Stochastic mean-field dynamics for fermions in the weak-coupling limit

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Assuming that the effect of the residual interaction beyond the mean field is weak and has a short memory time, two approximate treatments of correlation in fermionic systems by means of the Markovian quantum jump are presented. A simplified scenario for the introduction of fluctuations beyond the mean field is presented first. In this theory, part of the quantum correlations between the residual interaction and the one-body density matrix are neglected and jumps occur between many-body densities formed of pairs of states $D = |\Phi_a\rangle\langle\Phi_b|/\langle\Phi_b|\Phi_a\rangle$, where $|\Phi_a\rangle$ and $|\Phi_b\rangle$ are antisymmetrized products of single-particle states. The underlying stochastic mean-field theory is discussed and is applied to the monopole vibration of a spherical ^{40}Ca nucleus under the influence of a statistical ensemble of two-body contact interactions. This framework is however too simplistic to account for both fluctuation and dissipation. In the second part of this work, an alternative quantum jump method is obtained without making the approximation on quantum correlations. By restricting to two-particle–two-hole residual interactions, the evolution of the one-body density matrix of a correlated system is transformed into a Lindblad equation. The associated dissipative dynamics can be simulated by quantum jumps between densities written as $D = |\Phi\rangle\langle\Phi|$, where $|\Phi\rangle$ is a normalized Slater determinant. The associated stochastic Schrödinger equation for single-particle wave functions is given.

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I. INTRODUCTION

The description of quantum self-interacting systems with many degrees of freedom is common to many fields of physics, including Bose-Einstein condensates, atomic clusters, and nuclear systems. A striking aspect related to this problem is the emergence of well-ordered motion at the same time as complexity and chaos [1,2]. In many situations, the self-consistent mean-field theory provides a suitable framework to describe ordered motions. It also corresponds to one of the most useful methods for studying the static and dynamical properties of self-interacting systems [3–5]. However, it often turns out that the mean-field theory reproduces average properties of one-body observables but underestimates dissipative and fluctuating aspects. This can directly be assigned to the absence of two-body effects beyond the mean field. In the nuclear context, an extension of mean-field theory has been proposed by considering that one-body degrees of freedom represent a subsystem that is coupled to more complex internal degrees of freedom. By doing so, the problem of self-interacting systems has been mapped to an open quantum system problem. In nuclei, extensive work has been devoted to the formal derivation of dissipative quantum mechanics [6] and/or related stochastic equations for fermions, including Markovian and non-Markovian effects [7–14]. A common aspect of these approaches is that the residual part of the interaction introduces disorder on top of the mean field. These theories end with rather complex transport equations, which are hardly applicable in realistic situations [15]. In fact, only recently, the theory proposed in Ref. [11] has been applied to small-amplitude collective vibrations [16]. Its application to large-amplitude motion in nonequilibrated quantum many-body dynamics remains an open issue [15,17].

During the past decades, significant theoretical efforts have been devoted to the development of Monte Carlo methods to describe the static properties of many-body interacting systems [18]. Recent applications to nuclear physics have shown that stochastic methods can successfully be applied to describe the structure of nuclei [19]. These methods can also be extended to dynamical problems [5] and have been used recently to treat the exact dynamics of interacting bosons [20] and fermions [21] in schematic cases. As underlined in Ref. [22], it is highly desirable to provide approximate theory to describe dissipation in many-body systems by taking advantage of recent advances in Monte Carlo methods. The present work is an exploratory study devoted to the description of dissipation and fluctuations in dynamical problems using quantum jump techniques. Starting from a perturbative treatment of the residual interaction, two strategies are used to transform the many-body dynamics into a stochastic process. In the first strategy, neglecting part of the quantum correlations leads to a stochastic theory that may be economical in terms of numerical implementations. Although appropriate for treating fluctuations beyond the mean field, it is however not suitable for dissipation. In the second part of this article, we show that the approximate treatment of quantum correlations can be avoided, thereby leading to a more general framework. In that case, the dynamical equation of motion of one-body degrees of freedom can be mapped into a Lindblad equation [23,24] generally found in the theory of open quantum systems [25]. Finally, the associated jump process is discussed.

II. GENERALITIES ON PERTURBATION THEORY AND STOCHASTIC MECHANICS

We consider a many-body fermionic system described by a two-body Hamiltonian H. We assume that the mean-field

theory already provides a good approximation of its static and dynamical properties. In this case, the N-body wave function can be replaced by an antisymmetrized product of single-particle states interacting through an effective self-consistent mean field, denoted by $H_{\rm MF}$. Let us assume that the system is initially a Slater determinant, denoted by $|\Phi(t)\rangle$, and let us introduce the mean-field propagator $U_{\rm MF}(t', t)$. The great advantage of mean-field theory is that the propagated many-body state $|\Phi(t')\rangle = U_{\rm MF}(t', t)|\Phi(t)\rangle$ remains a Slater determinant and the dynamical evolution of the system reduces to the evolution of its single-particle components. Thus, the many-body density D is approximated by $D \simeq |\Phi(t')\rangle\langle\Phi(t')|$. Accordingly, all the information on the system is contained in the one-body density matrix, denoted by ρ, whose matrix elements are defined by $\langle j|\rho|i\rangle = {\rm Tr}(a_i^+ a_j D) \equiv \langle a_i^+ a_j\rangle$. Mean-field theory does simplify the dynamical description of many-body systems by reducing significantly the number of degrees of freedom to follow in time.

