

Quantum Monte-Carlo methods and exact treatment of the two-body problem with Hartree-Fock Bogoliubov states

Denis Lacroix^{1,2}

¹*National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*

²*Laboratoire de Physique Corpusculaire, ENSICAEN and Université de Caen, IN2P3-CNRS, Blvd du Maréchal Juin, 14050 Caen, France*

(Dated: May 16, 2006)

In this article, we show that the exact two-body problem can be replaced by quantum jumps between densities written as $D = |\Psi_a\rangle\langle\Psi_b|$ where $|\Psi_a\rangle$ and $|\Psi_b\rangle$ are vacuum for different quasi-particles operators. It is shown that the stochastic process can be written as a Stochastic Time-Dependent Hartree-Fock Bogoliubov theory (Stochastic TDHFB) for the generalized density \mathcal{R} associated to D where $\mathcal{R}^2 = \mathcal{R}$ along each stochastic trajectory.

I. INTRODUCTION

The goal of this article is to prove that the dynamics of fermions interacting through a two-body interaction can be transformed into a stochastic process in the Hilbert space of Hartree-Fock Bogoliubov (HFB) states. Such a derivation is motivated by recent studies dedicated to the structure of nuclei. In nuclear physics, mean-field theories like Hartree-Fock and HFB already provide a good approximation of static and dynamical properties [1]. It also turns out that a deep understanding of nuclei requires the introduction of correlations beyond mean-field. Large theoretical developments are devoted for instance to Generator Coordinates Methods (GCM) [2]. In that case, some collective degrees of freedom are selected and the correlated ground state is constructed as a superposition of mean-field states (HF or HFB). It has been shown that the description of nuclear systems is greatly improved if pairing correlations are already accounted for, i.e. if the GCM is performed with HFB many-body states. Such a method has been successfully applied to nuclear structure when only few degrees of freedom are selected. However, applications of GCM techniques when many collective degrees of freedom are important are still numerically intractable.

Monte-Carlo techniques appear as an alternative way of treating correlation beyond mean-field. Shell model Monte-Carlo theory[3] is an example of such technique. Recently, starting from the Hartree-Fock theory, new formulations [4–6] have been proposed that combines the advantages of Monte-Carlo methods and mean-field theories. In that case, the exact evolution of fermionic (or bosonic) systems is replaced by an ensemble of stochastic mean-field evolutions. A possible improvement of such theory, which might be of great interest in the nuclear context, is to include pairing correlations in the trial set of wave functions, i.e. to consider quantum jumps between HFB states instead of HF states. A first step in this direction as been made in ref. [7] where stochastic dynamics between BCS states were introduced. In this article, we show that the dynamics of fermions interact-

ing through a general two-body Hamiltonian

$$H = \sum_{ij} \langle i|T|j\rangle c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} \langle ij|v_{12}|lk\rangle c_i^\dagger c_j^\dagger c_l c_k \quad (1)$$

can be mapped into a quantum jump process between HFB states. Here, c^+ operators correspond to creation operators associated to a complete single-particle basis, and v_{12} matrix elements are antisymmetrized.

In the following we first introduce quantities associated to "densities" written as a dyadic of two HFB state vectors, i.e. $D = |\Psi_a\rangle\langle\Psi_b|$. The flexibility of stochastic methods allows to consider densities with specific helpful properties which are precised in the first part of this work. Then a TDHFB equation is derived for D when correlations beyond mean-field are neglected. Finally, the full stochastic theory that accounts for all two-body effects is derived.

II. PRELIMINARY RESULTS AND NOTATIONS

In quantum Monte-Carlo approaches starting from an initial density $D = |\Psi\rangle\langle\Psi|$, the exact system evolution is recovered by averaging over an ensemble densities written as a product of two different state vectors

$$D = |\Psi_a\rangle\langle\Psi_b|. \quad (2)$$

The use of two different states is at the heart of exact stochastic methods. The advantage of these approaches is that states entering in D correspond generally to a specific class of trial wave-function. In previous applications, these states have been chosen as Hartree-Fock states[5].

