^{(\alpha)}$,

$$\langle \boldsymbol{\psi}_p^{(\alpha)} | \boldsymbol{\phi}_q^{(\alpha)} \rangle = \delta_{pq}. \tag{127}$$

If we substitute the expression for the projection (126) into the transforms for drift (116) and for potential (117), we obtain the stochastic equations

$$|\boldsymbol{\phi}_l^{(\alpha)}\rangle = \frac{1}{i\hbar}\{\hat{T} + \mathrm{Tr}_2(\hat{V}^{(A)} p^{(\alpha)})\}|\boldsymbol{\phi}_l^{(\alpha)}\rangle dt + \frac{1}{\sqrt{2i}} \sum_\gamma \sqrt{\omega_\gamma}(I - p^{(\alpha)})\hat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle dW_\gamma^{(\alpha)}, \tag{128}$$

$$d\Omega = -\frac{1}{i\hbar}\frac{1}{2}\mathrm{Tr}[p^{(1)}\mathrm{Tr}_2(\hat{V}^{(A)} p^{(1)})] - \left\{\frac{1}{i\hbar}\frac{1}{2}\mathrm{Tr}[p^{(2)}\mathrm{Tr}_2(\hat{V}^{(A)} p^{(2)})]\right\}^*. \tag{129}$$

Here the one-body operator $\langle r|\mathrm{Tr}_2(\hat{V}^{(A)} p^{(\alpha)})|u\rangle = \sum_{sv} V^{(A)}_{rsuv}\langle v|p^{(\alpha)}|s\rangle$. We observe that these equations are exactly the same as that obtained in [3] (with the minor difference that in [3] the potential term (117) is not isolated from the drift).

B. Optimal observable evolution method of Lacroix [6]

As another example, we consider the problem of constructing the trace-conserving stochastic representation. The conventional approach is to require the conservation of trace of the operator basis (12) along each random trajectory. That is, we require

$$\mathrm{Tr}\hat{\Lambda} = \det M = \mathrm{const}, \tag{130}$$

where M is the overlap matrix (34). Therefore, it is enough to satisfy the constraints

$$\langle \boldsymbol{\phi}_p^{(2)} | \boldsymbol{\phi}_q^{(1)} \rangle = \mathrm{const} \tag{131}$$

for all p and q in the range $1, \ldots, N$.

Before we proceed further, let us recall that the constraint

$$f(\Omega, \Omega^*, z, z^*) \equiv f(\underline{\Omega}, \underline{z}) = \mathrm{const}, \tag{132}$$

of which (131) is a special case, means that we require that the differential $df(\underline{\Omega}, \underline{z}) = 0$ along each stochastic trajectory. Therefore, we employ the complex Ito lemma [9] to find $df(\underline{\Omega}, \underline{z})$,

$$df(\underline{\Omega}, \underline{z}) = \left\{\sum_\alpha \underline{V}'_\alpha \frac{\partial}{\partial \underline{\Omega}_\alpha} + \sum_{\alpha j} \underline{A}'_{\alpha j} \frac{\partial}{\partial \underline{z}_{\alpha j}} + \frac{1}{2}\sum_{\alpha\beta}\sum_{jk} \underline{\underline{D}}'_{\alpha\beta jk} \frac{\partial}{\partial \underline{z}_{\alpha j}} \frac{\partial}{\partial \underline{z}^*_{\beta k}}\right\} f(\underline{\Omega}, \underline{z}) dt + \sum_\alpha \sum_{jp} \underline{B}'_{\alpha jp} \frac{\partial f(\underline{\Omega}, \underline{z})}{\partial \underline{z}_{\alpha j}} dW_p, \tag{133}$$

where we suppose that the modified (transformed) and stochastically unraveled QME is written in the compound index notation (51). The compound indices are j and $k = (\beta l r)$, $p = (\beta\omega)$; here β is a type of orbital, l is a orbital index, r is a orbital component, and ω is a Wiener increment component; $\underline{\Omega} = (\Omega, \Omega^*)$ and $\underline{V}' = (V', V'^*)$, where V' is a potential term [which is the drift of the variable Ω, as it is stated by Eq. (111)]. The noise matrix $\underline{B}'_{\alpha jp}$ is defined as $\underline{B}'_{1jp} \equiv B'_{jp}$ and $\underline{B}'_{2jp} \equiv B^*_{jp}$. To satisfy the constraint (132), we have to equal to zero the coefficients before dt and dW_k in Eq. (133).

