Exact BCS stochastic schemes for a time dependent many-body fermionic system

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The exact quantum state evolution of a fermionic gas with binary interactions is obtained as the stochastic average of BCS-state trajectories. We find the most general Ito stochastic equations which reproduce exactly the dynamics of the system and we obtain some conditions to minimize the stochastic spreading of the trajectories in the Hilbert space. The relation between the optimized equations and mean-field equations is analyzed. The method is applied to a simple two-site model. The simulations display effects that cannot be obtained in the mean-field approximation.

I. INTRODUCTION

The numerical solution of a time dependent many-body problem is a formidable task for large quantum systems. For example, for a system of an arbitrary number of fermions with M possible modes of the quantum field, e.g. in a lattice model, the dimension of the Hilbert space is 2^M so that both the computer time and the memory requirements scale exponentially with the number of modes and becomes rapidly intractable when M increases. A similar situation occurs also in classical mechanics, when we describe the dynamics as the evolution of a probability distribution.

To circumvent the problem on the memory requirement in classical physics, an approach is not to solve numerically the equation of motion of the probability distribution, but to solve the statistical evolution of the variables and to evaluate the mean value of some quantities over a finite number of realizations. Such a Monte Carlo approach can be used also in quantum mechanics, the most famous example being the Path Integral Monte Carlo based on the Feynman's path integral formulation [1]. However, apart from notable exceptions (such as the imaginary time evolution of bosons with real Hamiltonians, or the imaginary time evolution of some models of fermions [2]), for a general quantum problem, the known Quantum Monte Carlo methods do not solve the computer time problem, which remains exponentially long because an exponentially large number of Monte Carlo realizations is usually required [3]. For fermions, this problem is the celebrated sign problem, which has been the subject of many efforts, both for real-time and imaginary-time simulations [4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

In Monte Carlo techniques with path integral, the randomly generated states are generally mutually orthogonal. In the original formulation of Feynman, they are the eigenvectors of the particle coordinates. As an alternative, we can use to randomly explore an over-complete set of states. Since the dynamics of degenerate bosonic gas with weak interactions is approximatively described by the evolution of a Hartree-Fock state, it can be convenient to evaluate the exact dynamics using a superposition of paths of Hartree-Fock states [14]. A similar approach has been used for fermion systems [15]. In Reference [14] the case of bosonic coherent states is also studied.

The number of random paths necessary to describe the dynamics can be reduced by increasing the number of elements of the over-complete set. In the extreme limit where every state of the Hilbert state is an element of the explored set, the dynamics can be described with a single, deterministic path: this corresponds to solving directly the Schrödinger equation, but this faces again the memory problem. As an intermediate possibility, we can choose a set of elements whose single path is a better approximation to the exact solution than the Hartree-Fock ansatz, but which is still numerically tractable. Attractive interactions in a fermionic gas can lead to the condensation of Cooper pairs in the superfluid state, as currently investigated experimentally in atomic gases close to a Feshbach resonance [16]. It is expected that such a superfluid state is reasonably well described by a BCS-state, much better indeed than by a Hartree-Fock state. For this reason we study here an exact stochastic approach with BCS states.

In this article we consider the dynamics in real-time of a system of fermions with binary interactions on a spatial lattice. The Hamiltonian is

$$\hat{\mathcal{H}} = \sum_{kl} h_{kl} \hat{c}_k^\dagger \hat{c}_l + \frac{1}{2} \sum_{kl} V_{kl} \hat{c}_k^\dagger \hat{c}_l^\dagger \hat{c}_l \hat{c}_k, \tag{1}$$

h and V are hermitian and real symmetric matrices, respectively, and $\hat{c}_k$, $\hat{c}_k^\dagger$ are Fermi annihilation and creation operators. The mode index k labels the spin state σ_k and the lattice node in position r_k. In what follows, we shall denote as m_s the total number of lattice nodes.

We wish to obtain the dynamical evolution of the quantum state as the average of stochastic trajectories of BCS states. The exact evolution is achieved by averaging an infinite number of stochastic trajectories. The BCS state

ansatz that we use is

$$|\Omega,\gamma\rangle \equiv \Omega S(\gamma)|0\rangle \equiv \Omega\, e^{\frac{1}{2}\sum_{kl}\gamma_{kl}\hat{c}_k^\dagger\hat{c}_l^\dagger}|0\rangle, \tag{2}$$

γ being an antisymmetric matrix, involving for spin 1/2 fermions a number of variables $2m_s(2m_s-1)/2$, and Ω being a multiplicative complex variable. Note that the state in Eq. (2) is in general not normalized. We shall consider the case where both γ and Ω are stochastic variables solving Ito stochastic equations [17].

In Section II we find the necessary and sufficient conditions on the stochastic equations in order to have an exact description of the dynamics. These constraints do not fix univocally the stochastic scheme, thus we shall use this freedom to reduce the statistical spreading of the trajectories. In Section III we construct explicit stochastic schemes. The growth rate of the spreading is evaluated and an upper limit for the statistical error on the observables is established, which shows that the statistical uncertainty is finite at every finite time. In Section IV the stochastic approach is illustrated on a two-site model.

