Quantum dynamics of Bose-Fermi mixtures via the stochastic-wave-function approach

Paweł Zin*
National Center for Nuclear Research, ul. Hoża 69, 00-681 Warsaw, Poland

(Received 12 April 2018; published 4 October 2018)

We present a reformulation of the nonrelativistic many-body quantum dynamics of Bose-Fermi mixtures via stochastic wave functions. We show that, within a wide range of two-particle interactions and a certain class of greater-than-two-particle interactions, the quantum dynamics can be mapped exactly onto a set of single-particle wave functions, with their evolution governed by a stochastic process.

DOI: 10.1103/PhysRevA.98.043608

I. INTRODUCTION

In recent years, considerable progress has been made in simulating the dynamics of many-body systems via stochastic equations. In the case of bosons, extensive use of the positive P representation has been made (see Ref. [1] and references therein). This representation allows for exact reformulation of the many-body quantum dynamics via stochastic equations if certain conditions are met. A different (technically simpler) derivation of similar stochastic equations using so-called stochastic wave functions has been presented in Ref. [2]. These stochastic equations have been used in simulating many-body quantum dynamics of interacting ultracold bosonic gases [3]. In the fermionic case, there are formulations of quantum dynamics using a stochastic-wave-function approach [4–8]. The stochastic equations obtained were rederived by using generalized phase-space representations [9]. A different approach was presented in Ref. [10] and uses Gaussian phase-space representations for fermions. There, within two-body interactions, the authors of Ref. [10] mapped quantum operator evolution onto stochastic processes in phase space. This method was generalized to Bose-Fermi systems and applied to the dissociation of bosonic molecules into a pair of fermionic atoms [11]. Apart from these methods there exists a variety of other methods simulating quantum many-body dynamics. We mention recently developed time-dependent variational Monte Carlo methods [12] and real-time full configuration Monte Carlo [13].

In the present paper, we generalize the stochastic-wave-function approach to Bose-Fermi mixtures. We show that the evolution under a Hamiltonian with a wide-range two-body interaction can be represented by stochastic equations. Additionally, we extend such a representation to a special form of greater-than-two-body interactions.

The method presented below uses many-body states of the particularly simple form

$$|\Psi_s\rangle = |\psi, N_b\rangle|\{\phi\}, N_f\rangle, \tag{1}$$

where $|\psi, N_b\rangle = |\psi\rangle^{\otimes N_b}$ is a product of single-particle orbitals $|\psi\rangle$ of N_b bosons while $|\{\phi\}, N_f\rangle$ denotes a Slater determinant of N_f single-particle orbitals $\{\phi\}$. The first ingredient of the method is based on the fact that the temporal evolution under a single-particle operator transforms such state into the same kind of state with single-particle orbitals changed (in the fermionic case such a statement is called Thouless's theorem [14]). Such an evolution is easy to implement numerically because we only need to evolve $1 + N_f$ *single-particle orbitals* (one for bosons and N_f for fermions) and not whole many-body states (which is usually impossible to even keep in computer memory).

The second idea of the method presented is to represent the evolution under two-body and greater-than-two-body operators as a sum over evolutions under single-particle operators. Here comes the stochastic ingredient of the method: In each time step Δt of the evolution, the single-particle operator is multiplied by a variable chosen by a random draw from a given probability distribution. In a finite time, there are many random draws of variables, which constitutes a stochastic process. Thus, the evolution under the full Hamiltonian is represented as a sum over stochastic processes, each of them given by a single-particle evolution. A single component of such a sum transforms the initial state $|\Psi_s\rangle$ given by Eq. (1) into a state of the same form $|\Psi'_s\rangle$. Thus, taking $|\Psi_s\rangle$ as an initial many-body state, the quantum evolution leads to a state

$$|\Psi\rangle = \lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} |\Psi'_{s,j}\rangle, \tag{2}$$

where M denotes the number of stochastic trajectories. Each of the functions $|\Psi'_{s,j}\rangle$ is obtained via single-particle evolution defined by a stochastic process (i.e., the single-particle orbitals defining state $|\Psi'_s\rangle$ depend of the values of the variables drawn in a single realization of the process), so $|\Psi'_{s,j}\rangle$ is called a "stochastic wave function" and the whole method is called the "stochastic-wave-function approach." We now describe each of the ingredients of the method in more detail.