Given a specific choice of trial wave-functions, it turns out that stochastic reformulation is generally not unique. This flexibility might be used for instance to optimize quantum jumps and reduce the number of paths (see for instance [8]). Here we will consider HFB state as trial state vectors and use this flexibility in a different way. Indeed, it turns out that the two-body problem can be reformulated as a stochastic process imposing additional relations between the states $|\Psi_a\rangle$ and $|\Psi_b\rangle$ along each path. These additional constraints, given below, lead to

simplified equations and derivations without restricting the exactness of the formulation.

A. Choice of a subclass of densities

Let us assume that D has the form (2) where $|\Psi_a\rangle$ and $|\Psi_b\rangle$ can be written as a product of quasi-particle operators, i.e. $|\Psi_a\rangle = \Pi a_\alpha^+ |0\rangle$ and $|\Psi_b\rangle = \Pi b_\alpha^+ |0\rangle$. D will be referred in the following as a density although it does not necessarily meet all required properties to be considered as a density matrix. For each quasi-particle operator, two sets of single-particle wave-functions, denoted by $|\alpha_{a,b}\rangle$ and $|\bar{\alpha}_{a,b}\rangle$, are introduced. They define the transformation between quasi-particle states and a complete set of particle states as

$$\begin{aligned} a_\alpha &= \sum_i c_i \langle \bar{\alpha}_a | i \rangle + \langle i | \alpha_a \rangle c_i^+, \\ b_\alpha &= \sum_i c_i \langle \bar{\alpha}_b | i \rangle + \langle i | \alpha_b \rangle c_i^+. \end{aligned} \quad (3)$$

Note that, we can recover the matrix notations U, V often used in the HFB theory through the relation ${}^{a,b}U_{i\alpha} = \langle \bar{\alpha}_{a,b} | i \rangle$ and ${}^{a,b}V_{i\alpha} = \langle i | \alpha_{a,b} \rangle$.

As usual [1, 9], we introduce vector notations $\mathbf{a} = \{a, a^+\}$, $\mathbf{b} = \{b, b^+\}$ and $\mathbf{c} = \{c, c^+\}$. Above linear transformations can then be written as matrix transformations $\mathbf{a} = \mathcal{W}_a^+ \mathbf{c}$ and $\mathbf{b} = \mathcal{W}_b^+ \mathbf{c}$. In opposite to the standard HFB theory, we do not impose the transformations to be canonical but instead restrict ourselves to a subclass of quasi-particles and vacuums having two specific properties. We first assume that

$$\mathcal{W}_a \mathcal{W}_b^+ = \mathcal{W}_a^+ \mathcal{W}_b = 1, \quad (4)$$

which gives the inverse transformations $\mathbf{c} = \mathcal{W}_b \mathbf{a} = \mathcal{W}_a \mathbf{b}$. As a consequence, although the a and a^+ operators (respectively the b and b^+) do not necessarily fulfill fermionic anti-commutation rules, because of (4) we have

$$[a_\alpha, b_\beta]_+ = [a_\alpha^+, b_\beta^+]_+ = 0, \quad [a_\alpha, b_\beta^+]_+ = \delta_{\alpha\beta}. \quad (5)$$

The second important assumption is that $|\Psi_a\rangle$ and $|\Psi_b\rangle$ are both vacuum for all a_α and b_α . As we will see in the following such properties might occur without any simple relations between the two sets of annihilation operators.

We introduce the generalized density matrix \mathcal{R}_{ab} defined as

$$\mathcal{R}_{ab} = \begin{pmatrix} \langle \Psi_b | c_i^+ c_j | \Psi_a \rangle & \langle \Psi_b | c_i c_j | \Psi_a \rangle \\ \langle \Psi_b | c_i^+ c_j^+ | \Psi_a \rangle & \langle \Psi_b | c_i c_j^+ | \Psi_a \rangle \end{pmatrix}. \quad (6)$$

From the two assumptions, it can be shown that

$$\mathcal{W}_b^+ \mathcal{R} \mathcal{W}_a = \mathcal{L} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (7)$$

or equivalently:

$$\begin{aligned} \langle a_\alpha b_\beta \rangle &= \langle a_\alpha^+ b_\beta \rangle = \langle a_\alpha^+ b_\beta^+ \rangle = 0, \\ \langle a_\alpha b_\beta^+ \rangle &= \delta_{\alpha\beta}. \end{aligned}$$