II. STOCHASTIC EQUATIONS

A. Conditions for the stochastic evolution to be exact

We want to evaluate exactly the quantum state evolution using a superposition of the BCS states $|\Omega,\gamma\rangle \equiv \Omega|\gamma\rangle$ with a stochastic evolution of γ and Ω. For an infinitesimal variation of γ and Ω we calculate the variation of the ansatz by expanding $|\Omega+\Delta\Omega,\gamma+\Delta\gamma\rangle$ in powers of $\Delta\Omega$ and $\Delta\gamma$: we have from Eq. (A4) that

$$\Delta|\Omega,\gamma\rangle = \left[\frac{\Delta\Omega}{\Omega} + \frac{1}{2}\sum_{ij}\Delta\gamma_{ij}\hat{c}_i^\dagger\hat{c}_j^\dagger + \frac{1}{8}\sum_{ijkl}\Delta\gamma_{ij}\Delta\gamma_{kl}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_k^\dagger\hat{c}_l^\dagger + \frac{1}{2\Omega}\sum_{ij}\Delta\Omega\Delta\gamma_{ij}\hat{c}_i^\dagger\hat{c}_j^\dagger + ...\right]|\Omega,\gamma\rangle, \tag{3}$$

On the other side, the Hamiltonian evolution during Δt of the state equal to $|\Omega,\gamma\rangle$ at time t is given to first order in Δt by Schrödinger's equation:

$$-\mathrm{i}\hat{\mathcal{H}}\Delta t|\Omega,\gamma\rangle = \left[\frac{\mathrm{i}}{2}\sum_{ijkl}V_{ij}\gamma_{ik}\gamma_{jl}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_k^\dagger\hat{c}_l^\dagger\Delta t - \mathrm{i}\sum_{ij}\left(\frac{1}{2}V_{ij}\gamma_{ij} + \sum_k h_{ik}\gamma_{kj}\right)\hat{c}_i^\dagger\hat{c}_j^\dagger\Delta t\right]|\Omega,\gamma\rangle \tag{4}$$

where we used Eq. (A5) to express $\hat{c}|\Omega,\gamma\rangle$ in terms of $\hat{c}^\dagger|\Omega,\gamma\rangle$ and where we took $\hbar = 1$. If γ and Ω satisfy a deterministic equation, it is obvious that the first term of the right hand side of Eq. (4) does not in general coincide with the third term of the right hand side of Eq. (3). As we shall prove, Eq.(4) and Eq.(3) can become equal when we consider stochastic equations and we average Eq.(3) over every possible realization of the stochastic variation during Δt:

$$\overline{\Delta|\Omega,\gamma\rangle} = -\mathrm{i}\hat{\mathcal{H}}\Delta t|\Omega,\gamma\rangle. \tag{5}$$

Since $S(\gamma)$ is invertible, we have to find a stochastic equation for Ω and γ that satisfies the equality

$$\left[\frac{\overline{\Delta\Omega}}{\Omega} + \frac{1}{2}\sum_{ij}\overline{\Delta\gamma_{ij}}\hat{c}_i^\dagger\hat{c}_j^\dagger + \frac{1}{8}\sum_{ijkl}\overline{\Delta\gamma_{ij}\Delta\gamma_{kl}}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_k^\dagger\hat{c}_l^\dagger + \frac{1}{2\Omega}\sum_{ij}\overline{\Delta\Omega\Delta\gamma_{ij}}\hat{c}_i^\dagger\hat{c}_j^\dagger\right]|0\rangle =$$
$$\left[\frac{\mathrm{i}}{2}\sum_{ijkl}V_{ij}\gamma_{ik}\gamma_{jl}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_k^\dagger\hat{c}_l^\dagger\Delta t - \mathrm{i}\sum_{ij}\left(\frac{1}{2}V_{ij}\gamma_{ij} + \sum_k h_{ik}\gamma_{kj}\right)\hat{c}_i^\dagger\hat{c}_j^\dagger\Delta t\right]|0\rangle. \tag{6}$$

Equation (6) is equivalent to the following ones,

$$\frac{\overline{\Delta\Omega}}{\Omega} = 0 \tag{7}$$

$$\overline{\Delta\gamma_{ij}} = -\frac{1}{\Omega}\overline{\Delta\Omega\Delta\gamma_{ij}} - \mathrm{i}V_{ij}\gamma_{ij}\Delta t - \mathrm{i}\sum_k h_{ik}\gamma_{kj}\Delta t + \mathrm{i}\sum_k h_{jk}\gamma_{ki}\Delta t \tag{8}$$

$$\sum_{\text{permutation of } ijkl}(-1)^p\left[\frac{1}{8}\overline{\Delta\gamma_{ij}\Delta\gamma_{kl}} - \frac{\mathrm{i}}{2}V_{ij}\gamma_{ik}\gamma_{jl}\Delta t\right] = 0 \tag{9}$$

where $(-1)^p$ is the signature of the permutation. The first equation implies that the deterministic term of Ω is zero. The second equation gives the deterministic term for γ, the last one gives a condition for the noise term of γ. This last condition can be written explicitly

$$\begin{aligned}\overline{\Delta\gamma_{ij}\Delta\gamma_{kl}} + \overline{\Delta\gamma_{jk}\Delta\gamma_{il}} + \overline{\Delta\gamma_{ik}\Delta\gamma_{lj}} + \mathrm{i}\Delta t(V_{ij}+V_{kj}+V_{il}+V_{kl})\gamma_{ik}\gamma_{lj} \\ +\mathrm{i}\Delta t(V_{ik}+V_{kj}+V_{il}+V_{jl})\gamma_{ij}\gamma_{kl} + \mathrm{i}\Delta t(V_{ik}+V_{lk}+V_{ij}+V_{lj})\gamma_{jk}\gamma_{il} = 0\end{aligned} \tag{10}$$

Note that this equation is automatically fulfilled when two of the four indices $ijkl$ are equal.

