Exact Stochastic Mean-Field Approach to the Fermionic Many-Body Problem

O. Juillet[1] and Ph. Chomaz[2]

[1]*LPC/ISMRA, Boulevard du Marechal Juin, F-14050 Caen Cedex, France*

[2]*Grand Accélérateur National d'Ions Lourds, BP 5027, F-14076 Caen Cedex 5, France*

(Received 19 July 2001; published 22 March 2002)

We investigate a reformulation of the dynamics of interacting fermion systems in terms of a stochastic extension of time-dependent Hartree-Fock equations. From a path-integral representation of the evolution operator, we show that the exact N-body state can be interpreted as a coherent average over Slater determinants evolving in a random mean-field. The imaginary time propagation is also presented and gives a similar scheme which converges to the exact ground state. In addition, the growth of statistical errors is examined to show the stability of this stochastic formulation.

DOI: 10.1103/PhysRevLett.88.142503 PACS numbers: 24.10.Cn, 05.40.Ca, 21.60.Jz, 24.60.Ky

Even with present-day computing facilities, the theoretical study of the structure and the dynamics of many-fermion systems, such as nuclei, atomic clusters, or quantum dots, remains a formidable task which requires approximations to step down to feasibility. In such a context, Hartree-Fock (HF) theory [1] is usually considered as the basic tool. The complex many-body problem is then reduced to an effective single-particle description in which the interaction is communicated through a common and self-consistent mean-field. In nuclear physics, static HF calculations provide a very good starting point to investigate many properties of the ground state [2]. The time-dependent model (TDHF) is also successful at low energy in heavy-ion reactions [2] and for the nonlinear electron dynamics in metal clusters [3]. Nevertheless, the HF description only treats in average the two-body interaction and various schemes have been developed to take into account correlation effects beyond the HF approximation [4–8].

The aim of this Letter is to present a new formulation of the many-fermion problem in terms of mean-field equations with a one-particle–one-hole ($1p$-$1h$) Gaussian white noise. The stochastic one-body process has an average identical to the exact solution and can be used for spectroscopic or dynamical studies as illustrated in exactly soluble models.

To begin, let us consider the building of correlations on a Slater state $|\Psi\rangle$ during a small time step Δt and under a general Hamiltonian $H = \sum_{ij} T_{ij} a_i^+ a_j - \frac{1}{4}\sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_k a_l$ containing a two-body interaction. Introducing the occupied states $|\alpha\rangle$ and the orthogonal particle orbitals $|\overline{\alpha}\rangle$, it follows immediately from the Schrödinger equation that

$$U(\Delta t)|\Psi\rangle = \left(1 + \frac{\Delta t}{i\hbar} H^{(0)}\right)|\Psi\rangle + \frac{\Delta t}{i\hbar} \sum_{\alpha_1 \overline{\alpha}_1} H^{(1)}_{\overline{\alpha}_1 \alpha_1} a^+_{\overline{\alpha}_1} a_{\hat{\alpha}_1} |\Psi\rangle + \frac{\Delta t}{i\hbar} \sum_{\alpha_1 \alpha_2 \overline{\alpha}_1 \overline{\alpha}_2} H^{(2)}_{\overline{\alpha}_1 \overline{\alpha}_2 \alpha_1 \alpha_2} a^+_{\overline{\alpha}_1} a^+_{\overline{\alpha}_2} a_{\hat{\alpha}_1} a_{\hat{\alpha}_2} |\Psi\rangle, \quad (1)$$

where $U(\Delta t)$ is the evolution operator and $|\hat{\alpha}\rangle$ the biorthogonal hole basis which satisfies $\langle \hat{\alpha}_1 | \alpha_2 \rangle = \delta_{\alpha_1 \alpha_2}$ to take into account a possible nonorthogonality of the occupied states $|\alpha\rangle$. In addition, the coefficients in the expansion (1) are given by