II. DECOMPOSITION OF QUANTUM EVOLUTION

We now focus our attention on the decomposition of the evolution under the Hamiltonian into a sum of evolutions under single-particle operators. First, let us analyze the evolution under a quite general two-particle interaction. The first

*pawel.zin@ncbj.gov.pl

step is to decompose the interaction part of the Hamiltonian into single-particle operators. To do it, let us first consider a two-particle interaction potential $V_{1,2}$ where 1 and 2 denote the first and second particle degrees of freedom (position, spin projection). In the Appendix we show (repeating the reasoning given in Refs. [4,5]) that, for general boson-boson and fermion-fermion interaction potentials, $V(1,2)$ can be decomposed as

$$V(1,2) = \sum_r \omega_r O^r(1) O^r(2), \tag{3}$$

where ω_r is real number and O^r are functions of position and spin projection. In the case of boson-fermion interactions we restrict our considerations to the potentials of the form given by Eq. (3). From now on, we use the second-quantized form of the Hamiltonian and all operators. The formulation of the method in this language is easier since it takes into account symmetry properties. As shown in the Appendix the decomposition given by Eq. (3) enables us to decompose the two-body-interaction Hamiltonian as

$$\hat{H}_2 = \sum_r \omega_{r;b} \hat{O}^r_b \hat{O}^r_b + \sum_r \omega_{r;f} \hat{O}^r_f \hat{O}^r_f + \sum_r \omega_{r;bf} \hat{O}^r_{b;bf} \hat{O}^r_{f;bf} + \hat{H}_{1,ad},$$

where the first three terms on the right-hand side correspond to boson-boson, fermion-fermion, and boson-fermion interactions. The operators $\hat{O}^r_i$ are single-particle operators of the form

$$\hat{O}^r_b = \sum_i O_b(i) \hat{n}_{b,i}, \tag{4}$$

where $i = (\mathbf{r}, m)$ denotes the position and spin projections and $\hat{n}_{b,i} = \hat{a}^\dagger_i \hat{a}_i$ is a number operator. Here $\mathbf{r}$ is a position on a lattice. In the above equation $\hat{H}_{1,ad}$ denotes a single-particle operator which comes from the use of commutation relations. In what follows we add this operator into the single-particle Hamiltonian $\hat{H}_1$ and therefore from now on it is not present in $\hat{H}_2$.

Having done that, we use it in the decomposition of the evolution under two-body operators into single-particle evolution. To do it we analyze small time step Δt evolution. Up to linear terms in Δt we have

$$\exp(i\hat{H}\Delta t) \simeq \exp(-i\hat{H}_1\Delta t)(1 - i\hat{H}_2\Delta t), \tag{5}$$

where $\hat{H} = \hat{H}_1 + \hat{H}_2$ and $\hat{H}_{1,2}$ denote the single-particle- and two-body-interaction parts of the Hamiltonian. We now introduce the operators

$$\hat{U}_\alpha(\{\zeta\}) = \exp\left(\sqrt{-i\Delta t} \sum_r \zeta_{r;\alpha} \hat{O}^r_\alpha\right),$$
$$\hat{U}_{\alpha;bf}(\{\zeta\}) = \exp\left(\sqrt{-i\Delta t} \sum_r \zeta_{r;bf} \hat{O}^r_{\alpha;bf}\right), \tag{6}$$

where $\alpha = b,\ f$, and ζ are complex variables defined together with the single variable probability distribution $\rho(\zeta)$, $\int d^2\zeta\ \rho(\zeta) = 1$. We additionally define the operator

$$\hat{U}_2(\{\zeta\}) = \hat{U}_b(\{\zeta^*\})\hat{U}_b(\{\zeta\})\hat{U}_f(\{\zeta^*\})\hat{U}_f(\{\zeta\}) \times \hat{U}_{b;bf}(\{\zeta^*\})\hat{U}_{f;bf}(\{\zeta\}) \tag{7}$$

together with the average defined as

$$\langle \ldots \rangle_s = \int \prod_r d^2\zeta_{r,b}\, \rho(\zeta_{r,b}) \int \prod_r d^2\zeta_{r,f}\, \rho(\zeta_{r,f}) \times \int \prod_r d^2\zeta_{r,bf}\, \rho(\zeta_{r,bf}) \cdots .$$