B. Growth of the statistical error

To estimate the statistical error of the method, we consider the growth rate of the mean squared distance between the true state of the system and a single realization of the stochastic ansatz, $\overline{\Delta||\psi\rangle - |\Omega,\gamma\rangle|^2} = \overline{\Delta M}$, where

$$M = \langle\Omega,\gamma|\Omega,\gamma\rangle. \tag{11}$$

This will allow to prove that the statistical error remains finite at all finite evolution times and this will provide a strategy to identify optimal stochastic schemes in trying to minimize the growth rate $\overline{\Delta M}/M$.

To the first order in Δt,

$$\overline{\Delta M} = \overline{(\Delta\langle\Omega,\gamma|)}|\Omega,\gamma\rangle + \langle\Omega,\gamma|\overline{(\Delta|\Omega,\gamma\rangle)} + \overline{(\Delta\langle\Omega,\gamma|)(\Delta|\Omega,\gamma\rangle)}. \tag{12}$$

In the right hand side, the sum of the first two terms gives exactly zero, since by construction $\overline{\Delta|\Omega,\gamma\rangle} = -\mathrm{i}\Delta t\hat{\mathcal{H}}|\Omega,\gamma\rangle/\hbar$. In the last term, we can replace $\Delta|\Omega,\gamma\rangle$ by its stochastic component:

$$\begin{aligned}\Delta|\Omega,\gamma\rangle^{\mathrm{stoch}} &\equiv \Delta|\Omega,\gamma\rangle - \overline{\Delta|\Omega,\gamma\rangle} \\ &= \left[\frac{\Delta\Omega}{\Omega} + \frac{1}{2}\sum_{ij}\Delta\gamma_{ij}^{\mathrm{stoch}}\,\hat{c}_i^\dagger\hat{c}_j^\dagger\right]|\Omega,\gamma\rangle,\end{aligned} \tag{13}$$

where we used the fact that $\Delta\Omega$ is purely stochastic and where $\Delta\gamma_{ij}^{\mathrm{stoch}}$ is the stochastic part of $\Delta\gamma_{ij}$. Equation (12) leads to

$$\frac{\overline{\Delta M}}{M} = \frac{||\Delta|\Omega,\gamma\rangle^{\mathrm{stoch}}||^2}{\langle\Omega,\gamma|\Omega,\gamma\rangle} \tag{14}$$

which can be evaluated using Wick's theorem:

$$\frac{\overline{\Delta M}}{M} = \left|\frac{\Delta\Omega}{\Omega} + \frac{1}{2}\sum_{ij}\Delta\gamma_{ij}^{\mathrm{stoch}}\langle\hat{c}_i^\dagger\hat{c}_j^\dagger\rangle\right|^2 + \frac{1}{2}\sum_{ijkl}\overline{\Delta\gamma_{ij}^*\Delta\gamma_{kl}}\langle\hat{c}_i\hat{c}_k^\dagger\rangle\langle\hat{c}_j\hat{c}_l^\dagger\rangle. \tag{15}$$

where the expectation value is taken in the ansatz, $\langle\ldots\rangle = \langle\Omega,\gamma|\ldots|\Omega,\gamma\rangle/M$. A clear step for the minimization of the error growth is to choose $\Delta\Omega$ in order to set to zero the first term in the right hand side of the above expression:

$$\frac{\Delta\Omega}{\Omega} = -\frac{1}{2}\sum_{kl}\Delta\gamma_{kl}^{\mathrm{stoch}}\langle\hat{c}_k^\dagger\hat{c}_l^\dagger\rangle. \tag{16}$$

We shall always choose $\Delta\Omega$ in this way in what follows. It is then easy to show [see Eq. (13)] that

$$\overline{\Delta M} = \Delta M, \tag{17}$$

i.e., the stochastic terms of ΔM are exactly zero. Furthermore the deterministic part of $\Delta\gamma$ is now slaved to the stochastic part of $\Delta\gamma$, according to Eq.(8): the only increments that remain to be specified to fully determine the stochastic scheme are $\Delta\gamma_{ij}^{\mathrm{stoch}}$, and this we shall do in the next section.

III. EXPLICIT EXACT STOCHASTIC SCHEMES

A. Our solution for an arbitrary interaction potential

This most general solution relies on the following ansatz for the stochastic increment:

$$\Delta\gamma_{ij}^{\rm stoch} = (\Delta f_i + \Delta f_j)\gamma_{ij} \tag{18}$$

where the noise terms Δf_k are independent of γ_{ij}. Inserting this ansatz in the validity condition Eq.(10), we find that if the noise terms have the following correlation function,

$$\overline{\Delta f_i \Delta f_j} = -{\rm i}V_{ij}\Delta t, \tag{19}$$

this validity condition is satisfied [21]. Since the matrix V_{ij} is real symmetric it can be diagonalized; a noise having this correlation function may then be explicitly constructed using the corresponding eigenbasis.