This again can be seen as a generalization of the HFB case and implies $\mathcal{R}_{ab}^2 = \mathcal{R}_{ab}$. In addition, the generalized density \mathcal{R}_{ab} takes a simplified form compared to the one generally obtained for transition densities [1]. Here, we have

$$\mathcal{R}_{ab} = \begin{pmatrix} \rho_{ab} & \kappa_{ab} \\ -\kappa_{ab}^* & 1 - \rho_{ab}^T \end{pmatrix}, \quad (8)$$

where ρ_{ab}^T denotes the transposed matrix of ρ_{ab} . In the following, to simplify notations we will omit the subscript "ab". Different operators matrix elements can be expressed as

$$\rho = \sum_\alpha |\alpha_a\rangle \langle \alpha_b|, \quad (9)$$

$$1 - \rho = \sum_\alpha |\bar{\alpha}_a\rangle \langle \bar{\alpha}_b|, \quad (10)$$

$$\kappa = \sum_\alpha |\alpha_a \bar{\alpha}_b\rangle = - \sum_\alpha |\bar{\alpha}_a \alpha_b\rangle, \quad (11)$$

with the convention $\kappa_{ij} = \sum_\alpha \langle ij | \alpha_a \bar{\alpha}_b \rangle$.

Finally, we will also use the notation $|{}^{a,b}W_\alpha\rangle$ and $|{}^{a,b}V_\alpha\rangle$ (taken from ref. [9]). We have in particular

$$\begin{aligned} \mathcal{R} &= \sum_\alpha |{}^a W_\alpha\rangle \langle {}^b W_\alpha|, \\ 1 - \mathcal{R} &= \sum_\alpha |{}^a V_\alpha\rangle \langle {}^b V_\alpha|, \end{aligned} \quad (12)$$

with $\langle {}^a W_\beta | {}^b W_\alpha \rangle = \langle {}^a V_\beta | {}^b V_\alpha \rangle = \delta_{\alpha\beta}$ and $\langle {}^a V_\beta | {}^b W_\alpha \rangle = 0$. This completes the different properties associated with the subclass of densities considered here.

B. Expression of the Hamiltonian and generalized TDHFB equation

Using the previous properties, the action of the two-body Hamiltonian on the vacuum $|\Psi_a\rangle$ can be recast as

$$H |\Psi_a\rangle = \{ \langle H \rangle + h_L + H_{res}^L \} |\Psi_a\rangle, \quad (13)$$

where we have used the compact notation $\langle H \rangle = \langle \Psi_b | H | \Psi_a \rangle$ and where h_L is a one-body effective Hamiltonian given by

$$h_L = \sum_{\alpha\beta} \left\{ \langle \bar{\alpha}_b | h | \beta_a \rangle a_\alpha^+ b_\beta^+ + \frac{1}{2} \Delta_{\bar{\alpha}_b \bar{\beta}_b} a_\alpha^+ a_\beta^+ - \frac{1}{2} \Delta_{\alpha_a \beta_a}^* b_\alpha^+ b_\beta^+ \right\} \quad (14)$$

h and Δ correspond respectively to matrix elements

$$h_{ij} = T_{ij} + \langle i | Tr_2(v_{12}\rho_2) | j \rangle, \quad (15)$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \langle ij | v_{12} | kl \rangle \kappa_{kl}, \quad (16)$$

which will be called mean-field and pairing field in analogy to HFB theory. Note that expression (14) differs from the one generally obtained in HFB using the Wick theorem because of the coexistence of two sets of quasi-particle operators. Starting from (14), the effective Hamiltonian can be recast as

$$h_L = \frac{1}{2} \begin{pmatrix} c^+ & c \end{pmatrix} (1 - \mathcal{R}) \mathcal{H} \mathcal{R} \begin{pmatrix} c \\ c^+ \end{pmatrix}, \quad (17)$$

where \mathcal{H} stands for the generalized HFB Hamiltonian [1, 9]:

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^T \end{pmatrix}. \quad (18)$$