$$\begin{aligned} H^{(0)} &= \mathrm{tr}\left[\rho T + \frac{1}{2}\rho \overline{V}(\rho)\right], \\ H^{(1)}_{\overline{\alpha}_1 \alpha_1} &= \langle \overline{\alpha}_1 | T + \overline{V}(\rho) | \alpha_1 \rangle, \end{aligned} \quad (2a)$$

$$H^{(2)}_{\overline{\alpha}_1 \overline{\alpha}_2 \alpha_1 \alpha_2} = -\frac{1}{4}\sum_{ijkl} \langle \overline{\alpha}_1 | i \rangle \langle \overline{\alpha}_2 | j \rangle \times V_{ijkl} \langle k | \alpha_1 \rangle \langle l | \alpha_2 \rangle, \quad (2b)$$

where the notation tr corresponds to a trace over the one-body space. $\rho = \sum_\alpha |\alpha\rangle\langle\hat{\alpha}|$ is the one-body density and $\overline{V}(\rho)$ the Hartree-Fock mean-field potential with matrix elements $\langle i|\overline{V}(\rho)|j\rangle = \sum_{kl} V_{ikjl}\rho_{lk}$. Furthermore, given any two-body interaction, it is always possible in a finite dimensional one-body space to find Hermitian one-body operators O_s so that the $2p$-$2h$ amplitude (2b) is written as

$$H^{(2)}_{\overline{\alpha}_1 \overline{\alpha}_2 \alpha_1 \alpha_2} = \frac{1}{4}\sum_s \hbar\omega_s \langle \overline{\alpha}_1 | O_s | \alpha_1 \rangle \langle \overline{\alpha}_2 | O_s | \alpha_2 \rangle. \quad (3)$$

The evolution (1) of the Slater state $|\Psi\rangle$ to first order in the time step Δt becomes

$$U(\Delta t)|\Psi\rangle = \exp\left(\frac{\Delta t}{i\hbar} H^{(0)}\right) \exp\left(\frac{\Delta t}{i\hbar} \sum_{\alpha,\overline{\alpha}} H^{(1)}_{\overline{\alpha}\alpha} a^+_{\overline{\alpha}} a_{\hat{\alpha}}\right) \times \prod_s \exp\left[\frac{i\omega_s \Delta t}{4} (O_s^{(\mathrm{ph})})^2\right] |\Psi\rangle, \quad (4)$$

with $O_s^{(\mathrm{ph})} = \sum_{\alpha,\overline{\alpha}} \langle \overline{\alpha} | O_s | \alpha \rangle a^+_{\overline{\alpha}} a_{\hat{\alpha}}$. The dynamics can then be linearized with the help of a Hubbard-Stratonovitch transformation [9–11] allowing us to interpret each evolution under the square of a $1p$-$1h$ operator as an infinite superposition of one-body evolutions, each of them in a fluctuating auxiliary field σ distributed with a Gaussian

weight

$$\exp(ixO^2) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} d\sigma \, \exp(-\sigma^2/2) \times \exp[(1 + i\,\mathrm{sgn}(x))\sqrt{|x|}\,\sigma O], \quad (5)$$

where x is real and O is an operator. Defining the vector $\vec{\sigma}$ of all the auxiliary fields σ_s that are introduced by the path integral (5) to linearize the evolution (4), and introducing the shorthand notation $d\vec{\sigma}G(\vec{\sigma}) = \prod_s d\sigma_s(2\pi)^{-1/2} \times \exp(-\sigma_s^2/2)$, we finally obtain

$$U(\Delta t)\,|\Psi\rangle = \exp\left(\frac{\Delta t}{i\hbar} H^{(0)}\right) \int d\vec{\sigma}\, G(\vec{\sigma}) \times \exp\left(\sum_{\alpha,\overline{\alpha}} \Delta Z_{\overline{\alpha}\alpha}(\vec{\sigma}) a^+_{\overline{\alpha}} a_{\hat{\alpha}}\right) |\Psi\rangle, \quad (6)$$

where

$$\Delta Z_{\overline{\alpha}\alpha}(\vec{\sigma}) = \frac{\Delta t}{i\hbar} H^{(1)}_{\overline{\alpha}\alpha} + \sum_s a_s \sigma_s \sqrt{\Delta t}\,\langle\overline{\alpha}|O_s|\alpha\rangle, \qquad a_s = \frac{1 + i\,\mathrm{sgn}(\omega_s)}{2}\sqrt{|\omega_s|}. \quad (7)$$