In the specific case of a discrete δ interaction potential between two opposite spin components:

$$V_{ij} = V_0\delta_{r_i,r_j}\delta_{\sigma_i,-\sigma_j} \tag{20}$$

where r_i and σ_i are the lattice position and the spin component of the mode of index i, the following explicit noise may be used:

$$f_i = (-{\rm i}V_0)^{1/2}\left[\Delta\xi_{r_i}\delta_{\sigma_i,\uparrow} + \Delta\xi_{r_i}^*\delta_{\sigma_i,\downarrow}\right] \tag{21}$$

where the $\Delta\xi_r$'s are statistically independent complex Gaussian noises of variance Δt. For this specific noise implementation, $\overline{f_i^* f_j} = |V_0|\Delta t\,\delta_{ij}$, so that the growth rate of the statistical error can be expressed by the simple formula [22]:

$$\frac{\Delta M}{M} = |V_0|\Delta t\sum_k \langle\hat{c}_k\hat{c}_k^\dagger\rangle\langle\hat{c}_k^\dagger\hat{c}_k\rangle \leq \frac{1}{2}|V_0|\Delta t\, m_s \tag{22}$$

where m_s is the number of lattice nodes and where we used the Eqs. (A8,A11, A9). $\Delta M/(M\Delta t)$ has a constant as an upper bound, thus the norm squared of $|\Omega,\gamma\rangle$ is bounded at every time by $\exp(|V_0|m_s t/2)$ times its initial value. A similar bound was derived in the stochastic Hartree-Fock scheme in [15], with a larger exponent [18]. Consequently, the Monte Carlo statistical variance of an observable O is finite when ${\rm Tr}[O^2]$ is finite [see Ref. [19], Eq. (30)].

To be complete we also give the corresponding deterministic part of the evolution of γ:

$$\overline{\Delta\gamma_{ij}}/\Delta t = -{\rm i}V_{ij}\gamma_{ij} - {\rm i}\sum_k (h_{ik}\gamma_{kj} + h_{jk}\gamma_{ik}) - {\rm i}\sum_k (V_{ik}+V_{jk})\langle\hat{c}_k^\dagger\hat{c}_k\rangle\gamma_{ij}. \tag{23}$$

We note that the last sum over k in the righthand side is simply the Hartree mean-field term.

B. Case of an off-diagonal γ and a delta interaction

We now restrict to useful limiting cases where the one-body Hamiltonian h is spin-diagonal, the interaction potential is an on-site discrete δ between two distinct spin components, as defined in Eq.(20), and where the matrix γ in the ansatz has initially zero matrix elements between identical spin components. We have then identified exact stochastic schemes that preserve at any time this block off-diagonal structure of γ.

1. The solution that we have found with minimal error growth

A general strategy to find the 'best' stochastic scheme among a very large number of possibilities is to try to minimize the growth rate of the statistical error Eq.(14). Whereas this program is easily fulfilled for bosons [14] it seems to be more difficult to achieve for the stochastic BCS ansatz. Here we report the solution that we have found with minimal error growth. It is possible that a better solution exists. The stochastic increment is given by

$$\Delta\gamma_{\uparrow r_i,\downarrow r_j}^{\rm stoch} = ({\rm i}V_0)^{1/2}(\Delta\xi_{r_i} - \Delta\xi_{r_j})\gamma_{\uparrow r_i,\downarrow r_j} \tag{24}$$

where the $\Delta\xi_r$ are m_s independent real Gaussian noises of variance Δt. The corresponding growth rate of the statistical error is exactly given by

$$\frac{\Delta M}{M} = \Delta t |V_0| \sum_r \left[\langle \hat{c}^\dagger_{\uparrow r} \hat{c}_{\uparrow r} \rangle \langle \hat{c}_{\uparrow r} \hat{c}^\dagger_{\uparrow r} \rangle + \langle \hat{c}^\dagger_{\downarrow r} \hat{c}_{\downarrow r} \rangle \langle \hat{c}_{\downarrow r} \hat{c}^\dagger_{\downarrow r} \rangle - 2 \langle \hat{c}^\dagger_{\uparrow r} \hat{c}^\dagger_{\downarrow r} \rangle \langle \hat{c}_{\downarrow r} \hat{c}_{\uparrow r} \rangle \right] \tag{25}$$

which is indeed smaller than the general result Eq.(22) because of the occurrence of a negative term involving anomalous averages. In this scheme the deterministic part of the evolution of γ is given by

$$\overline{\Delta\gamma_{\uparrow r_i,\downarrow r_j}}/\Delta t = -\mathrm{i} V_0 \gamma_{\uparrow r_i,\downarrow r_j} [\langle \hat{c}^\dagger_{\downarrow r_i} \hat{c}_{\downarrow r_i} \rangle - \langle \hat{c}^\dagger_{\uparrow r_i} \hat{c}_{\uparrow r_i} \rangle - \{ i \leftrightarrow j \}] - \mathrm{i} V_0 \delta_{r_i,r_j} \gamma_{\uparrow r_i,\downarrow r_j} - \mathrm{i} \sum_{r_k} (h_{\uparrow r_i,\uparrow r_k} \gamma_{\uparrow r_k,\downarrow r_j} + h_{\downarrow r_j,\downarrow r_k} \gamma_{\uparrow r_i,\downarrow r_k}) \tag{26}$$