We will see that expression (17) is central for further developments. The last term of equation (13), called hereafter residual Hamiltonian reads

$$H_{res}^L = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \bar{\alpha}_b \bar{\beta}_b | v_{12} | \delta_a \gamma_a \rangle a_\alpha^+ a_\beta^+ b_\gamma^+ b_\delta^+. \quad (19)$$

Performing a similar decomposition of $\langle \Psi_b | H$ leads to

$$\langle \Psi_b | H = \langle \Psi_b | \{ \langle H \rangle + h_R + H_{res}^R \}, \quad (20)$$

with

$$h_R = \frac{1}{2} \begin{pmatrix} c^+ & c \end{pmatrix} \mathcal{R} \mathcal{H} (1 - \mathcal{R}) \begin{pmatrix} c \\ c^+ \end{pmatrix}, \quad (21)$$

while

$$H_{res}^R = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha_b \beta_b | v_{12} | \bar{\delta}_a \bar{\gamma}_a \rangle a_\alpha a_\beta b_\gamma b_\delta. \quad (22)$$

C. Evolution of the generalized density \mathcal{R}

Starting from the initial density (2), the evolution of the system is considered assuming first that the effect of the residual interaction can be neglected. After one time-step, due to the one-body nature of h_L , the state $|\Psi_a + d\Psi_a\rangle = e^{\frac{dt}{i\hbar} h_L} |\Psi_a\rangle$ is a vacuum for the new quasi-particles $a'_\alpha = a_\alpha + da_\alpha = e^{\frac{dt}{i\hbar} h_L} a_\alpha e^{-\frac{dt}{i\hbar} h_L}$. Similarly,

$\langle \Psi_b + d\Psi_b | = \langle \Psi_b | e^{-\frac{dt}{i\hbar} h_R}$ is a vacuum for the new quasi-particles $b'_\alpha = b_\alpha + db_\alpha = e^{\frac{dt}{i\hbar} h_R} b_\alpha e^{-\frac{dt}{i\hbar} h_R}$.

Since the residual interaction is neglected, all the information on the system is contained in the evolution of \mathcal{R} . From standard rules of creation-annihilation operator transformations [9–11], we obtain:

$$[h_L, \mathbf{c}] = -(1 - \mathcal{R}) \mathcal{H} \mathcal{R} \mathbf{c}, \quad (23)$$

$$[h_R, \mathbf{c}] = -\mathcal{R} \mathcal{H} (1 - \mathcal{R}) \mathbf{c}. \quad (24)$$

With the help of the above anti-commutation relationships, we can express $e^{-\frac{dt}{i\hbar} h_L} \mathbf{c} e^{\frac{dt}{i\hbar} h_L}$ and $e^{\frac{dt}{i\hbar} h_R} \mathbf{c} e^{-\frac{dt}{i\hbar} h_R}$, and deduce the evolution of \mathcal{R} . Using the fact that initially $\mathcal{R}^2 = \mathcal{R}$ and $(1 - \mathcal{R}) \mathcal{R} = 0$, we end with

$$\begin{aligned} i\hbar \frac{d\mathcal{R}}{dt} &= (1 - \mathcal{R}) \mathcal{H} \mathcal{R} - \mathcal{R} \mathcal{H} (1 - \mathcal{R}) \\ &= [\mathcal{H}, \mathcal{R}], \end{aligned} \quad (25)$$

which is nothing but a TDHFB equation generalized to densities given by eq. (2). Without going into further details, it can be shown that the density \mathcal{R} fulfills all properties listed above and thus remains in the subclass of densities previously described. Therefore, the considerations made for single time step can be extended to the long-time dynamics.

III. INTRODUCTION OF QUANTUM MONTE-CARLO METHODS

In the previous section, we have introduced general properties of densities given by eq. (2) which will be helpful for the forthcoming discussion. In addition, we have shown that the dynamics reduces to a TDHFB-like equation when the residual interaction is neglected. The aim of this section is to show that the residual interaction can be treated by introducing stochastic processes between densities described in section II.