According to Thouless's theorem [1], the evolution of the Slater determination $|\Psi\rangle$ under any of the fluctuating $1p$-$1h$ Hamiltonians (6) gives another Slater determinant. To first order in Δt, the correlated wave function (6) can thus be brought, with the help of (2a) and (2b), to the form

$$U(\Delta t)\,|\Psi\rangle = \int d\vec{\sigma}\, G(\vec{\sigma}) \prod_\alpha a^+_{\alpha+\Delta\alpha(\vec{\sigma})}|\,\rangle, \quad (8)$$

with the following variation of the hole states:

$$|\Delta\alpha(\vec{\sigma})\rangle = \frac{1}{i\hbar}\left[T + \overline{V}(\rho) - \frac{1}{2}\rho\overline{V}(\rho)\right]|\alpha\rangle\Delta t + \sum_s a_s\sigma_s\sqrt{\Delta t}\,(1-\rho)O_s|\alpha\rangle. \quad (9)$$

In the end, the full dynamics of an uncorrelated state $|\Psi\rangle$, during a small time step Δt under a one- and two-body Hamiltonian, can be represented as the coherent average of Slater determinants that have evolved with a mean-field Hamiltonian $h_{\mathrm{mf}} = T + \overline{V}(\rho) - \frac{1}{2}\rho\overline{V}(\rho)$ supplemented with a $1p$-$1h$ noise $\eta(\vec{\sigma}) = \sum_s a_s\sigma_s\sqrt{\Delta t}\,(1-\rho)O_s$. This fluctuating potential is non-Hermitian and depends linearly on external number fields, each distributed with a unit Gaussian weight. We also emphasize that the deterministic part differs from the standard Hartree-Fock approach by including the term $-\frac{1}{2}\rho\overline{V}(\rho)$, which in fact arises naturally to take into account the difference between the total mean-field energy and the sum of the HF eigenvalues [2]. The formulation (8),(9) of the dynamics can be extended to many time steps and then corresponds to the discretized realization of a Markovian Langevin equation in the one-body Hilbert space [12]. In consequence, going to the continuous limit $\Delta t \to 0$, and denoting by $E(\cdots)$ the expectation of a random functional, we can state that

$$U(t)\,|\Psi\rangle = E\left(\prod_\alpha a^+_{\alpha(t)}|\,\rangle\right), \quad (10)$$

where the evolution of the hole states $|\alpha(t)\rangle$ is determined by the following Itô stochastic differential equation with the initial condition $|\alpha(0)\rangle = |\alpha\rangle$:

$$d|\alpha\rangle = \frac{1}{i\hbar}\left[T + \overline{V}(\rho) - \frac{1}{2}\rho\overline{V}(\rho)\right]|\alpha\rangle\,dt + \sum_s a_s(1-\rho)O_s|\alpha\rangle\,dW_s, \quad (11)$$

where W_s refers to independent real Wiener processes with vanishing ensemble averages and that obey to the Itô stochastic calculus [12]

$$E(dW_s(t)) = 0, \qquad dW_{s_1}(t)\,dW_{s_2}(t) = dt\,\delta_{s_1 s_2}. \quad (12)$$