In nuclear physics, the mean field is often adequate for describing average properties of one-body observables but fails to account for fluctuations. At the wave-function level, this corresponds to a deviation of the mean-field trajectory from the exact dynamics [26,27].

To illustrate this effect, we denote by δv_{12} the residual two-body interaction defined through $\delta v_{12} = H - H_{\rm MF}$. In the weak-coupling regime, this deviation can be treated in perturbation theory and the state at time t' reads [12]

$$|\Psi(t')\rangle = |\Phi(t')\rangle - \frac{i}{\hbar}\int \delta v_{12}(s)|\Phi(s)\rangle ds - \frac{1}{2\hbar^2} T\left(\iint \delta v_{12}(s')\delta v_{12}(s) ds' ds |\Phi(s)\rangle\right), \quad (1)$$

where $\delta v_{12}(s)$ corresponds to the residual interaction written in the interaction picture, $\delta v_{12}(s) = U^+_{\rm MF}(s, t)\delta v_{12}(t) U_{\rm MF}(s, t)$. At the mean-field level, $|\Psi(t')\rangle$ is replaced by $|\Phi(t')\rangle$, but owing to the accumulated effect of δv_{12} in time, it is expected that the exact state becomes a more and more complex superposition of a large number of Slater determinants. Accordingly, information on the system can no longer be reduced to only knowledge of the one-body density matrix and higher order correlations must be accounted for. A natural extension of mean-field theory is to enlarge the number of degrees of freedom considered. This is done for instance in the time-dependent density matrix (TDDM) theory, where both the one-body density matrix and the two-body correlation operator are followed in time [28]. These theories are however rarely applied because of the large number of degrees of freedom to consider [29].

An alternative way to account for correlations beyond the mean field is to use stochastic methods. Several strategies have been proposed to introduce noise on top of the mean field, based on a statistical ensemble of one-body densities [7,10,11], based on random two-body interactions or phase shifts [8,9], or directly from Fermi's golden rule [12–14]. The goal in all cases is to simulate the dynamics of correlated system by averaging over an ensemble of mean-field trajectories. The great advantage in that case is that the number of degrees of freedom to follow along each path is not increased compared to standard mean-field theory. However, these theories are rather complex and methods for numerical implementations are still lacting.

The aim of the present work is to discuss again the possibility of replacing correlated dynamics by quantum jumps in the Hilbert space of Slater determinants. We use Eq. (1) as a starting point and we restrict the discussion to the Markovian limit. To illustrate this hypothesis, we follow Refs. [8,9]. We assume that the residual interaction induces random transitions treated as a statistical ensemble of two-body interactions acting on top of the mean field. Equation (1) is then replaced by a set of evolutions with the same initial state and mean field but with different residual interactions. We assume that the two-body operator has a Gaussian distribution with a mean value $\overline{\delta v_{12}} = 0$ and a second moment denoted by $\overline{\delta v_{12}^2}$. Here, the average is taken over different values of δv_{12}. In nuclear systems, the residual interaction is expected to induce transitions on a shorter time scale (called correlation time and denoted by τ) than the time associated with the mean-field evolution (denoted by $\tau_{\rm rel}$) [17,30]. τ is related to the average autocorrelation function $\overline{\delta v_{12}(s')\delta v_{12}(s)}$, which is approximated by [8,9]

$$\overline{\delta v_{12}(s')\delta v_{12}(s)} \propto \overline{\delta v_{12}^2(s)} e^{-(s-s')^2/2\tau^2}. \quad (2)$$

Using this approximation, we consider a time scale Δt much larger than the time τ but smaller than $\tau_{\rm rel}$. In the following, this limit will be called the "Markovian" or "short memory time" approximation.

Using approximation (2), we consider in the following two limits for which the wave-function evolution as given by (1) can be replaced by quantum jumps between Slater determinants. The first case is a simplified scenario where part of the quantum correlations between δv_{12} and ρ is neglected along the path. In this case, it is shown that the evolution can be formulated in terms of quantum jumps between many-body densities formed of pairs of Slater determinants. In a second part, we show that the perturbative dynamics can still be transformed into a quantum jump process even if quantal correlations are not neglected. In both cases, all equations necessary for applications are given explicitly.