Let us compute the gradient vectors for the case when $f(\underline{\Omega}, \underline{z}) = \langle \boldsymbol{\phi}_p^{(2)} | \boldsymbol{\phi}_q^{(1)} \rangle$:

$$\frac{\partial f}{\partial \underline{\Omega}} = \left(\frac{\partial f}{\partial \Omega}, \frac{\partial f}{\partial \Omega^*}\right) = 0, \tag{134}$$

$$\frac{\partial f}{\partial \underline{z}_{\alpha j}} \equiv \frac{\partial f}{\partial \underline{z}_{\alpha\beta lr}} = \begin{cases} \phi^{(2)*}_{pr} & \text{for } \alpha = 1,\ \beta = 1,\ l = q, \\ \phi^{(1)}_{qr} & \text{for } \alpha = 2,\ \beta = 2,\ l = p, \\ 0 & \text{otherwise.} \end{cases} \tag{135}$$

If we substitute $\partial f / \partial \underline{z}$ in the noise part of the Ito lemma (133), we obtain the sufficient constraints,

$$B'^{(12)}_p = B'^{(21)}_p = 0, \tag{136}$$

$$\langle \boldsymbol{\phi}_q^{(1)} | B'^{(22)}_p = 0, \tag{137}$$

and

$$\langle \boldsymbol{\phi}_p^{(2)} | B'^{(11)}_q = 0, \tag{138}$$

for any p and q. Suppose that we start from the initial state with $\langle \boldsymbol{\phi}_p^{(2)} | \boldsymbol{\phi}_q^{(1)} \rangle = \delta_{pq}$. Then, we can satisfy the constraints (137) and (138) by employing the projective transform (115) with the projections

$$p_l^{(\alpha)} \equiv p^{(\alpha)} = \sum_q |\boldsymbol{\phi}_q^{(\alpha)}\rangle\langle \boldsymbol{\phi}_q^{(\bar{\alpha})}|. \tag{139}$$

The resulting stochastic equations coincide with (128) and (129), with the only difference that $p^{(\alpha)}$ is now given by (139). As the last step, we need to verify that the deterministic part of the Ito lemma (133) is zero. We inspect the contribution from the term with drift vector $\underline{A}$ and find that it is vanishing for the gradient vector (135). To evaluate the contribution from the term with diffusion matrix $\underline{\underline{D}}$, we calculate the Hessian matrix

$$\frac{\partial^2 f}{\partial \underline{z}_{\alpha j} \partial \underline{z}^*_{\beta k}} \equiv \frac{\partial^2 f}{\partial \underline{z}_{\alpha\gamma lr} \partial \underline{z}^*_{\beta\delta ms}} = 0 \quad \text{if } \gamma = \delta, \tag{140}$$

and we find that this contribution is vanishing, since the modified diffusion matrix has the block-diagonal form (136). Therefore, formally we have completed the construction of the trace-conserving representation. We note that the terms on the right-hand side of Eq. (129) cancel each other, and our stochastic equations coincide with the equations obtained in [6], where they were derived from entirely different considerations.

C. Norm-preserving stochastic time-dependent Hartree-Fock [5]

Currently, all the stochastic wave-function methods share a common problem. The generalized phase space, in which the diffusion happens, is infinite. As a consequence, the quasiprobability distribution is continuously being smeared out, and the variance of the Monte Carlo simulation results grows with simulation time. Moreover, for the quantum systems with pairwise interactions, the diffusion matrix depends quadratically on the phase-space variables. This fact leads to at least exponential growth of the variance [3,8,9]. Therefore, the simulation time, which is reachable within the reasonable computational effort, is limited. It is called the useful simulation time [10]. Tessieri *et al.* [5] have made an attempt to solve this problem by restricting the available phase space to a manifold of finite volume. In this section, we reformulate their reasoning in terms of gauge transformations.

Let us consider the unit sphere in the one-body Hilbert space H, which is defined by the equation

$$f_l^{(\alpha)}(\underline{z}) = \exp\left(\frac{1}{N}\,\mathrm{Re}\Omega\right)\langle\boldsymbol{\phi}_l^{(\alpha)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle = 1 \tag{141}$$

for $\alpha = 1,\ldots,2$ and $l = 1,\ldots,N$. Actually, we have $2N$ spheres: one sphere for each type of orbital. Now, suppose that the initial density matrix $\widehat{\rho}_N$ is represented by a quasiprobability distribution $\mathcal{P}(z,z^*)$ which is concentrated on these spheres. If we find such a gauge transformation of the QME that the constraints (141) are satisfied, then (formally) we have the phase-space representation on a finite manifold, and the useful simulation time should be significantly increased. Let us construct this gauge transformation.