According to Eq. (6), to get the linear terms in Δt we need to expand the operator given by Eq. (7) up to quadratic terms in ζ. Taking

$$\langle \zeta_{r,i} \rangle_s = 0, \quad \langle \zeta_{r,i}\zeta_{r',j} \rangle_s = 0, \quad \langle \zeta^*_{r;i}\zeta_{r',j} \rangle_s = \omega_{r;i}\delta_{r,r'}\delta_{i,j}, \tag{8}$$

where $i, j = b,\ f,\ bf$, we obtain up to linear terms

$$\langle \hat{U}_2(\{\zeta\}) \rangle_s \simeq 1 - i\hat{H}_2\Delta t. \tag{9}$$

Introducing the operator

$$\hat{U}(\{\zeta\}) = \exp(-i\hat{H}_1\Delta t)\hat{U}_2(\{\zeta\}), \tag{10}$$

we end up with

$$\exp(-i\hat{H}\Delta t) \simeq \langle \hat{U}(\{\zeta\}) \rangle_s, \tag{11}$$

where we used Eqs. (5) and (9). In a finite time we have

$$\exp(-i\hat{H}t) \simeq \prod_{j=1}^{t/\Delta t} \langle \hat{U}(\{\zeta\}_j) \rangle_{j,s}, \tag{12}$$

where $\{\zeta\}_j$ and $\langle \ldots \rangle_{j,s}$ denote a set of ζ and the average in a jth time step, respectively. The equality in the above equation is obtained in the limit $\Delta t \to 0$. To simplify the notation we use $\{\zeta\}_{t,\Delta t}$ as a set combining all sets $\{\zeta\}_j$ for $j = 1 \ldots t/\Delta t$, the total average $\langle \ldots \rangle_s$ combining all averages, and additionally

$$\hat{U}(\{\zeta\}_{t,\Delta t}, t, \Delta t) = \prod_{j=1}^{t/\Delta t} \hat{U}(\{\zeta\}_j) \tag{13}$$

as an evolution operator consisting of all subsequent evolutions under single-particle operators. Upon inserting the above in Eq. (12) we arrive at

$$\exp(-i\hat{H}t) \simeq \langle \hat{U}(\{\zeta\}_{t,\Delta t}, t, \Delta t) \rangle_s. \tag{14}$$

We now discuss the average $\langle U(\{\zeta\}_{t,\Delta t}, t, \Delta t) \rangle_s$. It is the multidimensional integral over the whole set $\{\zeta\}_{t,\Delta t}$ with the number of dimensions growing with the decrease of Δt. In such case the use of Monte Carlo sampling is adequate. There the multidimensional integral is approximated by a finite sum, i.e.,

$$\langle \hat{U}(\{\zeta\}_{t,\Delta t}, t, \Delta t) \rangle_s \simeq \frac{1}{M} \sum_{k=1}^{M} \hat{U}(\{\zeta_k\}_{t,\Delta t}, t, \Delta t), \tag{15}$$

where $\{\zeta_k\}_{t,\Delta t}$ denotes the whole set $\{\zeta\}_{t,\Delta t}$ in the kth term in the sum. This set is obtained by drawing all ζ constituting the set $\{\zeta_k\}_{t,\Delta t}$, each with the same single-variable probability

density ρ. The equality in the above sum is obtained in the limit $M \to \infty$. Upon inserting Eq. (15) into Eq. (14) we arrive at

$$\exp(-i\hat{H}t) \simeq \frac{1}{M}\sum_{k=1}^{M}\hat{U}(\{\zeta_k\}_{t,\Delta t}, t, \Delta t). \tag{16}$$

Thus, we decomposed the evolution under the Hamiltonian with a quite general two-body interaction into a sum of operators, each describing the evolution under a single-particle operator. Consequently, we obtained the second crucial ingredient of the method described in the introduction. As we see above, the single-particle evolution operator $\hat{U}(\{\zeta\}_{t,\Delta t}, t, \Delta t)$ depends on the set of random variables $\{\zeta\}_{t,\Delta t}$. Because we deal with temporal evolution we in fact deal with stochastic process where each set $\{\zeta\}_{t,\Delta t}$ is a realization of such a process with $\langle \ldots \rangle_s$ being an average over realizations.