It is also important to specify that such a formulation provides a reinterpretation of the exact evolution of the N-body density operator $D(t)$ in terms of a mean over dyadics in which the bra and the ket are different Slater determinants $|\Psi(t)\rangle = \prod_\alpha a^+_{\alpha(t)}|\,\rangle$, $|\Psi'(t)\rangle = \prod_{\alpha'} a^+_{\alpha'(t)}|\,\rangle$ with $|\alpha(t)\rangle$ and $|\alpha'(t)\rangle$ evolving independently under the stochastic Hartree-Fock equation (11):

$$D(t) = E(|\Psi(t)\rangle\langle\Psi'(t)|). \quad (13)$$

The necessary use of pairs of stochastic uncorrelated wave functions to reconstruct the exact full density operator constitutes the originality of our approach in comparison with previous schemes [8] where a quantum incoherent propagation of states was assumed. By a totally different way and for fermion systems, we end up with a representation of the N-body density matrix analogous to those assumed in Ref. [13] for the dynamics of Bose-Einstein condensates. Furthermore, our path-integral point of view provides a derivation of the stochastic term to be included in the mean-field dynamics.

Finally, the stochastic mean-field interpretation (10),(11) of the evolution process can be extended to imaginary time to obtain the following representation of the Boltzmann operator when it acts on a Slater determinant $|\Psi\rangle = \prod_\alpha a^+_\alpha|\,\rangle$:

$$\exp(-\beta H)\,|\Psi\rangle = E\left(\prod_\alpha a^+_{\alpha(\beta)}|\,\rangle\right), \quad (14)$$

with $|\alpha(0)\rangle = |\alpha\rangle$ and

$$d|\alpha\rangle = \left[T + \overline{V}(\rho) - \frac{1}{2}\rho\overline{V}(\rho)\right]|\alpha\rangle d\beta + \sum_s a_s(1-\rho)O_s|\alpha\rangle\,dW_s, \quad (15)$$

$$a_s = \sqrt{\frac{\hbar|\omega_s|}{2}}\begin{cases} 1, & \omega_s > 0, \\ i, & \omega_s < 0. \end{cases}$$

The correlated many-body ground state can then be obtained in the limit of large β where $\exp(-\beta H)$ behaves like a projector eliminating all the overlaps with excited eigenstates. For example, realistic nuclear structure

problems could be studied with the scheme (14),(15) in the context of the quantum Monte Carlo diagonalization method [5]. Using the closure relation over Slater determinants, the representation (14),(15) also allows one to reconstruct the Boltzmann operator by a similar method as those recently proposed for Bose-Einstein condensates [14]. Finally, the time-dependent stochastic Hartree-Fock equations (10),(11), provide the theoretical basis of equivalent Monte Carlo methods for dynamical problems.

We now examine statistical errors in the stochastic scheme (10),(11). This can be achieved by calculating the average of the norm of the deviation between the exact evolution and a stochastic realization. Using Eq. (10), we are thus interested in the indicator:

$$\chi(t) = E(\langle \Psi(t) \,|\, \Psi(t) \rangle) - 1 \text{ with } |\Psi(t)\rangle = \prod_{\alpha} a^{+}_{\alpha(t)} |\,\rangle . \tag{16}$$

Furthermore $\langle \Psi(t) \,|\, \Psi(t) \rangle$ is the determinant of the overlap matrix $g_{\alpha_1\alpha_2}(t) = \langle \alpha_1(t) \,|\, \alpha_2(t) \rangle$ associated to the Fermi sea of $|\Psi(t)\rangle$. But, with the help of Itô's differentiation rules [12], $g_{\alpha_1\alpha_2}$ evolves according to

$$dg_{\alpha_1\alpha_2}(t) = \frac{dt}{2} \sum_s |\omega_s| \langle \alpha_1(t)| O_s (1 - \rho(t)) O_s |\alpha_2(t)\rangle . \tag{17}$$