2. *The solution that we have found with minimal memory requirement*

In the case when the one-body Hamiltonian h is totally spin independent and when the off-diagonal block $\gamma_{\uparrow r_i,\downarrow r_j}$ is initially a symmetric or antisymmetric matrix (under the exchange of r_i and r_j), we have found a stochastic scheme which preserves this symmetry property at all times, which allows to save a factor of two on the memory requirement;

$$\Delta\gamma^{\mathrm{stoch}}_{\uparrow r_i,\downarrow r_j} = i(iV_0)^{1/2} (\Delta\xi_{r_i} + \Delta\xi_{r_j}) \gamma_{\uparrow r_i,\downarrow r_j} \tag{27}$$

where the $\Delta\xi_r$ are m_s independent real Gaussian noises of variance Δt. In this case, the growth rate of the statistical error is

$$\frac{\Delta M}{M} = \Delta t |V_0| \sum_r \left[\langle \hat{c}^\dagger_{\uparrow r} \hat{c}_{\uparrow r} \rangle \langle \hat{c}_{\uparrow r} \hat{c}^\dagger_{\uparrow r} \rangle + \langle \hat{c}^\dagger_{\downarrow r} \hat{c}_{\downarrow r} \rangle \langle \hat{c}_{\downarrow r} \hat{c}^\dagger_{\downarrow r} \rangle + 2 \langle \hat{c}^\dagger_{\uparrow r} \hat{c}^\dagger_{\downarrow r} \rangle \langle \hat{c}_{\downarrow r} \hat{c}_{\uparrow r} \rangle \right] \leq \Delta t |V_0| m_s \tag{28}$$

which is larger than for the two previous schemes. In this scheme the deterministic part of the evolution of γ is given by

$$\overline{\Delta\gamma_{\uparrow r_i,\downarrow r_j}}/\Delta t = -\mathrm{i} V_0 \gamma_{\uparrow r_i,\downarrow r_j} \left[\langle \hat{c}^\dagger_{\downarrow r_i} \hat{c}_{\downarrow r_i} \rangle + \langle \hat{c}^\dagger_{\uparrow r_i} \hat{c}_{\uparrow r_i} \rangle + \{ i \leftrightarrow j \} \right] - \mathrm{i} V_0 \delta_{r_i,r_j} \gamma_{\uparrow r_i,\downarrow r_j} - \mathrm{i} \sum_{r_k} (h_{\uparrow r_i,\uparrow r_k} \gamma_{\uparrow r_k,\downarrow r_j} + h_{\downarrow r_j,\downarrow r_k} \gamma_{\uparrow r_i,\downarrow r_k}) \tag{29}$$

C. Link with the mean-field approximation

In the three explicit stochastic schemes given in this section, the deterministic part of the evolution for γ_{ij} did not coincide with the mean-field evolution. This in contrast with the optimized stochastic Hartree-Fock schemes obtained for bosons [14] and for fermions [15]. For a general stochastic BCS ansatz with the optimizing choice Eq.(16), we found the following relation between the deterministic evolution of γ_{ij} and its mean field evolution (given in Appendix B):

$$\overline{\Delta\gamma_{ij}} - \Delta\gamma^{\mathrm{mean\ field}}_{ij} = \sum_{kl} \overline{\Delta\gamma_{ik} \Delta\gamma_{jl}} \langle \hat{c}^\dagger_k \hat{c}^\dagger_l \rangle \tag{30}$$

by inserting the expression Eq. (16) of $\Delta\Omega$ into Eq. (8) and by using Eq. (10) to eliminate $\overline{\Delta\gamma_{ij}\Delta\gamma_{kl}}$. This shows that finding a stochastic scheme where the deterministic and mean field evolutions coincide is not straightforward.

IV. STOCHASTIC APPROACH FOR A TWO-SITE SYSTEM

In order to illustrate the method, we apply it to a simple system with two sites, corresponding to the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_\sigma \left[\hat{c}^\dagger_{\sigma 1} \hat{c}_{\sigma 2} + \hat{c}^\dagger_{\sigma 2} \hat{c}_{\sigma 1} \right] + V \left[\hat{c}^\dagger_{\uparrow 1} \hat{c}^\dagger_{\downarrow 1} \hat{c}_{\downarrow 1} \hat{c}_{\uparrow 1} + \hat{c}^\dagger_{\uparrow 2} \hat{c}^\dagger_{\downarrow 2} \hat{c}_{\downarrow 2} \hat{c}_{\uparrow 2} \right] \tag{31}$$

where the spin index σ takes the values $\uparrow$ and $\downarrow$. There is no interparticle interaction when the two particles are in different wells. A physical system that may be described by this model is a set of two Fermi particles in a double-well potential.