We again consider the Ito lemma (133). We calculate the gradients and the Hessian matrices of the constraint functions (141) and substitute them into the Ito lemma. Then the noise part of the lemma gives us the condition on the noise matrix

$$\mathrm{Re}\langle\boldsymbol{\phi}_l^{(\alpha)}|B_l'^{(\alpha\beta)} = 0 \tag{142}$$

for all β. The deterministic part of the lemma gives us the condition on the potential and on the drift

$$\frac{1}{N}\exp\left(\frac{1}{N}\mathrm{Re}\Omega\right)\|\boldsymbol{\phi}_l^{(\alpha)}\|^2\mathrm{Re}V' + 2\mathrm{Re}\langle\boldsymbol{\phi}_l^{(\alpha)}|A_l'^{(\alpha)}\rangle = -\sum_{r\beta\gamma}|B_{lr,\gamma}'^{(\alpha\beta)}|^2. \tag{143}$$

To satisfy the condition on the noise matrix (142), it is sufficient to set $B_l'^{(12)} = B_l'^{(21)} = 0$ and to find such an equivalent transformation that

$$\langle\boldsymbol{\phi}_l^{(\alpha)}|B_l'^{(\alpha\alpha)} = 0. \tag{144}$$

This equation can be satisfied by the projective transform of the noise matrix (115), with the projection

$$\bar{p}_l^{(\alpha)} = \frac{|\boldsymbol{\phi}_l^{(\alpha)}\rangle\langle\boldsymbol{\phi}_l^{(\alpha)}|}{\|\boldsymbol{\phi}_l^{(\alpha)}\|^2}. \tag{145}$$

We calculate the modified drift vector according to (91), (101), (103), and (112) with $\boldsymbol{\kappa}_{lq}^{(\alpha)} = \delta_{lq}\boldsymbol{\phi}_l^{(\alpha)*}/\|\boldsymbol{\phi}_l^{(\alpha)}\|^2$:

$$A_l'^{(\alpha)} = \frac{1}{2i}\sum_\gamma\omega_\gamma\sum_{p\neq l}\frac{1}{\|\boldsymbol{\phi}_p^{(\alpha)}\|^2}\langle\boldsymbol{\phi}_p^{(\alpha)}|\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_p^{(\alpha)}\rangle \times\left\{\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle - \frac{1}{2\|\boldsymbol{\phi}_l^{(\alpha)}\|^2}|\boldsymbol{\phi}_l^{(\alpha)}\rangle\langle\boldsymbol{\phi}_l^{(\alpha)}|\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle\right\}. \tag{146}$$

Note that this expression is essentially the same as (116) and (117), with the only difference being that the potential term is not isolated, i.e., $V' = 0$. If we substitute this expression into (143), we find that $\mathrm{Re}\langle\boldsymbol{\phi}_l^{(\alpha)}|A_l'^{(\alpha)}\rangle = 0$. Therefore, the condition on drift (143) is not satisfied by (146). To rectify the situation, we apply the scalar homogeneity transform (96) with traceless matrix $\omega_{lp}^{(\alpha)}$ (so that no potential term appears). By adding $\boldsymbol{A}_l^{\Delta(\alpha)}$ [Eq. (96)] to the left-hand side of Eq. (143), we obtain the condition on $\omega_{lp}^{(\alpha)}$:

$$-\mathrm{Re}\sum_p\omega_{lp}^{(\alpha)}\langle\boldsymbol{\phi}_l^{(\alpha)}|\boldsymbol{\phi}_p^{(\alpha)}\rangle = -\frac{1}{4}\sum_\gamma|\omega_\gamma|\left\{\langle\boldsymbol{\phi}_l^{(\alpha)}|\widehat{O}^{(\gamma)2}|\boldsymbol{\phi}_l^{(\alpha)}\rangle - \frac{1}{\|\boldsymbol{\phi}_l^{(\alpha)}\|^2}\langle\boldsymbol{\phi}_l^{(\alpha)}|\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle^2\right\}. \tag{147}$$

