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Nuclear pairing correlations by a quantum Monte Carlo method

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Abstract

A quantum Monte Carlo approach is applied to the treatment of the pairing force in nuclear systems. The method makes possible the calculation of the pairing energy and the pair occupation probabilities for the ground state. It is computationally efficient, and also very simple to implement. The reliability of the method is checked with the use of two exactly solvable schematic shell models. The computed pairing energy is also compared with the predictions of several approximation methods of common use. Numerical results for some nuclei with a realistic interaction are also provided.

IPNO/TH 92-103 December 1992

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1. Introduction

A number of nuclear features such as the gap in the excitation spectrum of even-even nuclei, moments of inertia, and even-odd mass differences have been interpreted as the consequence of correlations between the nucleons in the nucleus, and are traditionally described by the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [1]. Because of its simplicity, BCS has been widely used as a first step in nuclear structure calculations involving pairing forces, and it is quite satisfactory when the number of valence nucleons is large and the pairing strength is large compared to the level spacing. However, when this is not the case, it suffers from two inherent drawbacks:

i) It introduces a non-negligible error in the pairing energy caused by the particle number fluctuation (the BCS wave function is not an eigenstate of the number operator).

ii) In some cases, there may be a critical value of the pairing force below which the BCS equations have no non-trivial solution. However, exact calculations show that this kind of phase transition is spurious.

Many attempts have been made in the past to improve the BCS method by projecting out that component of the BCS wave function which corresponds to the right number of particles (e.g. the work of Kerman, Lawson, and Macfarlane [2], or that of Unna and Weneser [3]). Also, other methods were developed in order to eliminate the effects of the number fluctuation such as the Lipkin-Nogami method [4, 5], and the Kamlah method [6]. A review of these questions can be found in ref. [7].

The exact solution of this problem is only available for some very simple systems, such as a single-level or a two-level model (see e.g. [7]). Richardson and Sherman [8] have also developed a method for determining the exact eigenstates and eigenvalues of the pairing force Hamiltonian when the pairing strength G is constant. It is based on the idea of reformulating the problem into a many-boson system with a N-body interaction (which includes the effect of the Pauli principle). They applied the method to various problems such as the case of a single- or a double-level model, or a system of N particles in N equispaced doubly-degenerate levels. However, no exact method is available for the case of a general pairing interaction (G not constant).

In a previous paper [9], we proposed to apply a Monte Carlo technique to the treatment of the pairing force in nuclei. The quantum Monte Carlo method has been used to study a variety of problems in condensed matter, nuclear and high-energy physics. It has proven to be a powerful tool for investigating the properties of quantum systems with many degrees of freedom (see [10] or [11] for a review). It has been applied to liquid helium [12, 13, 14], molecules [15], the electron gas [16], nuclear systems [17, 18, 19, 20, 21, 22], and lattice gauge theories [23, 24, 25, 26, 27]. Thus it seems natural to resort to a Monte Carlo technique for studying the pairing-force Hamiltonian in nuclei. Our method makes possible an *exact* calculation of the pairing energies and pair occupation probabilities, at least in principle. It was restricted in ref. [9] to the case of a pure pairing force of constant strength. In this paper, we generalize this Monte Carlo method to G not constant, and show that it is computationally efficient for

treating realistic cases.

Let us consider for the moment the case of a system of N particles with a pairing force of constant strength G. It is instructive to consider the two limiting cases of a strong and a weak coupling strength:

i) If $G \gg d$, where d represents the characteristic spacing between the single-particle levels, the solution tends to that of the seniority scheme (see [7]) for a single-level system (when all the states are degenerate). The pairing Hamiltonian of the seniority scheme has the form

$$H_{pair} = -G \sum_{m,m'>0}^{\Omega} a^{\dagger}_{m'} a^{\dagger}_{-m'} a_{-m} a_{m} \ , \tag{1}$$

where $\Omega = j + 1/2$ (j being the spin of the level) is the total number of conjugate state pairs $(m, -m)$. The exact energy eigenvalues of this Hamiltonian are given by

$$E = -\frac{G}{4}(N - s)(2\Omega + 2 - N - s) \ , \tag{2}$$

where s stands for the seniority quantum number. Thus the pairing energy of the ground state ($s = 0$) is given by

$$E_{sen} = n(\Omega - n + 1)G \ , \tag{3}$$

where $n = N/2$ stands for the number of pairs. This expression, derived from group theory calculations, can also be obtained with the help of an elementary method, as noted in ref. [28]. Let us take one of the many configurations C which contribute to the ground state wave function of the pairing Hamiltonian H_{pair}, and count how many times the single configuration is repeated by the action of H_{pair}. The resulting repetition factor (which we call ω), multiplied by the strength G of the pairing interaction, yields exactly the pairing energy. This property is evident, since all the configurations C play the same role in the ground state. It is clear that the pairing Hamiltonian H_{pair} annihilates a pair of particles (n possibilities) and creates a pair either on the same place (one possibility) or on an available orbit ($\Omega - n$ possibilities). Thus, the number of different annihilation-creation actions, i.e., $\omega = n(\Omega - n + 1)$, multiplied by G is just the pairing energy (see equation 3) as expected.