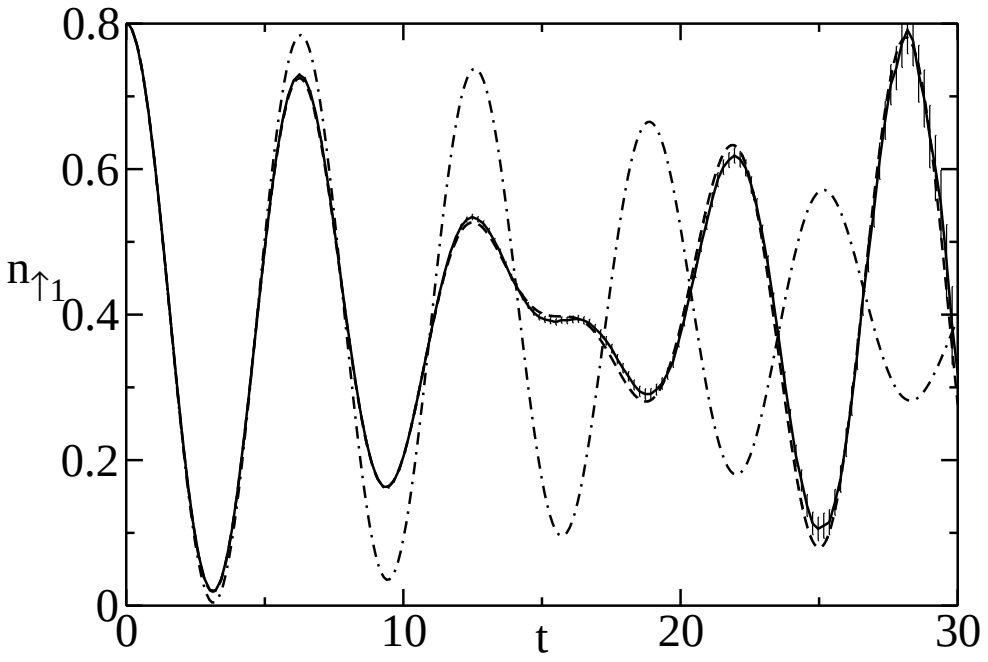

FIG. 1: Mean value of the population in the state $1\uparrow$ as a function of time. The solid and dashed lines are evaluated using the schemes of §III B 1 and §III B 2, respectively. The number of realizations is 10^5 and $V = 0.2$. The dashed-dotted line is the BCS mean-field prediction. The widths of the error bars are the standard deviations.

At the initial time, we choose a BCS state with the elements of γ equal to zero, apart from $\gamma_{1\uparrow,1\downarrow} = -\gamma_{1\downarrow,1\uparrow} \equiv \gamma_0 = 2$. The state is a superposition of the vacuum and the state with two atoms in the site 1. The direct numerical solution of the dynamics is obtained writing the Hamiltonian in the basis of the Fock states of the operators $\hat{c}_{i,s}$ and $\hat{c}^\dagger_{i,s}$. The integration is simplified by the fact that the interaction cannot flip the spin and the amplitude of some states remains zero. In Fig. 1 we report the mean value of the population in the state $\uparrow 1$ as a function of time. We have set $V_0 = 0.2$. The dashed-dotted line is evaluated with the mean-field equations (as given in Appendix B), the dashed line is the direct numerical solution and the solid line is the stochastic solution. The widths of the error bars are the standard deviations. We have used 10^5 realizations with the scheme of §III B 1. In the mean-field approximation, the evolution has a damped oscillation with a revival for $t > 30$. The collapse and revival of the oscillations of the exact solution occur with a shorter time scale. The stochastic approach is able to display very well this behavior. In Fig. 2 we report $\overline{\langle \Omega, \gamma | \Omega, \gamma \rangle}$ as a function of time. The solid dashed and dotted lines are evaluated using the schemes of §III B 1 §III A and §III B 2, respectively. The dashed-dotted line is the upper bound of Eq. (25) for the first two schemes. As expected, the optimized scheme has a smaller spreading.

Note that the growth rate of $\overline{M}$ is zero at the initial time for the scheme of §III B 1 (see inset of Fig. 2), because of the presence of the last term in Eq. (25), which cancels the other contributions in the initial state considered here of particles localized on a site. The spreading of the trajectories grows exponentially and it increases for larger interparticle interactions. We have done similar calculations for a stronger interaction, e.g. for $V = 2$; the stochastic method agrees with the direct numerical solution, with a higher growth rate of the statistical error for increasing V, as expected.