The trivial solution to this system is obtained by choosing $\omega_{lp}^{(\alpha)}$ to be a table of real functions such that $\omega_{lp}^{(\alpha)}\langle\boldsymbol{\phi}_l^{(\alpha)}|\boldsymbol{\phi}_p^{(\alpha)}\rangle$ does not depend on p. This gives us one possible solution,

$$\omega_{lp} = \frac{1}{4}\sum_\gamma|\omega_\gamma|\frac{\langle\boldsymbol{\phi}_l^{(\alpha)}|\widehat{O}^{(\gamma)2}|\boldsymbol{\phi}_l^{(\alpha)}\rangle - \frac{1}{\|\boldsymbol{\phi}_l^{(\alpha)}\|^2}\langle\boldsymbol{\phi}_l^{(\alpha)}|\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle^2}{(N-1)\mathrm{Re}\langle\boldsymbol{\phi}_l^{(\alpha)}|\boldsymbol{\phi}_p^{(\alpha)}\rangle}, \tag{148}$$

for $l \neq p$, and

$$\omega_{ll} = 0. \tag{149}$$

Now, formally the phase-space representation on a finite manifold is constructed. Bringing together all the ingredients, we obtain the stochastic equations of [5]:

$$|\boldsymbol{\phi}_l^{(\alpha)}\rangle = \frac{1}{i\hbar}\left\{\widehat{T}|\boldsymbol{\phi}_l^{(\alpha)}\rangle + A_q'^{(\alpha)} - \sum_p|\boldsymbol{\phi}_p^{(\alpha)}\rangle\omega_{pl}^{(\alpha)}\right\}dt + \frac{1}{\sqrt{2i}}\sum_\gamma\sqrt{\omega_\gamma}\left(I - \frac{|\boldsymbol{\phi}_l^{(\alpha)}\rangle\langle\boldsymbol{\phi}_l^{(\alpha)}|}{\|\boldsymbol{\phi}_l^{(\alpha)}\|^2}\right)\times\widehat{O}^{(\gamma)}|\boldsymbol{\phi}_l^{(\alpha)}\rangle dW_\gamma^{(\alpha)}. \tag{150}$$

D. "Simple scheme" for fermions

Here we present an additional stochastic method. The purpose of doing this is to demonstrate that the stochastic Hartree-Fock methods, which converge towards exact quantum dynamics, do exist. We call it the "simple scheme" for fermions because its structure and convergence properties are similar to that of the simple scheme for bosons, which was invented in the work of Carusotto *et al.* [8] and which was proven to be free from systematic errors in [9].

We start from the general projectively transformed family of SDEs (118), (119), and (120) and employ the same parameter $\boldsymbol{\kappa}_{lq}^{(\alpha)}$ as in the method of Tessieri *et al.* [5]:

$$\boldsymbol{\kappa}_{lq}^{(\alpha)} = \delta_{lq}\boldsymbol{\phi}_l^{(\alpha)*}/\left\|\boldsymbol{\phi}_l^{(\alpha)}\right\|^2. \tag{151}$$

We obtain the stochastic equations

$$\begin{aligned}\left\langle r\middle|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle =& \frac{1}{i\hbar}\langle r|\widehat{T}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle dt + \frac{1}{2i\hbar}\sum_{p\neq l}\frac{1}{\left\|\boldsymbol{\phi}_p^{(\alpha)}\right\|^2}\\ &\times \left(r,\boldsymbol{\phi}_p^{(\alpha)}|\widehat{V}|\boldsymbol{\phi}_l^{(\alpha)},\boldsymbol{\phi}_p^{(\alpha)}\right)dt\\ &+ \sum_\gamma\sqrt{\frac{\omega_\gamma}{2i}}\left(1-\frac{1}{\left\|\boldsymbol{\phi}_l^{(\alpha)}\right\|^2}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle\left\langle\boldsymbol{\phi}_l^{(\alpha)}\right|\right)\\ &\times \widehat{O}^{(\gamma)}\left|\boldsymbol{\phi}_l^{(\alpha)}\right\rangle dW_\gamma^{(\alpha)},\end{aligned} \tag{152}$$