In consequence the variation of χ during an infinitesimal time dt is given by

$$\begin{aligned} d\chi(t) &= E[\langle \Psi(t) \,|\, \Psi(t) \rangle \operatorname{tr}(dg(t) g^{-1}(t))] \\ &= \frac{dt}{2} E\left(\langle \Psi(t) \,|\, \Psi(t) \rangle \sum_s |\omega_s| \sigma_s^2(t) \right), \end{aligned} \tag{18}$$

where $\sigma_s(t)$ refers to the quantal fluctuations of the one-body operators O_s in the uncorrelated stochastic wave function $|\Psi(t)\rangle$. Such a result then implies that the approach will never explode in a finite dimensional one-body space: in this case, a trivial upper bound for the variance $\sigma_s^2(t)$ is in fact given by the square of the largest eigenvalue λ_s of the one-body observable O_s in the N-body space and thus, after time integration,

$$\chi(t) \leq \exp\left(\frac{t}{2} \sum_s |\omega_s| \lambda_s^2 \right). \tag{19}$$

As a first step towards the use of the previous stochastic formulation in practical problems, we investigate some numerical implementations in exactly soluble models. More precisely, we consider a system of Ω fermions distributed among a number n of energy orbitals $i = 0, \ldots, n-1$, each of which is Ω degenerate. In addition, the Hamiltonian of the system is expanded onto the bilinear operators $G_{ij} = \sum_{\omega=1}^{\Omega} a^{+}_{i\omega} a_{j\omega}$ which generates a $U(n)$ Lie algebra. This nontrivial model corresponds to a generalization of the Lipkin-Meshkov-Glick model [15] which is often used to check the validity of approximate many-body techniques. We first focus on the three-level model with the usual Hamiltonian:

$$H = \sum_{i=0}^{2} \varepsilon_i G_{ii} - \frac{1}{2} V \sum_{\substack{i,j=0 \\ i \neq j}}^{2} G_{ij}^2 . \tag{20}$$

In addition we choose equidistant levels ($\varepsilon_0 = 0$, $\varepsilon_1 = \varepsilon$, $\varepsilon_2 = 2\varepsilon$) and set $\eta = \Omega V/\varepsilon = 2$ where the mean-field dynamics is a mixture of integrable and chaotic trajectories [16]. Figure 1 presents the evolution of $\Omega = 10$ fermions equally shared among the three levels in a Slater determinant at the initial time. 5×10^7 simulations trajectories have been performed. We have shown only the mean number of particles in the ground orbital but other observables have also been considered: In all cases, the expectation values obtained in the stochastic mean-field scheme are in agreement with the exact dynamics within the error bars. Let us now test the description of the ground state. The implementation of the propagation in imaginary time (14),(15) has been realized in the model (20) where the ground state and Hartree-Fock energies are, respectively, $E_o = -1.6836$ and $E_{\mathrm{HF}} = -1.25$ in units of ε. By an average over many simulations, the mean energy $\overline{E}(\beta)$ calculated with the stochastic one-body scheme rapidly converges to the exact binding energy E_o: For $\beta\varepsilon = 2$ and 10^6 realizations we have found $\overline{E}(\beta) = -1.6876 \pm 0.0078$ in perfect agreement with the exact ground state. We have also checked the method for a more correlated system ($\Omega = 3$, $\varepsilon = V = 1$): In this case, $E_o = -1.7016$, $E_{\mathrm{HF}} = -1$, and we obtain $\overline{E}(\beta) = -1.705\,01 \pm 0.009\,39$ at $\beta = 1.5$ and after 10^6 simulations. Finally, to study the dynamics of an initial correlated state, a coupling between the stochastic evolutions in real and imaginary time is investigated in the