V. CONCLUSIONS

In this article we have shown that the state evolution of a fermionic gas with binary interactions can be obtained in an exact way as the average of stochastic trajectories of BCS states. We have derived the general Ito stochastic

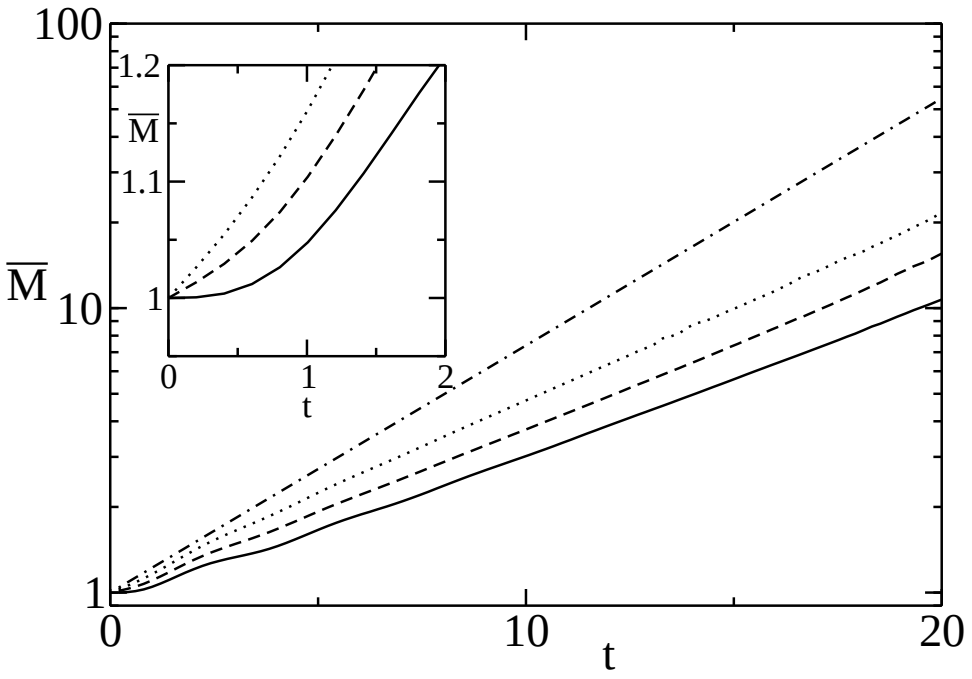

FIG. 2: Average of $M = \langle \Omega, \gamma | \Omega, \gamma \rangle$ over the stochastic realisations, as a function of time, evaluated using the scheme of §III B 1 (solid line), of §III A (dashed line) and of §III B 2 (dotted line). The dashed-dotted line is the upper bound of Eq. (25) for the first two schemes. At the initial time the growth of $\overline{M}$ is zero for the first scheme (see inset).

equations which give the exact evolution of the system and we have found a condition on some parameters of these equations to reduce the statistical spreading of the trajectories in the Hilbert space. The upper bound that we have found on the spreading for a particular scheme is similar to the one obtained for the Hartree-Fock ansatz in [15], with a smaller value. We have illustrated the method on a two-site model and we have shown that the quantum effects, which cannot be obtained with a mean-field approximation, are displayed by the results of the stochastic approach.

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APPENDIX A: SOME PROPERTIES OF BCS STATES

First we prove that the BCS states form a complete family for the states with an even number of atoms. The set of states with a definite number of atoms in each mode constitutes an orthonormal basis of the Hilbert space. It is sufficient to show that each element of this set is equal to a superposition of BCS states. An element has the following form

$$|\{k_n, l_n\}\rangle \equiv \Big(\prod_{n=1}^{N_p} \hat{c}^\dagger_{k_n} \hat{c}^\dagger_{l_n}\Big)|0\rangle, \tag{A1}$$

where we have grouped the atoms in pairs. The n-th pair has the atoms in the k_n and l_n modes. N_p is the number of pairs. $k_n \neq k_m \neq l_n \neq l_m$ when $n \neq m$, whereas $k_n \neq l_m$ for every n and m. It is easy to prove that

$$|\{k_n, l_n\}\rangle = K \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 ... \int_0^{2\pi} d\phi_{N_p} e^{-\mathrm{i}\sum_{n=1}^{N_p}[\phi_n + \exp(\mathrm{i}\phi_n)\hat{c}_{k_n}^\dagger \hat{c}_{l_n}^\dagger]}|0\rangle, \tag{A2}$$

where K is a normalization constant. Thus, the BCS states form a complete family. Actually, it is over-complete.

It is possible to demonstrate that (see Section 2.2 of Ref. [20]) [23]

$$\tilde{M} \equiv \langle \bar{\Omega}, \bar{\gamma} | \Omega, \gamma \rangle = \bar{\Omega}^* \Omega \det[\mathbb{1} + \bar{\gamma}^\dagger \gamma]^{1/2} \tag{A3}$$

and

$$\frac{\partial}{\partial \gamma_{kl}} |\Omega, \gamma\rangle = \hat{c}_k^\dagger \hat{c}_l^\dagger |\Omega, \gamma\rangle, \tag{A4}$$

$$\hat{c}_k |\Omega, \gamma\rangle = \sum_l \gamma_{kl} \hat{c}_l^\dagger |\Omega, \gamma\rangle. \tag{A5}$$

From Eq. (A3) we have

$$\frac{\partial}{\partial \gamma_{ij}} \tilde{M} = -[\bar{\gamma}^\dagger (\mathbb{1} + \gamma \bar{\gamma}^\dagger)^{-1}]_{ij} \tilde{M}. \tag{A6}$$