$$V^{(\alpha)} = -\frac{1}{4i\hbar}\sum_{l\neq p}\frac{1}{\left\|\boldsymbol{\phi}_l^{(\alpha)}\right\|^2\left\|\boldsymbol{\phi}_p^{(\alpha)}\right\|^2}\left(\boldsymbol{\phi}_l^{(\alpha)},\boldsymbol{\phi}_p^{(\alpha)}\middle|\widehat{V}\middle|\boldsymbol{\phi}_l^{(\alpha)},\boldsymbol{\phi}_p^{(\alpha)}\right), \tag{153}$$

$$d\Omega = dt\sum_\alpha \bar{V}^{(\alpha)}. \tag{154}$$

VII. CONVERGENCE TOWARDS EXACT QUANTUM DYNAMICS

In this section we discuss the conditions where a stochastic Hartree-Fock method is guaranteed to reproduce the exact quantum dynamics (in terms of expected values of the observables).

First of all, we need to ensure that the SDE of a stochastic Hartree-Fock method satisfy the conditions of the existence of a solution. We recall that the SDE of a general form (50) possesses a solution $z(t)$ which is valid at all times $t \in [0,\infty)$ (nonexploding), if the following restriction on the growth order is satisfied [31],

$$\|\boldsymbol{A}(z,z^*)\|^2 + \|B(z,z^*)\|^2 \leqslant K(1+\|z\|^2), \tag{155}$$

where K is some positive constant. The SDE which violates this restriction can exhibit exploding trajectories (the so-called spikes [32]). It is known from the experience with phase-space methods that the appearance of the spiking solutions is usually accompanied with the emergence of slowly decaying power-law tails of $\mathcal{P}(z,z^*,t)$ [32]; thus, the stochastic method does not reproduce the exact quantum dynamics (as it is discussed in Secs. IV B and IV C). However, we note that Eq. (155) is a sufficient condition. It does not mean automatically that the SDE which violates this condition will exhibit the spiking trajectories. Moreover, according to the current developments in mathematics [33,34], we can expect the emergence of more general and flexible conditions than Eq. (155) in the near future. Nevertheless, currently, any method violating Eq. (155) should be considered as having unclear status and as requiring a special investigation.

The next point to be checked is the uniqueness of the solution. The sufficient condition for this is the generalized Lipshitz condition [31]: For every $p > 0$ there should exist such a constant K_p that

$$\begin{aligned}&\|\boldsymbol{A}(z,z^*) - \boldsymbol{A}(z',z'^*)\| + \|B(z,z^*)\\ &\quad - B(z',z'^*)\| \leqslant K_p\|z-z'\|\end{aligned} \tag{156}$$

for all times and for all z such that $\|z\| \leqslant p$. The violation of this condition jeopardizes the numerical computations: The latter rely on the discretized approximations of the continuous stochastic process. However, if the generalized Lipshitz condition is violated, the discretized process is not guaranteed to converge towards the continuous one as we decrease the time step. Another difficulty is that the initial-value problem may become ill defined.

The last, and usually the most difficult, task is to prove that the quasiprobabilities $\mathcal{P}(z,z^*,t)$, which correspond to the solutions of the SDE, and all the spatial derivatives of $\mathcal{P}(z,z^*,t)$ do not have the power-law tails and that their tails are uniformly dominated. In fact, currently there is no well-established mathematical tool for doing that. We refer the interested reader to [33,34] for (we believe) the relevant current developments in mathematics.

In the following, we check these conditions for each of the stochastic Hartree-Fock methods mentioned in Sec. VI.

A. Method of Juillet and Chomaz [3]

Since the projections (126) have unit norm, $\|\bar{p}^{(\alpha)}\| = 1$, the growth restriction (155) is satisfied by the stochastic equations of Juillet and Chomaz (128) and (129). However, we have problems with the generalized Lipshitz condition Eq. (156). The problems come from the projections $\bar{p}^{(\alpha)}$: The dimension of the image $\dim\mathrm{im}\,\bar{p}^{(\alpha)}$ equals to the number of linearly independent orbitals in the set $(\boldsymbol{\phi}_1^{(\alpha)},\ldots,\boldsymbol{\phi}_N^{(\alpha)})$. Therefore, when these orbitals continuously evolve, the number of independent orbitals can suddenly change. This means that the derivatives $\partial\bar{p}^{(\alpha)}/\partial z$ become singular, which is incompatible with the generalized Lipshitz condition (156). Moreover, it can be argued that in the vicinity of the locus, where the change of the $\dim\mathrm{im}\,\bar{p}^{(\alpha)}$ happens, the derivative diverges as $\|\partial\bar{p}^{(\alpha)}/\partial z\| \sim 1/s$, where s is the distance to the locus. Whereas the test calculations for an exactly solvable model system in the work [3] do not show systematic discrepancies, in the absence of the detailed studies of the singularities of $\partial\bar{p}^{(\alpha)}/\partial z$ and their influence on the solutions and numerical methods, we should consider the status of this method as uncertain.