III. FLUCTUATIONS BEYOND THE MEAN FIELD IN A SIMPLIFIED STOCHASTIC SCENARIO

Let us first consider the perturbative evolution of an initial Slater determinant. Under the assumptions of Eq. (2) and the short memory time approximation, the meanfield does not change over Δt. Then, the average evolution of the state, denoted by $\overline{\Delta|\Psi\rangle} = \overline{|\Psi(t+\Delta t)\rangle} - |\Phi(t)\rangle$, reduces to

$$\overline{\Delta|\Psi\rangle} = \frac{\Delta t}{i\hbar} H_{\rm MF}|\Phi(t)\rangle - \frac{\tau\Delta t}{2\hbar^2}\overline{\delta v_{12}^2}|\Phi(t)\rangle. \quad (3)$$

This expression can also be regarded as an average over Markovian stochastic processes in many-body wave-function space. To give a deeper insight we define the ensemble of antisymmetrized two-body residual interactions as

$$\delta v_{12}(\sigma) = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ \langle\alpha\beta|\delta v_{12}(\sigma)|\,\delta\gamma\rangle a_\gamma a_\delta. \quad (4)$$

Here, $\sigma \equiv \{\sigma_i\}_{i=1,N}$, where all components are stochastic variables sampled according to Gaussian probabilities with mean zero and $\overline{\sigma_i^2} = 1$. The number N of stochastic components defines the complexity of the process. The definition (4) includes the force proposed in Ref. [9]. Equation (3) can be interpreted as the average over the quantum diffusion

$$\Delta|\Psi\rangle = \left\{ \frac{\Delta t}{i\hbar} H_{\rm MF} + \Delta B \delta v_{12} + \frac{1}{2} (\Delta B \delta v_{12})^2 \right\} |\Phi(t)\rangle, \quad (5)$$

where $\Delta B = i\sqrt{\tau \Delta t}/\hbar$. In the following, we will consider the last expression as a differential stochastic equation in Hilbert space [25,31]. We use the notation dB instead of ΔB and use the Ito rules of stochastic calculus [32]. Because of the two-body nature of δv_{12}, Eq. (5) induces complex reorganization of single-particle degrees of freedom. After the jump, the state is not a priori a single Slater determinant. For applications, it is highly desirable to preserve the simple initial form of the state along the stochastic path. This can be achieved by invoking the additional approximations described in the following. Following Refs. [20–22], we consider an initial density

$$D = \frac{|\Phi_a\rangle\langle\Phi_b|}{\langle\Phi_b|\Phi_a\rangle}, \quad (6)$$

where $|\Phi_a\rangle = \mathcal{A}(\Pi_i|\alpha_i\rangle)$ and $|\Phi_b\rangle = \mathcal{A}(\Pi_i|\beta_i\rangle)$ are two nonorthogonal Slater determinants formed of products of single-particle wave packets denoted, respectively, by $|\alpha_i\rangle$ and $|\beta_i\rangle$. The notation $\mathcal{A}(.)$ corresponds to the antisymmetrized product. We assume that both states follow the diffusion process described by Eq. (5) but with two independent sets of Gaussian stochastic variables, denoted, respectively, by $\sigma_{\mathbf{a}}$ and $\sigma_{\mathbf{b}}$. This case will be referred in the following as the "uncorrelated noise." The use of different sets of stochastic variables is at variance with standard quantum Monte Carlo procedures that simulate density evolution given by Lindblad equations [25]. However, this assumption has been shown to be crucial for describing the exact dynamics of interacting systems with stochastic methods [20,21].

A. Approximate stochastic mechanics in one-body density matrix space

To approximate the diffusion process, we first focus on single-particle degrees of freedom. Under the approximation

$$\left\langle a_i^+ a_j \delta v_{12}^2 \right\rangle \simeq \langle a_i^+ a_j \rangle \left\langle \delta v_{12}^2 \right\rangle + 2\langle a_i^+ a_j \delta v_{12} \rangle \langle \delta v_{12} \rangle - 2\langle a_i^+ a_j \rangle \langle \delta v_{12} \rangle^2, \quad (7)$$

the one-body density evolution [Eq. (5)] reduces to

$$d\langle a_i^+ a_j \rangle \simeq \frac{dt}{i\hbar} \langle [a_i^+ a_j, H_{\rm MF}] \rangle + dB_a (\langle a_i^+ a_j \delta v_{12} \rangle - \langle a_i^+ a_j \rangle \langle \delta v_{12} \rangle) + dB_b^* (\langle \delta v_{12} a_i^+ a_j \rangle - \langle a_i^+ a_j \rangle \langle \delta v_{12} \rangle). \quad (8)$$

It is interesting to notice that, although we consider a second order perturbation theory for the residual interaction, the second-order term exactly cancels out when approximation (7) is used. Equation (7) corresponds to a Gaussian approximation for quantal fluctuations. Therefore, Eq. (8) provides the stochastic equation of motion of one-body degrees of freedom associated with Eq. (5) when neglecting part of the quantal fluctuations. The corresponding stochastic evolution of ρ reads

$$d\rho = \frac{dt}{i\hbar} [h_{\rm MF}, \rho] + dB_a (1-\rho) U(\rho, \sigma_{\mathbf{a}}) \rho + dB_b^* \rho U'(\rho, \sigma_{\mathbf{b}}) (1-\rho), \quad (9)$$

where $h_{\rm MF}$ denotes the matrix elements associated with the mean-field Hamiltonian, and $U(\rho, \sigma_{\mathbf{a}}) = {\rm Tr}_2[\delta v_{12}(\sigma_{\mathbf{a}}) \rho_2]$ and $U'(\rho, \boldsymbol{\sigma}_b) = {\rm Tr}_2[\rho_2 \delta v_{12}(\boldsymbol{\sigma}_b)]$.