To continue our analysis, we assume that the initial many-body state $|\Psi(0)\rangle$ is given by $|\Psi_s\rangle$ defined by Eq. (1). We now use the first ingredient of the method mentioned in the introduction: the result of the action of the operator $U(\{\zeta_k\}_{t,\Delta t}, t, \Delta t)$ on the state $|\Psi_s\rangle$ is a wave function of the same form as $|\Psi_s\rangle$, which we denoted as $|\Psi_s', \{\zeta_k\}\rangle$ (it was denoted as $|\Psi_s'\rangle$ in the introduction). It reads

$$|\Psi_s', \{\zeta_k\}\rangle = \hat{U}(\{\zeta_k\}_{t,\Delta t}, t, \Delta t)|\Psi_s\rangle.$$

Combining the above together with Eq. (16) we arrive at

$$|\Psi\rangle = \exp(-i\hat{H}t)|\Psi_s\rangle \simeq \frac{1}{M}\sum_{k=1}^{M}|\Psi_s', \{\zeta_k\}\rangle,$$

which has exactly the same form as Eq. (2). As a result we obtained the many-body wave function as a sum of states $|\Psi_s\rangle$ defined by Eq. (1). The above equation constitutes the main result of the present paper.

To make the derivation of the method more transparent, let us consider an example of a bosonic two-mode model:

$$\hat{H} = U((\hat{a}_1^\dagger\hat{a}_1)^2 + (\hat{a}_2^\dagger\hat{a}_2)^2). \tag{17}$$

Here, we can clearly see that the two-body part of the Hamiltonian is already decomposed with $\hat{O}_b^r = \hat{a}_r^\dagger\hat{a}_r$ and $\omega_r = U$ where $r = 1, 2$. We denote the probability amplitudes of a single particle being located in modes 1, 2 as $\psi_{1,2}$. Thus, the N-particle state of the form $|\Psi_s\rangle$ given by Eq. (1) reads

$$\begin{aligned}|\psi_1, \psi_2; N\rangle &= \frac{1}{\sqrt{N!}}(\psi_1\hat{a}_1^\dagger + \psi_2\hat{a}_2^\dagger)^N|0\rangle \\ &= \sum_{n=1}^{N}\sqrt{\binom{N}{n}}{\psi_1}^n{\psi_2}^{N-n}|n, N-n\rangle, \end{aligned}\tag{18}$$

where $|0\rangle$ denotes the particle vacuum and $|n, N-n\rangle$ denotes the state of n and $N-n$ particles in the first and second mode, respectively. Now we use the just-derived stochastic method in a single time step Δt. That is, we wish to calculate the many-body wave function after time step Δt. According to the previous consideration, the evolution operator $\hat{U}_2$ given by Eq. (7) now takes the form

$$\hat{U}_2(\{\zeta\}) = \hat{U}_b(\{\zeta^*\})\hat{U}_b(\{\zeta\}), \tag{19}$$

where the set $\{\zeta\}$ consists of two complex variables $\zeta_{1,b}$ and $\zeta_{2,b}$. The method consists of applying this operator to the initial state $|\psi_1, \psi_2; N\rangle_s$, i.e.,

$$\hat{U}_2(\{\zeta\})|\psi_1, \psi_2; N\rangle = \hat{U}_b(\{\zeta^*\})\hat{U}_b(\{\zeta\})|\psi_1, \psi_2; N\rangle.$$

Because we deal with single-particle evolution, the resulting state is of the form $|\psi_1', \psi_2'; N\rangle$, i.e.,

$$|\psi_1', \psi_2'; N\rangle = U_b(\{\zeta^*\})U_b(\{\zeta\})|\psi_1, \psi_2; N\rangle, \tag{20}$$

where

$$\psi_r' = \exp(\sqrt{-i\Delta t}(\zeta_{r,b} + \zeta_{r,b}^*))\psi_r \tag{21}$$

for $r = 1, 2$. According to Eqs. (9), (19), and (20) we should obtain

$$(1 - i\hat{H}\Delta t)|\psi_1, \psi_2; N\rangle = \langle|\psi_1', \psi_2'; N\rangle\rangle_s.$$

We will show that this is indeed the case. From Eq. (18) we obtain

$$\langle|\psi_1', \psi_2'; N\rangle\rangle_s = \left\langle \sum_{n=1}^{N}\sqrt{\binom{N}{n}}{\psi_1'}^n{\psi_2'}^{N-n}|n, N-n\rangle \right\rangle_s.$$