A. Separable residual interaction

In the following discussion, we concentrate first on the evolution of $|\Psi_a\rangle$, keeping in mind that everything can be transposed to $\langle \Psi_b |$. Following the Stochastic mean-field approach [4–6], we consider that the residual part of the interaction can be written as a sum of separable interactions in the particle-hole channel:

$$\langle \bar{\alpha}_a \bar{\beta}_a | v_{12} | \delta_b \gamma_b \rangle = - \sum_m \langle \bar{\alpha}_a | O_m | \delta_b \rangle \langle \bar{\beta}_a | O_m | \gamma_b \rangle, \quad (26)$$

where O_m corresponds to a set of single-particle operators. Using relation (26), the residual interaction H_{res}^L can be recast as

$$H_{res}^L |\Psi_a\rangle = \frac{1}{4} \sum_m B_m^{ph} B_m^{ph} |\Psi_a\rangle, \quad (27)$$

where the set of one-body operators B_m are given by

$$B_m^{ph} = \sum_{\alpha\beta} \langle \bar{\alpha}_a | O_m | \beta_b \rangle a_\alpha^+ b_\beta^+. \quad (28)$$

Guided by previous section, we write it as

$$B_m^{ph} = \frac{1}{2} (c \ c^+) (1 - \mathcal{R}) \mathcal{B}_m^{ph} \mathcal{R} \begin{pmatrix} c^+ \\ c \end{pmatrix}, \quad (29)$$

where we have introduced the matrix \mathcal{B}_m^{ph} :

$$\mathcal{B}_m^{ph} = \begin{pmatrix} O_m & 0 \\ 0 & -O_m^T \end{pmatrix}. \quad (30)$$

Once H_{res}^L is written as (27), the introduction of stochastic process is rather straightforward. Introducing a set of stochastic variables $d\xi_m^L$ (which follow Ito rules of stochastic calculus [12]) with mean values equal to zero and variances satisfying

$$\overline{d\xi_m^{L,(n)} d\xi_{m'}^{L,(n)}} = \delta_{mm'} \frac{dt}{2i\hbar}. \quad (31)$$

Here the (n) exponent stands for a specific realization of the stochastic process. In the following, it will sometimes be omitted to simplify notations. The evolution of $|\Psi_a\rangle$ associated to H can then be written as an average over stochastic evolutions in the Hilbert space of HFB state vectors:

$$e^{\frac{dt}{i\hbar} H} |\Psi_a\rangle = e^{\frac{dt}{i\hbar} \langle H \rangle} \overline{e^{\frac{dt}{i\hbar} h_L + \sum_m d\xi_m^L B_m^{ph}} |\Psi_a\rangle} \quad (32)$$

$$= \overline{|\Psi_a^{(n)}(t + dt)\rangle}. \quad (33)$$

In this equation, same conventions as in ref. [6, 13] are used and $|\Psi_a^{(n)}(t + dt)\rangle$ correspond to different vacuum states. Introducing the notation

$$dS_{ph}^L = \frac{dt}{i\hbar} h_L + \sum_m d\xi_m^L B_m^{ph}, \quad (34)$$

according to the Thouless theorem, each $|\Psi_a^{(n)}\rangle$ is a vacuum for the quasi-particle $a'_\alpha = e^{dS_{ph}^L} a_\alpha e^{-dS_{ph}^L}$.

One can finally note that the stochastic evolution of $|\Psi_a\rangle$ should be completed by an equivalent stochastic evolution for $\langle \Psi_b |$. The associated propagator and stochastic variables are respectively denoted by dS_{ph}^R and $d\xi_m^R$. These variables should be taken statistically independent of $d\xi_m^L$ to properly account for the exact dynamics of D . More explicitly, we have

$$dS_{ph}^R = -\frac{dt}{i\hbar} h_R + \sum_m d\xi_m^R B_m^{ph}, \quad (35)$$

where

$$B_m^{ph} = \frac{1}{2} (c \ c^+) \mathcal{R} \mathcal{B}_m^{ph} (1 - \mathcal{R}) \begin{pmatrix} c^+ \\ c \end{pmatrix}, \quad (36)$$

and $\overline{d\xi_m^R d\xi_{m'}^R} = -\delta_{mm'} \frac{dt}{i\hbar}$.