ii) On the contrary, when $G \ll d$ (weak coupling limit), the ground state will tend asymptotically to the unperturbed one-body Hamiltonian ground state (i.e., with $G = 0$). It is obvious that the pairing energy in this case is simply given by

$$E_P = nG + \mathcal{O}(G^2) \ . \tag{4}$$

This result follows straightforwardly from the BCS solution with $\Delta = 0$ (i.e., the trivial solution). It can also been interpreted in terms of pair diffusion. Indeed, only virtual diffusions (i.e., when a pair is annihilated and created on the same state) can exist in this case, since real diffusions produce configurations which do not belong to the (asymptotic) ground state. Thus, the number of possible pair diffusions is clearly equal to n.

For a general case between these two extremes, it seems quite natural to look for a way to count all the possible pair diffusions, taking into account the fact that the diffusions associated with a large increase of the one-body energy are more hindered than others. The resulting pairing energy should lie somewhere between nG and ωG. This idea is at the basis of the method we propose in this paper. Moreover, as the number of diffusions for all the possible configurations is generally huge, a Monte Carlo approach is clearly appropriate to solve this problem. In fact, it can be considered as a procedure to *exactly* determine the lowest eigenvalue (and the corresponding eigenstate) of the pairing Hamiltonian, which could not be done with other methods since the dimension of the model space is huge in general.

Finally, it is interesting to note that, as the pairing force is traditionally interpreted in terms of pair diffusion, our method simply consists in simulating this diffusion in order to measure interesting quantities rather than calculating them directly. In particular, the pair occupation probabilities (the v_k^2 in BCS theory) are related to actual probabilities in the Monte Carlo process.

In Section 2, we introduce our Monte Carlo method. Section 2.1 is devoted to the case of a constant G, whereas Section 2.2 treats a general pairing interaction. In Section 2.3, we expose the Monte Carlo estimators for the pairing energy and the pair occupation probabilities. Then, we introduce a symmetrized form for the breakup of the evolution operator in Section 2.4. In Section 3, we present the implementation and the results of the method. The exactly solvable cases of a two-level model and of a system of equidistant levels are considered in Section 3.1 and 3.2 respectively, in order to check the reliability of the method. In Section 3.3, we apply the method to some nuclei with a realistic interaction. Finally, we conclude in Section 4. Statistical and systematic errors originating from the method are discussed in Appendix A.

2. The Monte Carlo method

2.1 PAIRING FORCE OF CONSTANT STRENGTH

For simplicity, we consider first the case of a many-body system with a pure pairing force of constant strength G (> 0). It is described by the Hamiltonian

$$H = \sum_{k>0}^{\Omega} \epsilon_k (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - G \sum_{k,k'>0}^{\Omega} a_{k'}^\dagger a_{\bar{k}'}^\dagger a_{\bar{k}} a_k \ , \tag{5}$$

where k and $\bar{k}$ are time-reversed conjugate states with energy ϵ_k. The indices k, k' run from 1 to Ω, where Ω is the total number of conjugate orbit pairs. Our purpose is to calculate the exact N-particles ground state energy of H by use of a Monte Carlo procedure. This method does not assume a particular functional form for the ground state wave function (such as the BCS ansatz), and is thus exact, at least in principle.

We work in a Fock space where the pair configurations denoted by $|C>$ constitute a basis, since one can assume that all particles are paired without loss of generality. We define

$$|C> = |\{n_k\}> \quad \text{with} \quad \sum_{k=1}^{\Omega} n_k = n \ , \quad n_k = 0 \text{ or } 1 \ , \tag{6}$$

where n_k are the pair occupation numbers and $n = \frac{\Omega}{2}$ is the number of pairs in the Ω conjugate orbit pairs $(k, \bar{k})$. The dimension of our basis is $\binom{\Omega}{n}$, which rapidly becomes very large for a reasonable model space. The ground state $|\Psi_0>$ of H can be expressed in this basis $\{|C>\}$ as

$$|\Psi_0> = \sum_C \alpha_C |C> , \tag{7}$$

where the coefficients α_C are to be calculated to obtain the ground state energy E_0 or other observables. This summation is impracticable as it involves a huge number of terms for usual model spaces, and an approximation is generally needed. However, we show that a Monte Carlo sampling procedure allows to estimate this sum by a partial exploration of the $|C>$ space, without need for a complete enumeration of the whole set of configurations $\{|C>\}$. Moreover, as the configurations $|C>$ contain the correct number of pairs n, the resulting ground state $|\Psi_0>$ will also have exactly n pairs. This is a great advantage compared to the BCS formalism (without projection) where the number of pairs is fixed only on average, which is a well known source of errors [2].