Using Eqs. (A4-A6) we find that

$$\frac{\langle \bar{\Omega}, \bar{\gamma} | \hat{c}_l \hat{c}_k^\dagger | \Omega, \gamma \rangle}{\langle \bar{\Omega}, \bar{\gamma} | \Omega, \gamma \rangle} = [(\mathbb{1} + \bar{\gamma}^\dagger \gamma)^{-1}]_{kl} \tag{A7}$$

$$\frac{\langle \bar{\Omega}, \bar{\gamma} | \hat{c}_k^\dagger \hat{c}_l | \Omega, \gamma \rangle}{\langle \bar{\Omega}, \bar{\gamma} | \Omega, \gamma \rangle} = [\bar{\gamma}(\mathbb{1} + \bar{\gamma}^\dagger \gamma)^{-1} \gamma^\dagger]_{lk} \tag{A8}$$

$$\frac{\langle \bar{\Omega}, \bar{\gamma} | \hat{c}_k \hat{c}_l | \Omega, \gamma \rangle}{\langle \bar{\Omega}, \bar{\gamma} | \Omega, \gamma \rangle} = -[\gamma(\mathbb{1} + \bar{\gamma}^\dagger \gamma)^{-1}]_{kl} \tag{A9}$$

$$\frac{\langle \bar{\Omega}, \bar{\gamma} | \hat{c}_l^\dagger \hat{c}_k^\dagger | \Omega, \gamma \rangle}{\langle \bar{\Omega}, \bar{\gamma} | \Omega, \gamma \rangle} = [\bar{\gamma}^\dagger (\mathbb{1} + \gamma \bar{\gamma}^\dagger)^{-1}]_{kl}. \tag{A10}$$

We note that Equation (A8) can be written in various forms using the matrix identities

$$\bar{\gamma}^\dagger \gamma (\mathbb{1} + \bar{\gamma}^\dagger \gamma)^{-1} = \bar{\gamma}^\dagger (\mathbb{1} + \gamma \bar{\gamma}^\dagger)^{-1} \gamma = [\gamma (\mathbb{1} + \bar{\gamma}^\dagger \gamma)^{-1} \bar{\gamma}^\dagger]^T \tag{A11}$$

where A^T is the transpose of matrix A.

APPENDIX B: MEAN-FIELD EQUATIONS

Using the results of section 9.9b of [20], we obtain the following equations of motion for γ in the mean-field approximation:

$$\dot{\gamma}_{ij} = -\mathrm{i}\sum_k (h_{ik}\gamma_{kj} + h_{jk}\gamma_{ik}) + \left[-\mathrm{i}\sum_k V_{ik} \langle \hat{c}_k^\dagger \hat{c}_k \rangle \gamma_{ij} + \mathrm{i}\sum_k V_{ik} \langle \hat{c}_k^\dagger \hat{c}_i \rangle \gamma_{kj} - (i \leftrightarrow j) \right] + \mathrm{i}\sum_{kl} V_{kl} \langle \hat{c}_k \hat{c}_l \rangle^* \gamma_{ki} \gamma_{jl} + \mathrm{i} V_{ij} \langle \hat{c}_i \hat{c}_j \rangle. \tag{B1}$$

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[17] One may be worried by the fact that the stochastic ansatz does not have a well defined number of particles. E.g. for bosons it was shown that using a Glauber coherent state ansatz (which is the bosonic analog of the BCS state) leads to divergences in the statistical error [19]. However, such a pathology cannot occur for fermions with a finite number of modes: the total number of fermions is bounded from above by the number of modes in the system. In a BCS ansatz, one has even that the variance of the number of particles is less than twice the mean number of particles. Furthermore, if the initial BCS state of the fermions corresponds to the limit of pairs localized on individual lattice sites, one shall find in the optimized scheme of §III B 1 that the initial growth rate of the statistical error is zero. This is not the case for the stochastic coherent scheme for bosons for an initial coherent state localized on a single lattice site.
[18] In [15] one has to write the interaction term as $\sum_s \hbar\omega_s O_s^2/4$, where O_s are Hermitian one-body operators. A natural choice is to take $s = r$ and $O_r = \hat{c}^\dagger_{\uparrow r}\hat{c}_{\uparrow r} - \hat{c}^\dagger_{\downarrow r}\hat{c}_{\downarrow r}$, and $\hbar\omega_r = -2V_0$. When expanding the square O_r^2 one indeed uses the fact (for fermions) that the square of an occupation number is equal to the occupation number, which allows to reincorporate the undesired terms into the one-body part of the Hamiltonian. From Eq.(19) of [15] one then gets $M(t) \leq \exp(t|V_0|m_s)$, so that the rate inside the exponent is two times larger than the one for the stochastic BCS ansatz.
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[21] Note that imposing such a correlation function on the f_i's is sufficient but not necessary; this is exemplified by the fact that the two other schemes of this section, though of the form Eq. (18), lead to Δf_i's with different correlation functions.
[22] To get the upper bound, we used the fact that $n_k(1-n_k) \leq 1/4$ where $n_k = \langle \hat{c}^\dagger_k \hat{c}_k \rangle$.
[23] The identity Eq. (A3) determines $\tilde{M}$ up to a sign. For the numerical example given in this paper, we have checked formally that the determinant in Eq. (A3) can be written as a square of a polynomial in the γ_{ij}'s and the $\bar{\gamma}_{ij}$'s, which allows to choose the correct determination by continuation from $\bar{\gamma} = 0$.