Inserting ψ_r' given by Eq. (21) into the above, expanding up to quadratic terms in ζ, and using $\langle|\zeta_{r,b}|^2\rangle_s = U$ we arrive at

$$\begin{aligned}\langle|\psi_1', \psi_2'; N\rangle\rangle_s \simeq \sum_{n=1}^{N}\sqrt{\binom{N}{n}}\{1 - iU\Delta t[n^2 + (N-n)^2]\} \\ \times\psi_1^n\psi_2^{N-n}|n, N-n\rangle.\end{aligned}$$

Because $U(n^2 + (N-n)^2)|n, N-n\rangle = \hat{H}|n, N-n\rangle$, the above reads

$$\begin{aligned}\langle|\psi_1', \psi_2'; N\rangle\rangle_s \simeq (1 - i\hat{H}\Delta t)\sum_{n=1}^{N}\sqrt{\binom{N}{n}} \\ \times\psi_1^n\psi_2^{N-n}|n, N-n\rangle.\end{aligned}$$

From Eq. (18) we find that the above reads

$$\langle|\psi_1', \psi_2'; N\rangle\rangle_s \simeq (1 - i\hat{H}\Delta t)|\psi_1, \psi_2; N\rangle,$$

which is what we wished to obtain.

III. TREATMENT OF GREATER-THAN-TWO-BODY INTERACTIONS

Note that the method presented above is capable of handling more than two-body interactions. The necessary criterion for the application of the above method is the possibility of decomposing the interaction Hamiltonian into single-particle operators. Consider an n-particle interaction (let us take bosons for simplicity) that can be decomposed [15]

$$\hat{H}_n = \sum_r \omega_r\prod_{j=1}^{n}\hat{O}_j^r. \tag{22}$$

The crucial part of the method consists of decomposing

$$(1 - i\hat{H}_n\Delta t) \simeq \left\langle\prod_j \exp(\hat{A}_j)\right\rangle_s, \tag{23}$$

where $\hat{A}_j$ are single-particle operators. The above needs to be satisfied to linear terms in Δt. When we look at the form of decomposition given by Eq. (22) it is straightforward to introduce

$$U_{n,i}(\{\zeta\}) = \exp\left(\sum_r (-i\,\Delta t\omega_r)^{1/n}\zeta_{i,r}\hat{O}_i^r\right),$$

with $i = 1, \ldots, n$ and random variables having the property

$$\left\langle \prod_{i=1}^{n} \zeta_{i,r} \right\rangle_s = 1, \tag{24}$$

with all the other terms up to order n equal to zero. Then we have

$$1 - i\,\Delta t\hat{H}_n \simeq \left\langle \prod_{i=1}^{n} U_{n,i}(\{\zeta\}) \right\rangle_s, \tag{25}$$

which is what we need. The above-defined random variables can be constructed in the following way: We take $\zeta_{i,r}$, $i = 1, \ldots, n-1$ as independent complex random variables with $\langle|\zeta_{i,r}|^2\rangle = 1$ and take $\zeta_n = \prod_{i=1}^{n-1}\zeta_{i,r}^*$.

The above results can be easily generalized to the bosonic Hamiltonian of the form

$$\hat{H} = \sum_{n=1}^{N_0} \hat{H}_n,$$

where each $\hat{H}_n$ has the form given by Eq. (22). In this case, the evolution operator up to terms linear in Δt can be decomposed as

$$1 - i\,\hat{H}\Delta t \simeq \prod_{n=1}^{N_0}(1 - i\,\hat{H}_n\Delta t).$$

Inserting Eq. (25) into the above and using $(1 - i\,\hat{H}_1\Delta t) \simeq \exp(-i\,\hat{H}_1\Delta t)$ we arrive at

$$\begin{aligned} 1 - i\,\hat{H}\Delta t &\simeq \exp(-i\,\hat{H}_1\Delta t)\prod_{n=2}^{N_0}\left\langle \prod_{i=1}^{n} U_{n,i}(\{\zeta\}) \right\rangle_s \\ &= \left\langle \exp(-i\,\hat{H}_1\Delta t)\prod_{n=2}^{N_0}\prod_{i=1}^{n} U_{n,i}(\{\zeta\}) \right\rangle_s \end{aligned}$$

where $\langle\ldots\rangle_s$ denotes now the global average. As we did before, we take the finite time evolution and approximate the overall average by the finite sum. Thus, as we did before, we end up with a decomposition of the evolution operator $\exp(-i\,\hat{H}t)$ by a sum of evolutions under single-particle operators. Starting from a state of the form $|\Psi_s\rangle$ we end up with the final wave function of the form given by Eq. (2).