IV. NATURE OF THE STOCHASTIC PROCESS

Similarly to the previous case, where the residual interaction was neglected, we do expect that along each path, the stochastic evolution of the system reduces to the stochastic evolution of \mathcal{R} . The explicit form of the stochastic evolution of \mathcal{R} can now be obtained using the commutation relationship [9–11]:

$$\begin{aligned} [e^{dS_{pp}^L}, \mathbf{c}] &= e^{-(1-\mathcal{R})[\frac{dt}{i\hbar} \mathcal{H} + \mathcal{B}^L]} \mathcal{R} \mathbf{c} \\ &= \mathbf{c} - (1 - \mathcal{R}) \left[\frac{dt}{i\hbar} \mathcal{H} + \mathcal{B}^L \right] \mathcal{R} \mathbf{c}, \end{aligned} \quad (37)$$

while

$$\begin{aligned} [e^{dS_{pp}^R}, \mathbf{c}] &= e^{-\mathcal{R}[-\frac{dt}{i\hbar} \mathcal{H} + \mathcal{B}^R](1-\mathcal{R})} \mathbf{c} \\ &= \mathbf{c} - \mathcal{R} \left[-\frac{dt}{i\hbar} \mathcal{H} + \mathcal{B}^R \right] (1 - \mathcal{R}) \mathbf{c}, \end{aligned} \quad (38)$$

where \mathcal{B}^L and \mathcal{B}^R stand for

$$\mathcal{B}^{L/R} = \sum_m d\xi_m^{L/R} \mathcal{B}_m^{ph}. \quad (39)$$

Note that equations (37) and (38) are exact thanks to the $(1 - \mathcal{R})$ term. Similarly, as in previous section and using expression (37) and (38), one gets the stochastic evolution of \mathcal{R} :

$$d\mathcal{R} = \frac{dt}{i\hbar} [\mathcal{H}, \mathcal{R}] + (1 - \mathcal{R}) \mathcal{B}^L \mathcal{R} + \mathcal{R} \mathcal{B}^R (1 - \mathcal{R}). \quad (40)$$

Such a stochastic process, called hereafter Stochastic TD-HFB, is similar to the Stochastic mean-field dynamics [14] except that the mean-field and normal densities are now replaced respectively by the HFB Hamiltonian \mathcal{H} and density \mathcal{R} . Starting from $\mathcal{R} = \sum_\alpha |^a W_\alpha\rangle \langle ^b W_\alpha|$, evolution of \mathcal{R} can be replaced by the set of equations

$$\begin{cases} |d^a W_\alpha\rangle = \left\{ \frac{dt}{i\hbar} \mathcal{H} + (1 - \mathcal{R}) \mathcal{B}^L \right\} |^a W_\alpha\rangle \\ \langle d^b W_\alpha| = \langle ^b W_\alpha| \left\{ -\frac{dt}{i\hbar} \mathcal{H} + \mathcal{B}^R (1 - \mathcal{R}) \right\} \end{cases} \quad (41)$$

Above expressions show that if initially fulfilled, the property $\langle ^a W_\beta | ^b W_\alpha \rangle = \delta_{\alpha\beta}$ is true all along each stochastic path. Again, it can be shown that all the properties of the class of densities considered in section II are preserved during the stochastic evolution (40). Therefore, we only have to initiate the quantum jump process with a density which satisfies the properties described in section II. This is the case if we start from an initial HFB

density $D = |\Psi\rangle\langle\Psi|$, which is the most convenient in practice. Note finally that the explicit form of the quasi-particle evolution can directly be obtained from eq. (41) while the stochastic evolution of ρ and κ can be deduced from (40).

A. Alternative form and $pp - hh$ separable interaction

In the previous section, we have developed quantum diffusion processes between HFB states assuming expression (26). However, recent studies in nuclear structure [15] support separable interactions in the particle-particle and hole-hole channels. For completeness, we introduce a set of one-body operators G_m and assume that the residual interaction now reads

$$\langle\bar{\alpha}_a\bar{\beta}_a|v_{12}|\delta_b\gamma_b\rangle = -\sum_m\langle\bar{\alpha}_a|G_m|\bar{\beta}_b\rangle\langle\delta_a|G_m|\gamma_b\rangle^* \quad (42)$$