It is easy to show that the coefficients α_C must be positive if $|\Psi_0>$ corresponds to the ground state of H. Let us apply the Hamiltonian to a given configuration $|C>$,

$$H|C> = E_C^{1-b}|C> - G \sum_{C'} |C'> , \tag{8}$$

where $E_C^{1-b} = \sum_{k=1}^{\Omega} 2\ n_k(C)\ \epsilon_k$ denotes the one-body energy of the configuration, and the summation, corresponding to the two-body part of H, runs over all the configurations $|C'>$ obtained from $|C>$ by moving one pair. As explained above, there are $\omega = n(\Omega - n + 1)$ such terms, corresponding to all the possible pair diffusions. Note that $n(\Omega - n)$ of these terms describe real diffusions (with $k \neq k'$), whereas the n remaining terms count the virtual diffusions associated to the diagonal terms ($k = k'$) of the double summation in H. Thus, separating the one-body and two-body parts, the matrix elements of H are clearly given by

$$\begin{aligned} < C'|H^{1-b}|C> &= \begin{cases} E_C^{1-b} & \text{if } C = C' , \\ 0 & \text{otherwise,} \end{cases} \\ < C'|H^{2-b}|C> &= \begin{cases} -G & \text{if } C \text{ and } C' \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases} \end{aligned} \tag{9}$$

where we consider C and C' as connected configurations if they differ at most by the position of one pair. Now, it appears clearly that the α_C are positive, by calculating

$$\begin{aligned} E_0 &= < \Psi_0|H|\Psi_0> / < \Psi_0|\Psi_0> \\ &= \left[\sum_C \sum_{C'} \alpha^*_{C'} \alpha_C \ < C'|H|C>\right] \Big/ \left[\sum_C |\alpha_C|^2\right] \\ &= \left[\sum_C |\alpha_C|^2\ E_C^{1-b} \ - G \sum_{\text{connected } C,C'} \alpha^*_{C'} \alpha_C\right] \Big/ \left[\sum_C |\alpha_C|^2\right] . \end{aligned} \tag{10}$$

We may arbitrarily define the α_C as real, and we see easily that changing α_C to $|\alpha_C|$ can only decrease the energy E_0, since $G > 0$. Thus the ground state $|\Psi_0>$ must have its components $\alpha_C \geq 0$, and a Monte Carlo procedure may be applied wherein each α_C is associated to the sampling probability of the configuration $|C>$. Note that, according to this probability interpretation, we impose here the normalization condition $\sum_C \alpha_C = 1$, slightly different from the standard condition $\sum_C |\alpha_C|^2 = 1$. So, the probabilities appearing in the Monte Carlo process are not the physical probabilities $|\alpha_C|^2$, and this fact will be important when computing the pair occupation probabilities.

In order to calculate the ground state properties of our Hamiltonian (see 5), we use a random walk algorithm based on the imaginary-time method (see [27] for a review). One applies the imaginary time evolution operator $e^{-t(H-E)}$ to filter the ground state $|\Psi_0>$ from an arbitrary initial state $|\Phi>$, that is

$$\begin{aligned} |\Psi_0> &= \lim_{t\to\infty} e^{-t(H-E)}|\Phi> \\ &= \lim_{\substack{\Delta t\to 0 \\ N\Delta t\to\infty}} \prod_{s=1}^{N} e^{-\Delta t(H-E)}\ |\Phi> , \end{aligned} \tag{11}$$

where E is a normalization energy which is adjusted along the random walk in order to keep the norm approximately constant during the time evolution of $|\Psi(t)>$. By inserting complete sets of configurations $|C>$ between the infinitesimal evolution operators, the product becomes

$$\begin{aligned} e^{-t(H-E)}|\Phi> = \sum_{C_N}\cdots\sum_{C_0} |C_N><C_N|e^{-\Delta t(H-E)}|C_{N-1}> \\ \cdots <C_2|e^{-\Delta t(H-E)}|C_1><C_1|e^{-\Delta t(H-E)}|C_0><C_0|\Phi> , \end{aligned} \tag{12}$$

yielding a multiple summation representation for $|\Psi_0>$. This allows one to express the expectation value of any observable as a multiple integral (in fact a summation in our discrete configuration space) which is then calculated stochastically using a random walk algorithm. This procedure is the classical Path Integral Monte Carlo method [27].