The stochastic one-body evolution given by Eq. (9) also contains part of the information on correlations. Indeed, an approximate evolution of the two-body density, whose matrix elements are $\langle a_i^+ a_j^+ a_l a_k \rangle = \langle kl|\rho_{12}|ij\rangle$, can be obtained through approximations similar to Eq. (7) but preserving the symmetry of the two-body density:

$$\begin{aligned} \langle a_i^+ a_j^+ a_l a_k v_{12} \rangle \simeq\ & \langle a_i^+ a_j^+ a_l a_k \rangle \langle v_{12} \rangle + (\langle a_i^+ a_k v_{12} \rangle \langle a_j^+ a_l \rangle \\ & - \langle a_i^+ a_l v_{12} \rangle \langle a_j^+ a_k \rangle) + (\langle a_i^+ a_k \rangle \langle a_j^+ a_l v_{12} \rangle \\ & - \langle a_i^+ a_l \rangle \langle a_j^+ a_k v_{12} \rangle) - 2(\langle a_i^+ a_k \rangle \langle a_j^+ a_l \rangle \\ & - \langle a_i^+ a_l \rangle \langle a_j^+ a_k \rangle) \langle v_{12} \rangle \end{aligned} \quad (10)$$

and

$$\begin{aligned} & \langle a_i^+ a_j^+ a_l a_k v_{12} v_{12} \rangle \\ & \simeq \langle a_i^+ a_j^+ a_l a_k \rangle \left\langle v_{12}^2 \right\rangle + 2(\langle a_i^+ a_k v_{12} \rangle \langle a_j^+ a_l v_{12} \rangle \\ & \quad - \langle a_i^+ a_l v_{12} \rangle \langle a_j^+ a_k v_{12} \rangle) - 2(\langle a_i^+ a_k \rangle \langle a_j^+ a_l \rangle \\ & \quad - \langle a_i^+ a_l \rangle \langle a_j^+ a_k \rangle) \langle v_{12} \rangle^2. \end{aligned} \quad (11)$$

Combining with Ito rules reduces the evolution of ρ_{12} to

$$d\langle a_i^+ a_j^+ a_l a_k \rangle \simeq d(\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li}), \quad (12)$$

indicating that the two-body evolution can be deduced from the stochastic evolution of ρ. Although Eq. (12) is similar to the mean-field case, it contains correlations beyond the mean field. A similar situation occurs in the exact reformulation of self-interacting fermions with quantum jumps [22].

In summary, the jump process described by Eq. (5) for both state vectors entering in D can be approximated by the jump process in one-body space given by Eq. (9) if part of the quantal fluctuations is neglected. The advantage of this approximation is that expression (6) for D is preserved along the stochastic path. In this work, we restrict ourselves to this limit and Eq. (9) will be referred to as the incoherent stochastic mean-field (SMF) dynamics. The properties of this diffusion process are described in the following.

We consider that the single-particle states of $|\Phi_a\rangle$ and $|\Phi_b\rangle$ initially verify

$$\langle \beta_j | \alpha_i \rangle = \delta_{ij}. \quad (13)$$

Equation (9) can be simulated by quantum jumps for single-particle states given by

$$\begin{cases} |d\alpha_i\rangle = \left[\frac{dt}{i\hbar} h_{\rm MF}(\rho) + dB_a (1-\rho) U(\rho, \sigma_{\mathbf{a}})\right] |\alpha_i\rangle, \\ \langle d\beta_j| = \langle \beta_j | \left[-\frac{dt}{i\hbar} h_{\rm MF}(\rho) + dB_b^* U'(\rho, \sigma_{\mathbf{b}})(1-\rho)\right]. \end{cases} \quad (14)$$

The latter quantum diffusion process has several attractive aspects. First, it can be easily verified that Eq. (13) is preserved

along the stochastic path. Thus, the one-body density reads at all time $\rho = \sum_i |\alpha_i\rangle\langle\beta_i|$. Consequently, the trace of the density is constant along the path: $\mathrm{Tr}(dD) = \mathrm{Tr}(d\rho) = 0$. In addition, ρ remains a projector (i.e., $\rho^2 = \rho$ at all time). Finally, the total entropy $S = -k_B \mathrm{Tr}(D \ln D)$ is constant along the path. Indeed, since the density is given by Eq. (6), $S(D)$ identifies with the one-particle entropy $S(\rho)$. Using Eq. (9) and Ito rules, we obtain $\overline{dS(\rho)} = 0$. Despite a constant entropy, the SMF induces correlations beyond the mean field. Indeed, starting from an initial two-body density $\rho_{12} = \mathcal{A}(\rho_1\rho_2)$, after one time step, the average evolutions of the one- and two-body density matrices read