where G_m should be a skew matrix (i.e. $G_m^T = -G_m$) to respect the antisymmetrization of v_{12} . The formulation of the two-body problem can equivalently be done starting from eq. (42). The final result is that \mathcal{R} still obeys a stochastic equation with similar form as (40), where $\mathcal{B}^{L/R}$ now reads

$$\mathcal{B}^{L/R} = \sum_m d\eta_m^{L/R} \mathcal{B}_m^{pp} + i \left(d\eta_m^{L/R} \right)^* \mathcal{B}_m^{hh}, \quad (43)$$

and $d\eta_m$ corresponds to stochastic variables with mean value zero and

$$\overline{d\eta_m^L (d\eta_{m'}^L)^*} = \delta_{mm'} \frac{dt}{2\hbar}, \quad (44)$$

while all other second moments are equal to zero. \mathcal{B}_m^{pp} and \mathcal{B}_m^{hh} are given by

$$\mathcal{B}_m^{pp} = \begin{pmatrix} 0 & G_m \\ 0 & 0 \end{pmatrix}, \quad \mathcal{B}_m^{hh} = \begin{pmatrix} 0 & 0 \\ -G_m^* & 0 \end{pmatrix}. \quad (45)$$

V. CONCLUSIONS

In this work, we have shown that the exact dynamics of interacting fermions can be replaced by a Monte-Carlo method in the Hilbert space of Hartree-Fock Bogoliubov states. In order to prove this reformulation, we have used an intermediate result, considering densities $D = |\Psi_a\rangle\langle\Psi_b|$ with specific properties. Neglecting the residual interaction, the evolution of D leads to a TD-HFB equation for \mathcal{R} . We then have proven that the introduction of correlations beyond the mean-field picture can be replaced by a Stochastic TDHFB equation for \mathcal{R} , generalizing the stochastic mean-field approach [5]. It should be noted that the reformulation is not unique and the selection of a sub-class of D is not absolutely necessary. However, in that case derivations and stochastic equations are more complicated.

The stochastic theory presented here is not restricted to dynamical problem and could also be useful to study static properties of interacting systems [5]. In that case, real time propagation is replaced by imaginary time evolution. Monte-Carlo methods has the advantage of not requiring an a priori knowledge of the relevant collective degrees of freedom and can eventually be used as an alternative to GCM. It should however be noted that Monte-Carlo methods still require large numerical efforts. Work is actually in progress to combine advantages of GCM and Monte-Carlo techniques.

Finally, we would like to mention that the above theory gives an indirect proof of the fact that densities described in section II form an over-complete set of densities to treat the two-body problem. This might be of great interest even for non stochastic methods which treat correlations beyond mean-field.

ACKNOWLEDGMENTS

The author is grateful to Thomas Duguet and Vincent Rotival for the careful reading of the manuscript and to Olivier Juillet for discussions during this work.

-
- [1] P. Ring and P. Schuck, *The Nuclear Many-Body Problem*, Springer-Verlag, New-York (1980).
 - [2] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
 - [3] S.E.Koonin, D.J.Dean, K.Langanke, Ann.Rev.Nucl.Part.Sci. **47** (1997) 463.
 - [4] I. Carusotto, Y. Castin and J. Dalibard, Phys. Rev. A **63** (2001) 023606.
 - [5] O. Juillet and Ph. Chomaz, Phys. Rev. Lett. **88** (2002) 142503.
 - [6] D. Lacroix, Phys. Rev. **C71**, 064322 (2005).
 - [7] A. Montina and Y. Castin, Phys. Rev. **A73**, 013618 (2006).
 - [8] D. Lacroix, Phys. Rev. A **72**, 013805 (2005).
 - [9] J.P. Blaizot and G. Ripka, Quantum Theory of Finite Systems, (MIT Press, Cambridge, Massachusetts, 1986).
 - [10] C. Bloch, lecture notes on Nuclear Many-Body problem, Bombay, (1962)
 - [11] R. Balian and E. Brezin, Nuovo Cimento **B64**, 37 (1969).
 - [12] W. Gardiner, "Handbook of Stochastic Methods", Springer-Verlag, (1985).
 - [13] H.P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
 - [14] O. Juillet, *in preparation*.
 - [15] T. Duguet, Phys. Rev. C **69**, 054317 (2004).