It is straightforward to generalize the above to Bose-Fermi mixtures in the case of an n-particle interaction (n_b bosons and n_f fermions) of the form

$$\hat{H}_{n_b,n_f} = \sum_r \omega_r \prod_{i=1}^{n_b}\hat{O}_{i,b}^r \prod_{j=1}^{n_f}\hat{O}_{j,f}^r, \tag{26}$$

where $n_f + n_b = n$. As above we introduce

$$U_{j;k}(\{\zeta\}) = \exp\left(\sum_r (-i\,\Delta t\omega_r)^{1/n}\zeta_{j,r,k}\hat{O}_{j,k}^r\right),$$

where $k = b,\ f$. In the above $j = 1, \ldots, n_b$ for $k = b$ or $j = 1, \ldots, n_f$ for $k = f$. We additionally take

$$\left\langle \prod_{i=1}^{n_b}\zeta_{i,r,b}\prod_{j=1}^{n_f}\zeta_{j,r,f} \right\rangle_s = 1.$$

Then, as in the bosonic case described above, we arrive at

$$1 - i\,\Delta t\hat{H}_n \simeq \left\langle \prod_{i=1}^{n_b} U_{i,b}(\{\zeta\})\prod_{j=1}^{n_f} U_{j,f}(\{\zeta\}) \right\rangle_s.$$

Using results that we have just obtained, we see that the method is capable of handling the Bose-Fermi Hamiltonians of the form

$$\hat{H} = \sum_{n_b,n_f} \hat{H}_{n_b,n_f},$$

where $\hat{H}_{n_b,n_f}$ is of the form given by Eq. (26).

We now briefly discuss the form of the probability distribution ρ. As we saw above we use complex random variables with the first and second moment defined. All the higher moments do not appear in the derivation. Thus the probability distribution is not unique. For simplicity of the numerical calculation we can take the Gaussian probability distribution.

IV. CALCULATION OF MEAN VALUES OF OBSERVABLES

As a last step let us discuss the calculation of mean values of observables. Looking at Eq. (2) it seems that, to calculate the mean values of observables, we need to store all wave functions $|\Psi'_{s,j}\rangle$ in computer memory. For large M this could be a serious obstacle for the method. However, we do not need to do it. We have

$$\langle\hat{O}\rangle = \langle\Psi|\hat{O}|\Psi\rangle = \lim_{M\to\infty}\frac{1}{M^2}\sum_{j,k=1}^{M}\langle\Psi'_{s,j}|\hat{O}|\Psi'_{s,k}\rangle.$$

Thus to calculate $\langle\hat{O}\rangle$ we need to calculate numerically $\langle\Psi'_{s,j}|\hat{O}|\Psi'_{s,k}\rangle$. This means that we need to run two independent stochastic processes obtaining two wave functions, which we can call $|\Psi'_{s,k}\rangle$ and $|\Psi'_{s,j}\rangle$. Having them stored in computer memory, we calculate $\langle\Psi'_{s,j}|\hat{O}|\Psi'_{s,k}\rangle$ and keep only the result of the calculation while deleting the two stochastic wave functions. Repeating this procedure and adding the obtained results we converge towards $\langle\hat{O}\rangle$.

As shown above the stochastic method always gives the mean values of observables when $M \to \infty$. In practical use, the crucial question is how fast, with increasing M, the numerical result converges towards the true value. In practice, for given M, there are ways to calculate the error connected with the obtained mean value of a given observable. The analog of the above-described method was used to calculate the properties of bosons and fermions independently. In the bosonic case, it was used to calculate the properties of atoms scattered in the collision of Bose-Einstein condensates. The

calculations were done for a few different systems with *true* experimental parameters, with the mean number of atoms being about 10^5 and the three-dimensional (3D) lattice consisting of about 10^6 points [3]. In this case it turned out that it was enough to have about 10^4 trajectories to obtain a reasonably small error for quantities such as the density of scattered atoms or the two-particle correlation function [16]. In the fermionic case, the ground-state properties of the unitary Fermi gas limit were calculated on the $8 \times 8 \times 8$ lattice with 42 atoms [7]. The above shows that the analog of the presented method was capable of obtaining a reasonably small error for many realistic systems. This is an important argument that the presented method is capable of handling calculations of interesting Bose-Fermi mixtures.