$$\begin{cases} d\overline{\rho} &= \frac{dt}{i\hbar}\,[h_{\mathrm{MF}}, \rho]\,, \\ d\overline{\rho_{12}} &= \frac{dt}{i\hbar}\,[h_{\mathrm{MF}}(1) + h_{\mathrm{MF}}(2), \rho_{12}] + dC_{12}, \end{cases} \tag{15}$$

where the labels "1" and "2" refer to the particle on which the operator is acting [33] and dC_{12} corresponds to correlations beyond the mean field associated with the stochastic one-body evolution given by Eq. (9). It reads

$$\begin{aligned} dC_{12} = -\frac{\tau dt}{\hbar^2}[&(1-\rho_1)(1-\rho_2)\overline{U_1(\sigma_{\mathbf{a}})U_2(\sigma_{\mathbf{a}})}\rho_{12} \\ &+ \rho_{12}\overline{U_1'(\sigma_{\mathbf{b}})U_2'(\sigma_{\mathbf{b}})}(1-\rho_1)(1-\rho_2)], \end{aligned} \tag{16}$$

where the density dependences are omitted in U and U'. Equation (16) clearly indicates that dC_{12} is a second-order term in perturbation. Note that its form is similar to that of the second moment of the initial stochastic correlation used in Ref. [11].

B. Illustration of the application

To illustrate the SMF theory, we consider the monopolar vibration of a ^{40}Ca nucleus. The system is initially prepared in a pure state $D = |\Phi\rangle\langle\Phi|$, where $|\Phi\rangle$ is a Slater determinant solution of a constrained Hartree-Fock (CHF) equation. The CHF equation is solved by assuming spherical symmetry and spin and isospin saturation. The Skyrme interaction of Ref. [34] is used in the mean field. We assume, in addition to the self-consistent mean field, a monopolar constraint λr^2, with $\lambda = 0.25$ MeV fm^{-2} at $t < 0$ fm/c [35]. At $t = 0$ fm/c, the constraint is relaxed and two dynamical calculations are considered. The first corresponds to the time-dependent Hartree-Fock (TDHF) evolution. In the second case, the SMF evolution described by Eq. (9) is performed with a statistical ensemble of contact interactions defined by one stochastic variable [i.e., $\delta v_{12}(\sigma) = \sigma v_{\mathrm{res}}$, where v_{res} is a contact interaction]. In this case, $U(\sigma, r)$ takes the form $U(\sigma, r) = \sigma g_0 \rho(r)$, where g_0 is a parameter measuring the strength of the perturbation. In both cases, evolutions are solved by assuming spherical symmetry.

The evolution of the root-mean-square (rms) radius obtained with TDHF evolution is presented in Fig. 1 (filled circles). The different lines displayed on the top part of Fig. 1 correspond to the evolution of the rms radius along several stochastic paths obtained with $g_0 = 500$ MeV/fm and a collision time $\tau = 0.01$ fm. In each case, the stochastic evolution differs significantly from the mean-field prediction. The bottom part of Fig. 1 shows a comparison between the TDHF evolution and the evolution of the rms radius obtained by averaging over the different stochastic trajectories. Interestingly enough, the average evolution tracks with the TDHF evolution. This example illustrates a special situation where the mean-field dynamics can be recovered from complex trajectories in many-body space [36]. However, significant fluctuations around the mean TDHF trajectories are observed. This is illustrated in Fig. 2, where the quantity $\Delta_r = (\overline{\langle r^2\rangle^2} - \overline{\langle r^2\rangle}^2)^{1/2}$

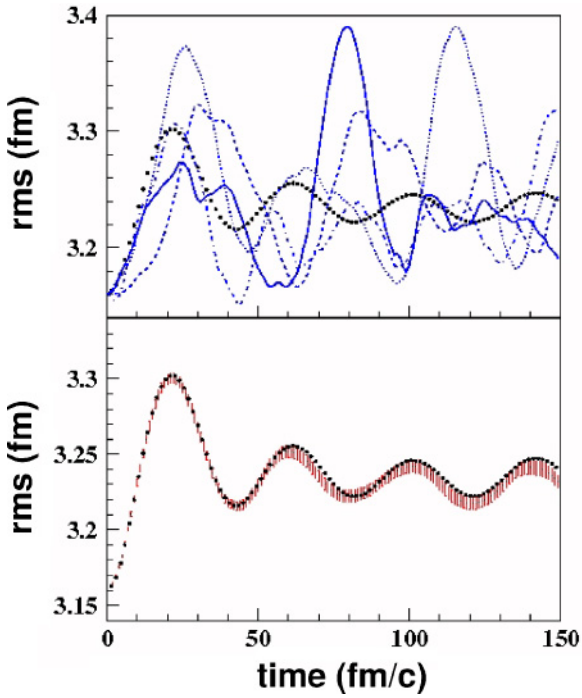

FIG. 1. (Color online) Top: Evolution of the rms radius as a function of time. Black circles correspond to the standard TDHF evolution, different lines correspond to different stochastic paths. Bottom: Error bars correspond to the rms evolution obtained by averaging over different paths; black circles correspond to the TDHF case. The stochastic simulation is performed for $g_0 = 500$ MeV/fm. The average is taken over 200 trajectories. The width of the error bars corresponds to the statistical fluctuations of the rms.