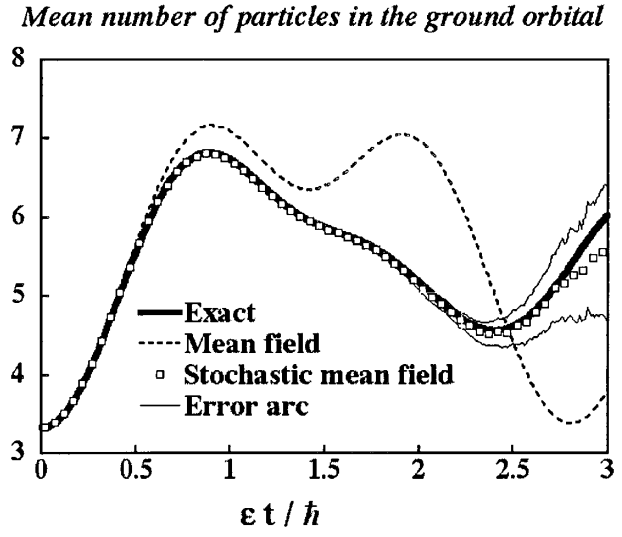

FIG. 1. Implementation of the stochastic Hartree-Fock scheme in the three-level Lipkin model for $\Omega = 10$ fermions with $\eta = \Omega V/\varepsilon = 2$. The stochastic mean-field dynamics is compared to the exact and Hartree-Fock evolution. We have considered 5×10^7 simulations for the initial Slater determinant $|\Psi\rangle = \prod_{\omega=1}^{\Omega} \frac{a^{+}_{0,\omega} + a^{+}_{1,\omega} + a^{+}_{2,\omega}}{\sqrt{3}} |\,\rangle$.

two-level Lipkin model. The Hamiltonian $H = \varepsilon J_z + VJ_x^2$ is expressed in terms of the quasispin algebra $J_x = (G_{10} + G_{01})/2$, $J_y = (G_{10} - G_{01})/2i$, and $J_z = (G_{11} - G_{00})/2$. The system is supposed to be in its ground state at time $t = 0$ when we suddenly change the sign of the two-body interaction. The results are shown in Fig. 2: An average over a large set of stochastic one-body simulations allows one to reconstruct the exact many-body solution with, however, larger statistical error bars than in the previous calculations due to the addition of the errors coming from the imaginary time evolution to the one introduced by the subsequent real time dynamics. It should be noticed that not only one-body observables are correctly predicted, but also two and three and in fact many-body quantities as shown in the lower part of the figure.