However, the main goal of the present paper is to show that the stochastic-wave-function approach, which is derived independently for bosons and fermions, can be easily generalized to Bose-Fermi mixtures and to greater-than-two-body interactions. It is worth mentioning, that within the stochastic-wave-function approach, there are many ways of mapping the quantum evolution on the stochastic process. The proposed method is only one way of doing so. It is important to add that, in the fermionic case, a mapping free of the famous "sign problem" was found [7]. The natural extension of the present paper would be to find a more general way of mapping, which can be probably done by considering the evolution of density matrices instead of wave functions [2].

We now comment on the choice of the initial many-body state. The above method was formulated for the initial state $|\Psi_s\rangle$ given by Eq. (1). However, it naturally extends to initial states being a superposition or mixtures of states $|\Psi_s\rangle$. It is known that any many-body state is a superposition of states $|\Psi_s\rangle$ [2,9,17], so in principle the above method can treat any initial state. However, in practice one is usually interested in thermal states as a starting point of the dynamics. So the first goal is to find the thermal state. This can be done by adopting the above-described method to imaginary time evolution as it was done in the case of bosons [3,18] and fermions [4].

V. SUMMARY

In the present paper, we generalized the stochastic wave function, which was recently formulated independently for bosonic and fermionic systems, to Bose-Fermi mixtures. In the case of a wide class of two-particle interactions, and certain class of more-than-two particle interactions, the quantum dynamics was mapped exactly onto set of single-particle wave functions with their evolution governed by a stochastic process.

ACKNOWLEDGMENT

This work was supported by the National Science Center Grant No. DEC-2011/01/D/ST3/00482.

APPENDIX: DECOMPOSITION OF TWO-BODY INTERACTION POTENTIAL OPERATOR

We consider two particle interaction potential $V(1,2)$ where 1, 2 denote degrees of freedom of a given particle. These degrees of freedom are, for example, position $\mathbf{r}$ and spin projection m (on a given quantization axis) of a particle, i.e., $1 = (\mathbf{r}_1, m_1)$. When both particles are identical bosons or fermions, the potential has to be symmetric with respect to the change of particles: $V(1,2) = V(2,1)$. If we think of the potential as a matrix, than to be Hermitian, the matrix needs to be real (because it is symmetric). Such a matrix can be diagonalized with real vectors O_r and real eigenvalues ω_r. It may be represented as

$$V(1,2) = \sum_r \omega_r O^r(1) O^r(2). \tag{A1}$$

The real eigenvector $O^r(\mathbf{r}, m)$ is a function of the degrees of freedom of a given particle.

As written in the main body of the paper in the case of the boson-fermion interaction, we restrict ourselves to the potential of the form

$$V_{bf}(1,2) = \sum_r \omega_{r;bf} O^r_{b,bf}(1) O^r_{f,bf}(2), \tag{A2}$$

where 1 and 2 denote the bosonic and fermionic degrees of freedom, respectively.

Now we use the above to decompose the two-particle-interaction part of the Hamiltonian $\hat{H}_2$ written in the second-quantized form. We have

$$\begin{aligned}\hat{H}_2 = &\frac{1}{2}\sum_r \omega_{r;b} \sum_{i,j} O^r_b(i) O^r_b(j) \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}_i \hat{a}_j \\ &+ \frac{1}{2}\sum_r \omega_{r;f} \sum_{i,j} O^r_f(i) O^r_f(j) \hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_i \hat{c}_j \\ &+ \frac{1}{2}\sum_r \omega_{r;bf} \sum_{i,j} O^r_{b,bf}(i) O^r_{f,bf}(j) \hat{a}^\dagger_i \hat{c}^\dagger_j \hat{a}_i \hat{c}_j,\end{aligned}$$

where $i, j = (\mathbf{r}, m)$ and j denotes degrees of freedom of a boson or fermion which is position and spin projection. Here we use $\mathbf{r}$ being defined on a lattice with $\hat{a}_i$ and $\hat{c}_i$ being bosonic and fermionic annihilation operators. Using the commutations relations we arrive at