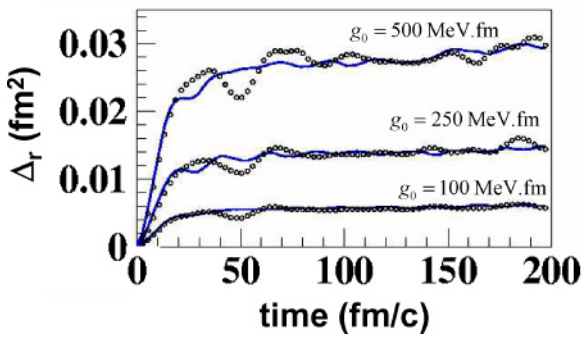

FIG. 2. (Color online) Evolution of the dispersion of the rms as a function of time for different values of g_0. The different curves from bottom to top correspond, respectively, to $g_0 = 100$, 250, and 500 MeV fm. Solid lines and open circles correspond, respectively, to initial constraints $\lambda = 0$ MeV fm^{-2} and $\lambda = 0.25$ MeV fm^{-2}.

is displayed as a function of time for different values of g_0 and λ. We also computed as a reference the mean-field width $\sigma_{\rm MF}$, corresponding to the quantal fluctuations of r^2 estimated in the mean-field approximation, leading to $\sigma_{\rm MF} = 6.3\,{\rm fm}^2$. As expected in the weak-coupling approximation, the additional fluctuations Δ_r induced by the stochastic term are much smaller than $\sigma_{\rm MF}$. It turns out that the dispersion is properly parametrized by the formula $\Delta_r = \Delta_0(1 - e^{-\Gamma_0 t})$, where Δ_0 is proportional to g_0 although Γ_0 is independent of it. Therefore, although the average evolution of the rms collective variables is not affected by the stochastic process, fluctuations around the mean value increase and saturate as expected in Brownian motion. Interestingly enough, the behavior observed here is very similar to the description of a quantum oscillator [37] with Nelson stochastic mechanics [38] replacing $(\hbar/m)^{1/2}$ by g_0. By assuming a single collective state and using similar techniques as in Ref. [37], an analytical expression can be obtained for Δ_r, where Δ_0 is indeed proportional to g_0 whereas Γ_0 depends only on the oscillator frequency. Note, however, that a complete understanding of the Brownian process presented here must pass through the linearization of Eq. (9) as in Ref. [17].

C. Critical discussion

In this section, we have shown that the presented SMF theory can be applied to account for fluctuations beyond the mean field. The previous example can only serve as an illustration owing to the very schematic residual interaction used and to the very small time τ (see estimation in Refs. [39,40]). Besides the simplicity of the force, it is important to note that the preceding theory only gives a partial answer to the simulation of correlations beyond the mean field for realistic nuclear systems. Indeed, as clearly seen in Fig. 1, although fluctuations of one-body observables are increased, the average evolution of the rms tracks with the TDHF case. Therefore, no additional damping is observed in the SMF, in contrast to what is obtained in extended TDHF dynamics [17]. Indeed, dissipative aspects present in the memory kernel of extended TDHF dynamics are not included in the present framework. A careful analysis demonstrates that the absence of a collision term could be assigned to the approximations made on quantal fluctuations [Eqs. (7), (10), and (11)].

Under these approximations, it is however possible to show that a fermionic system submitted to a statistical ensemble of residual interactions δv_{12} can be treated by a jump process related to its mean field [Eq. (9)]. The form of the noise is a second critical aspect for nuclear physics. In fact, it is expected that the residual interaction is dominated by the two-particle–two-hole (2p–2h) channels. Owing to the mean-field nature of the noise in Eq. (9), these components cancel out in the stochastic part. Therefore, although the SMF can be of great interest, some important aspects for nuclear physics are missing. In the next section, we discuss the possibility of using the quantum jump process in one-body space in a more general framework.

IV. STOCHASTIC MECHANICS WITH DISSIPATION

To generalize the stochastic method described previously, we consider directly the evolution of the many body density D associated with Eq. (1). Using the short memory time approximation for δv_{12}, the evolution of D can be recast as

$$\Delta D = \frac{\Delta t}{i\hbar}[H_{\rm MF}, D] - \frac{\tau\,\Delta t}{2\hbar^2}\overline{[\delta v_{12}, [\delta v_{12}, D]]}. \tag{17}$$

In the previous section, the term $\overline{\delta v_{12} D \delta v_{12}}$ has been neglected because the average evolution of wave functions were directly considered. This approximation made it possible to have uncorrelated noise for $|\Phi_a\rangle$ and $\langle\Phi_b|$. Here, this contribution is not neglected. As a consequence, the uncorrelated noise assumption is no longer possible.