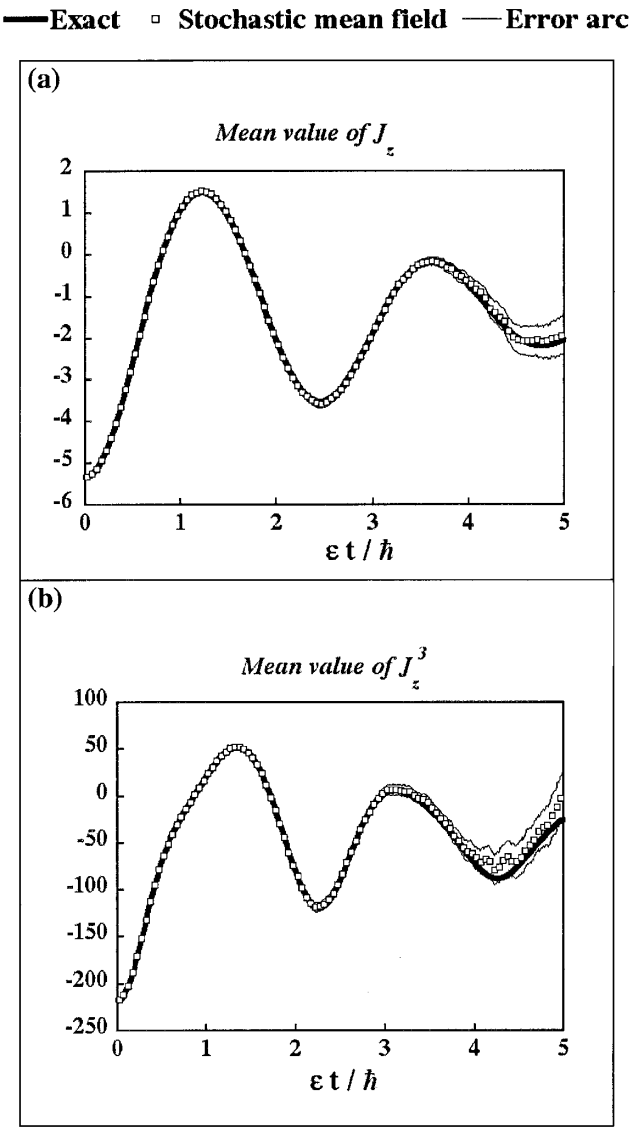

FIG. 2. Dynamics of an initial correlated wave function in the two-level Lipkin model for $\Omega = 20$ fermions. For $t < 0$, we suppose $\varepsilon = 1$, $V = -0.1$, and reconstruct the ground state using (15) until $\beta = 5$ and with the wave function $\prod_{\omega=1}^{\Omega} a_{1,\omega}^{+} | \rangle$ as a starting point. At time $t = 0^+$, the interaction is suddenly changed to $V = 0.1$ and we then apply the one-body evolution scheme (11) on each stochastic Slater determinant obtained with the propagation in imaginary time. An average over 10^8 of such simulations is compared to the exact dynamics of the one- and three-body observables J_z [part (a)], J_z^3 [part (b)]. Similar results have been obtained for the two-body operator J_z^2.

In conclusion, we have presented a new theoretical method to solve exactly the N-body Schrödinger equation for a fermionic system with binary interactions. In particular, we have shown that the full dynamics of an uncorrelated state can be formulated in terms of the coherent average of Slater determinants that have evolved following a stochastic Hartree-Fock equation. The noise comes from the linearization of the $2p$-$2h$ residual interaction through a Hubbard-Stratonovitch transformation. A similar stochastic one-body interpretation has been proposed for the Boltzmann operator and statistical errors have been investigated to show the stability of the scheme. Finally, by coupling an imaginary and a real-time fluctuating mean-field propagation, the exact dynamics of a correlated wave function can be reached. The numerical implementation in exactly soluble models has confirmed the formal results: In all the cases we have studied, the stochastic Hartree-Fock method when averaged over many simulations gives the correct result with a reasonable statistical spread. First applications to a realistic problem are under development.

O. J. acknowledges financial support from "Société de secours des amis des sciences." Discussions with D. Lacroix, P. Van Isacker, and F. Gulminelli on various aspects of this work are gratefully acknowledged.

[1] J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, Massachusetts, 1986).
[2] J. W. Negele, Rev. Mod. Phys. **54**, 913 (1982).
[3] F. Calvayrac, P.-G. Reinhard, E. Suraud, and C. A. Ullrich, Phys. Rep. **337**, 493 (2000).
[4] S. E. Koonin, D. J. Dean, and K. Langanke, Ann. Rev. Nucl. Part. Sci. **47**, 463 (1997).
[5] T. Otsuka, T. Mizusaki, and M. Honma, J. Phys. G **25**, 699 (1999).
[6] W. Cassing and U. Mosel, Prog. Part. Nucl. Phys. **25**, 235 (1990).
[7] D. Lacroix, P. Chomaz, and S. Ayik, Nucl. Phys. **A651**, 369 (1999).
[8] Y. Abe, S. Ayik, P.-G. Reinhard, and E. Suraud, Phys. Rep. **275**, 49 (1996).
[9] J. Hubbard, Phys. Lett. **3**, 77 (1959).
[10] R. D. Stratonovitch, Sov. Phys. Kokl. **2**, 416 (1958).
[11] A. K. Kerman, S. Levit, and T. Troudet, Ann. Phys. (N.Y.) **148**, 436 (1983).
[12] C. W. Gardiner, *Handbook of Stochastic Methods* (Springer-Verlag, Berlin, 1983).
[13] I. Carusotto, Y. Castin, and J. Dalibard, Phys. Rev. A **63**, 023606 (2001).
[14] I. Carusotto and Y. Castin, J. Phys. B **34**, 4589 (2001).
[15] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965).
[16] D. C. Meredith, S. E. Koonin, and M. R. Zirnbauer, Phys. Rev. A **37**, 3499 (1988).