$$\begin{aligned}\hat{H}_2 = &\sum_r \omega_{r;b} \hat{O}^r_b \hat{O}^r_b + \sum_r \omega_{r;f} \hat{O}^r_f \hat{O}^r_f \\ &+ \sum_r \omega_{r;bf} \hat{O}^r_{b;bf} \hat{O}^r_{f;bf} + \hat{H}_{1,ad},\end{aligned}$$

where

$$\hat{O}^r_b = \sum_i O_b(i) \hat{n}_{b,i}, \quad \hat{O}^r_f = \sum_i O^r_f(i) \hat{n}_{f,i},$$

$$\hat{O}^r_{b,bf} = \sum_i O^r_{b,bf}(i) \hat{n}_{b,i}, \quad \hat{O}^r_{f,bf} = \sum_i O^r_{f,bf}(i) \hat{n}_{f,i},$$

$$\hat{H}_{1,ad} = -\frac{1}{2}\sum_i V_b(i,i) \hat{n}_{b,i} - \frac{1}{2}\sum_i V_f(i,i) \hat{n}_{f,i},$$

where $\hat{n}_{b,i} = \hat{a}^\dagger_i \hat{a}_i$ and $\hat{n}_{f,i} = \hat{c}^\dagger_i \hat{c}_i$.

[1] P. Deuar and P. D. Drummond, J. Phys. A **39**, 1163 (2006); **39**, 2723 (2006).
[2] I. Carusotto, Y. Castin, and J. Dalibard, Phys. Rev. A **63**, 023606 (2001); I. Carusotto and Y. Castin, Ann. Henri Poincaré **4**, 783 (2003).
[3] P. D. Drummond, P. Deuar, and K. V. Kheruntsyan, Phys. Rev. Lett. **92**, 040405 (2004); P. Deuar and P. D. Drummond, *ibid.* **98**, 120402 (2007); V. Krachmalnicoff *et al.*, *ibid.* **104**, 150402 (2010); J.-C. Jaskula *et al.*, *ibid.* **105**, 190402 (2010); K. V. Kheruntsyan, J.-C. Jaskula, P. Deuar, M. Bonneau, G. B. Partridge, J. Ruaudel, R. Lopes, D. Boiron, and C. I. Westbrook, *ibid.* **108**, 260401 (2012).
[4] O. Juillet and P. Chomaz, Phys. Rev. Lett. **88**, 142503 (2002); O. Juillet, F. Gulminelli, and P. Chomaz, *ibid.* **92**, 160401 (2004).
[5] L. Tessieri, J. Wilkie, and M. Çetinbaş, J. Phys. A: Math. Gen. **38**, 943 (2005).
[6] D. Lacroix, Ann. Phys. (NY) **322**, 2055 (2007).
[7] O. Juillet, New J. Phys. **9**, 163 (2007).
[8] A. Montina and Y. Castin, Phys. Rev. A **73**, 013618 (2006).
[9] E. A. Polyakov, Phys. Rev. A **93**, 022116 (2016).
[10] J. F. Corney and P. D. Drummond, Phys. Rev. Lett. **93**, 260401 (2004); Phys. Rev. B **73**, 125112 (2006).
[11] P. D. Drummond, J. F. Corney, Comput. Phys. Commun. **169**, 412 (2005); M. Ogren, K. V. Kheruntsyan, and J. F. Corney, Europhys. Lett. **92**, 36003 (2010).
[12] G. Carleo, F. Becca, M. Schiro, and M. Fabrizio, Sci. Rep. **2**, 243 (2012); G. Carleo, L. Cevolani, L. Sanchez-Palencia, and M. Holzmann, Phys. Rev. X **7**, 031026 (2017).
[13] A. Nagy and V. Savona, Phys. Rev. A **97**, 052129 (2018).
[14] J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, MA, 1986).
[15] As an example we may take n-particle particle contact interaction on a lattice where r denotes a lattice site, $\omega_r = U$, and $\hat{O}_i^r = \hat{a}_r^\dagger \hat{a}_r$.
[16] P. Deuar (private communication).
[17] E. A. Polyakov and P. N. Vorontsov-Velyaminov, Phys. Rev. A **91**, 042107 (2015).
[18] I. Carusotto and Y. Castin, J. Phys. B **34**, 4589 (2001); Phys. Rev. Lett. **90**, 030401 (2003).