The one-body density matrix equation of motion associated with Eq. (17) is given by

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}\,[h_{\rm MF}(\rho), \rho] - \frac{g}{2}\mathcal{D}(\rho), \tag{18}$$

where $g = \tau/\hbar^2$ is a real constant. The $\mathcal{D}(\rho)$ term, called the "dissipator" hereafter, corresponds to the average effect of the residual interaction and reads

$$\langle j|\mathcal{D}|i\rangle = \overline{\langle[[a_i^+ a_j, \delta v_{12}], \delta v_{12}]\rangle}. \tag{19}$$

We assume that the system is initially in a pure state described by a Slater determinant $|\Phi(t)\rangle$ formed of N orthonormal single-particle states denoted by $|\alpha\rangle$. The associated initial one-body density matrix reads $\rho = \sum_\alpha |\alpha\rangle\langle\alpha|$. Having in mind the nuclear many-body problem, we assume that only 2p–2h components of δv_{12} are not equal to zero. Completing the hole states by a set of particle states, denoted by $|\tilde\alpha\rangle$, we have

$$\delta v_{12}(t) = \frac{1}{4}\sum_{\tilde\alpha\tilde\beta\alpha\beta} a_{\tilde\alpha}^+ a_{\tilde\beta}^+ \langle\tilde\alpha\tilde\beta|v_{12}(t)|\alpha\beta\rangle a_\alpha a_\beta. \tag{20}$$

$\mathcal{D}$ can then be recast as

$$\mathcal{D}(\rho) = {\rm Tr}_2\,[v_{12}, F_{12}]\,, \tag{21}$$

where F_{12} is equal to

$$\begin{aligned} F_{12} = \tfrac{1}{2}\,[&(1-\rho_1)(1-\rho_2)\,v_{12}\rho_1\rho_2 \\ &- \rho_1\rho_2 v_{12}\,(1-\rho_1)(1-\rho_2)]\,. \end{aligned} \tag{22}$$

Expression (21) takes a form similar to the collision term generally obtained in extended TDHF dynamics [17]. The dissipator $\mathcal{D}(\rho)$ can be further transformed. Indeed, δv_{12} given by Eq. (20) can always be decomposed as (see for instance [41])

$$\delta v_{12} = -\frac{1}{4}\sum_n \lambda_n \mathcal{O}_n^2, \tag{23}$$

where λ_n are real and the $\mathcal{O}_n$ correspond to a set of commuting Hermitian one-body operators written as $\mathcal{O}_n = \sum_{\tilde\alpha\alpha}\langle\tilde\alpha|O_n|\alpha\rangle a_{\tilde\alpha}^+ a_\alpha$. By using Eq. (21), $\mathcal{D}(\rho)$ can be recast as

$$\mathcal{D}(\rho) = \sum_{mn}\Gamma_{mn}\,(O_n O_m\rho + \rho O_n O_m - 2O_m\rho O_n)\,. \tag{24}$$

The coefficients Γ_{mn} are given by

$$\Gamma_{mn} = \tfrac{1}{2}\lambda_m\lambda_n {\rm Tr}[O_m(1-\rho)O_n\rho]. \tag{25}$$

We recognize in this expression the quantum covariance between the operator $\mathcal{O}_n$ and $\mathcal{O}_m$ (i.e., ${\rm Tr}[O_m(1-\rho)O_n\rho] =$

$\langle \mathcal{O}_m \mathcal{O}_n \rangle - \langle \mathcal{O}_m \rangle \langle \mathcal{O}_n \rangle$). Expression (24) has the form of the dissipator appearing usually in the Lindblad equation [25]. Therefore, we have shown that the evolution of one-body degrees of freedom associated with Eq. (17) can be identified with a Markovian quantum master equations generally obtained in quantum open systems. A large amount of work is devoted to the simulation of such master equations by quantum jump methods (see for instance [25,42–45]) and one can take advantage of the most recent advances in this field. This aspect has however rarely been discussed in the context of self-interacting systems. In the following, the associated diffusion process is made explicit and we show that it indeed corresponds to jumps between Slater determinants. The stochastic Schrödinger equation for the single-particle wave function is then given.

A. Explicit form of the stochastic process

Following Ref. [25], we introduce the Hermitian positive matrix Γ with components Γ_{mn}. An economical method for introducing the quantum jump process [25] is to use the unitary transformation u that diagonalizes Γ (i.e., $\Gamma = u^{-1}\gamma u$, where γ is the diagonal matrix of the eigenvalues of Γ). New operators A_k can be defined by the transformation $A_k = \sum_n u^{-1}_{kn} O_n$. The dissipator is then recast as

$$\mathcal{D}(\rho) = \sum_k \gamma_k \left(A_k^2 \rho + \rho A_k^2 - 2 A_k \rho A_k \right). \tag{26}$$

The last equation can be simulated using the average over the stochastic mean-field dynamics:

$$d\rho = \frac{dt}{i\hbar} [h_{\mathrm{MF}}(\rho), \rho] - g \frac{dt}{2} \mathcal{D}(\rho) + db_{\mathrm{sto}}, \tag{27}$$

where db_{sto} is a stochastic one-body operator, which, using Ito rules [32], reads

$$db_{\mathrm{sto}} = \sum_k [dW_k (1-\rho) A_k \rho + dW_k^* \rho A_k (1-\rho)]. \tag{28}$$

Here dW_k denotes stochastic variables given by $dW_k = -i d\xi_k \sqrt{g\gamma_k}$, where $d\xi_k$ corresponds to a set of real Gaussian stochastic variables with mean zero and $d\xi_k d\xi_{k'} = \delta_{kk'} dt$.