B. Optimal observable evolution method of Lacroix [6]

The stochastic equations of this method coincide with that of Juillet and Chomaz (128) and (129), except that the projections $p^{(\alpha)}$ are now given by Eq. (139). From the form of $p^{(\alpha)}$ we obtain that the drift vector and the noise matrix

are cubic in the components of $\phi_{lr}^{(\alpha)}$. Therefore, the growth restriction (155) is violated, and we expect that the method can exhibit systematic discrepancies with the exact quantum dynamics. This conclusion is supported by the numerical tests in the work [6].

C. Norm-preserving stochastic time-dependent Hartree-Fock [5]

The method of Tessieri *et al.* [5] violates both the growth and the generalized Lipshitz conditions: The matrix ω_{lp} (148), which enters the drift term in the Eq. (150), contains the inner product $\langle \boldsymbol{\phi}_l^{(\alpha)} | \boldsymbol{\phi}_p^{(\alpha)} \rangle$ in the denominator. If any two orbitals become nearly orthogonal, the drift coefficient will diverge. Therefore, we should consider the status of this method as uncertain.

D. "Simple scheme" for fermions

Finally, we consider the stochastic equations (152), (153), and (154). If we assume that the norms $\|\widehat{O}^{(\gamma)}\|$ and $\|\widehat{V}\|$ are finite, then we obtain that the growth restriction (155) is satisfied. Moreover, the generalized Lipshitz condition (156) is also satisfied. Therefore, these equations satisfy the conditions for the existence and uniqueness of the solution.

Now we prove that in this method there are no power-law tails. We proceed in the same way as in Sec. V of Ref. [9]. We consider the evolution of the function

$$f = \sum_{l=1}^{N} \langle \boldsymbol{\phi}_l^{(\alpha)} | \boldsymbol{\phi}_l^{(\alpha)} \rangle. \tag{157}$$

We substitute this function into the Ito lemma (133). We find that the noise term vanishes due to the choice of $\boldsymbol{\kappa}_{lq}^{(\alpha)}$ Eq. (151); in the deterministic part the drift contribution also vanishes. Therefore, we obtain

$$df = \sum_{lr\gamma} \left| B_{lr,\gamma}^{\prime(\alpha\alpha)} \right|^2 dt \leqslant \text{const} \times \max_{\gamma} \|\widehat{O}^{(\gamma)}\|^2 f\, dt. \tag{158}$$

Integrating this inequality, we get

$$f(t) \leqslant f(0) \exp(\text{const} \times \max_{\gamma} \|\widehat{O}^{(\gamma)}\|^2 t). \tag{159}$$

This means that if the initial quasiprobability $\mathcal{P}$ is vanishing outside the ball of radius R, then at any later time t it will be also vanishing outside the ball of a finite radius (although the radius is increasing exponentially). This concludes our proof that the simple scheme for fermions is a correct stochastic representation of the exact quantum dynamics.

Here it should be noted that we do not argue that this method is efficient, or that it should be used for simulations. We provide it here as a proof of concept, that a correct, well-defined, stochastic Hartree-Fock method is possible. Now the actual problem is to find the most efficient scheme possible, using the equivalent transformations described in the previous sections.

VIII. CONCLUSION

In this work, we have developed a rigorous and unified approach to the stochastic TDHF methods. Our approach is to explicitly consider the quasiprobability distributions which emerge in these methods. In the case of a quantum system with pairwise interactions, this approach has allowed us to completely describe the QMEs, the corresponding stochastic differential equations, and their equivalent transformations. Sufficient conditions, where the stochastic TDHF method is guaranteed to reproduce the exact quantum dynamics, are presented. It is shown that all the currently known methods reported in the literature have unclear status with respect to these conditions. Nevertheless, we explicitly construct an example method, which we call the "simple scheme for fermions," and prove that it is well defined and satisfies all the conditions.

We believe that the general forms of stochastic equations presented here will be useful in the development of efficient real and imaginary time Monte Carlo methods based on the Slater states (including the auxiliary field and other related methods [35–42]).

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