B. Nature of the stochastic process in Hilbert space

It is worth noticing that the proposed dissipative equation and its stochastic counterpart are only well defined if the density is initially prepared as a pure Slater-determinant state. We now turn to the essential properties of Eq. (27). First, it preserves the number of particles $\mathrm{Tr}\,(d\rho) = 0$. In addition, if initially $\rho^2 = \rho$, then

$$d\rho d\rho - g \frac{dt}{2} [\rho \mathcal{D}(\rho) + \mathcal{D}(\rho)\rho] = -g \frac{dt}{2} \mathcal{D}(\rho), \tag{29}$$

which is obtained using Ito stochastic rules and retaining only terms linear in dt. The last expression demonstrates that $(\rho + d\rho)^2 = \rho + d\rho$. Thus, ρ remains a projector along the stochastic path. As a consequence, the pure state nature of the many-body density matrix is preserved along the stochastic path [i.e., $D = |\Phi(t)\rangle\langle\Phi(t)|$, where $|\Phi\rangle$ is a normalized Slater determinant at all time]. The associated stochastic Schrödinger equation for single-particle states reads

$$d|\alpha\rangle = \left\{ \frac{dt}{i\hbar} h_{\mathrm{MF}}(\rho) + \sum_k dW_k (1-\rho) A_k - g \frac{dt}{2} \sum_k \gamma_k \left[A_k^2 \rho + \rho A_k \rho A_k - 2 A_k \rho A_k \right] \right\} |\alpha\rangle. \tag{30}$$

Eq. (30) can be directly used for practical applications.

In this section, assuming that the residual interaction can be written in terms of $2p-2h$ components, we have shown that the dissipative dynamics of one-body degrees of freedom can be simulated by quantum jumps. The stochastic method differs significantly from the simplified scenario considered in the previous section. First, the above theory does not require the introduction of the generalized many-body density matrix formed of two Slater determinants since $D = |\Phi(t)\rangle\langle\Phi(t)|$ along each path. As a counterpart, the numerical effort required to treat the new SMF, which includes dissipative aspects, is significantly increased. Indeed, in Sec. III B, we have shown that fluctuations can be introduced using a simplified residual interaction and a limited number of noise terms. In the new SMF, the numerical effort is directly proportional to the number of one-body operators entering in Eq. (23). This situation is similar to stochastic methods used in nuclear structure studies [19]. In that case, significant numerical effort is required. For instance, if we assume that a physical system is described in a mesh, then the number of noise terms is a priori as large as the number of mesh points. The numerical implementation of the quantum jump process in its full complexity is expected to remain difficult with present computer capacities. Therefore, specific numerical techniques as well as truncation procedures should be developed to implement the method in many-body dissipative dynamics.

V. CONCLUSION

In this work, we have presented a discussion on the possibility of replacing the dynamics of interacting fermions by quantum jumps. By assuming a weak-coupling approximation and a short memory time for the residual interaction, two scenarios have been considered. Focusing on one-body degrees of freedom, we have found two different approximations that lead to equations of motions for the one-body density matrix that can be treated by quantum jumps between Slater determinants.

In the first stochastic mean-field process, part of the quantal correlations between ρ and δv_{12} are neglected along the path. The SMF is illustrated in the monopolar vibration of a calcium nucleus. In this case, whereas expectation values of one-body observables are unchanged, fluctuations are increased compared to the mean field. In the presented application, the residual interaction is rather simple. However, more complex statistical ensembles, such as two-body random interactions, can be used. This method suffers from the absence

of dissipative effects and appears to be too simplified for the nuclear many-body problem.

In the second part of this work, we showed that the dynamics of correlated systems can be described by a quantum jump process even if no approximation on the quantal correlations are made. Restricting to 2p–2h residual interactions gives a guideline for transforming the evolution of the one-body density matrix evolution into a Lindblad equation. The stochastic process corresponds to quantum jumps between pure state densities $D = |\Phi\rangle\langle\Phi|$, where $|\Phi\rangle$ is a Slater determinant. The associated stochastic equation of motion for single-particle wave functions is given.

Finally, we would like to mention that the presented framework does not account for non-Markovian effects. It has however been shown in Ref. [15] that the memory effect might be important in the nuclear context. Promising work is being devoted to incorporating non-Markovian effects in quantum Monte Carlo methods [46–49].

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