The essential problem in our case is the difficulty of handling the infinitesimal evolution operator $e^{-\Delta t(H-E)}$ in configuration space. Indeed, applying $e^{-\Delta t\ H}$ to a given configuration $|C>$ obviously gives

$$e^{-\Delta t\, H}|C> = |C> - \Delta t\ H|C> + \frac{\Delta t^2}{2!}H^2|C> + \cdots , \tag{13}$$

where the second term in the r.h.s. contains configurations connected by 1 step (1 pair is moved), the third term contains configurations connected by 2 steps, etc..., finally yielding the whole set of $\binom{\Omega}{n}$ configurations. It is possible to consider only the 1st-order term in Δt of the expansion, just keeping the one-step diffusions; this is a good approximation if $\Delta t \cdot E_{max} \ll 1$. This constraint on Δt depends on the energy E_{max} of the most excited state, not on the solution $|\Psi_0>$, and makes thus the method impracticable.

We propose a solution of this problem by doing a breakup of H which provides a simple stochastical evaluation of the matrix elements $< C'|e^{-t(H-E)}|C >$, in analogy with what is done in ref. [29] and [30]. We write the Hamiltonian in the form $H = H^{1-b} + H^{2-b}$ and use the common breakup

$$e^{-\Delta t\ H} \simeq e^{-\Delta t\ H^{1-b}} \cdot e^{-\Delta t\ H^{2-b}} + \mathcal{O}(\Delta t^2)\ , \tag{14}$$

which is an approximation since H^{1-b} and H^{2-b} do not commute. However, the method is asymptotically exact since the commutator $[\Delta t\ H^{1-b}, \Delta t\ H^{2-b}]$ tends to 0 like Δt^2. The advantage of this breakup is that the matrix elements of $e^{-\Delta t\ H^{1-b}}$ and $e^{-\Delta t\ H^{2-b}}$ can be *exactly* evaluated separately (without truncating the expansion of the exponential). We will present in Section 2.4 a symmetrized form of this breakup which leads to a gain in accuracy of one more order in Δt.

For the time evolution operator associated with the one-body part H^{1-b}, we have obviously

$$e^{-\Delta t\ H^{1-b}}|C >= e^{-\Delta t\ E_C^{1-b}}|C >\ , \tag{15}$$

so that evolving $|C >$ comes to multiply by a factor depending on E_C^{1-b}. For the two-body part, we have

$$\begin{aligned} e^{-\Delta t\ H^{2-b}}|C >= |C > &+ G\Delta t \sum_{k,k'>0} a^\dagger_{k'} a^\dagger_{\bar{k}'} a_{\bar{k}} a_k |C > \\ &+ \frac{(G\Delta t)^2}{2!} \sum_{k,k',k'',k'''>0} a^\dagger_{k'''} a^\dagger_{\bar{k}'''} a_{\bar{k}''} a_{k''} a^\dagger_{k'} a^\dagger_{\bar{k}'} a_{\bar{k}} a_k |C > + \cdots , \end{aligned} \tag{16}$$

where the successive terms in the r.h.s. correspond to the contributions of 0-, 1-, 2-steps diffusions, etc... The matrix elements $< C'|e^{-\Delta t\ H^{2-b}}|C >$ cannot be obtained directly, but will be generated by a stochastic process going from $|C >$ to the destination configuration $|C' >$, such that the probability $P(C', C)$ of going from $|C >$ to $|C' >$ is proportional to $< C'| \cdot |C >$. We write

$$< C'|e^{-\Delta t\ H^{2-b}}|C >= \mathcal{N}(C)\ P(C', C)\ , \tag{17}$$

where $\mathcal{N}(C)$ is a normalization factor, and is a function of the configuration $|C >$ in general, and $P(C', C)$ is a probability distribution in $|C' >$.

In order to calculate this normalization factor, let us re-express equation (16) as

$$e^{-\Delta t\ H^{2-b}}|C >= \sum_{L=0}^{\infty} \sum_{\lambda=1}^{\omega^L} \frac{(G\Delta t)^L}{L!}\ |C_L^\lambda >\ , \tag{18}$$

where $|C_L^\lambda >$ represents the set of configurations reachable after a L-step diffusion. Of course, $|C_0^1 >= |C >$ for a 0-step diffusion. There are $\omega = n(\Omega - n + 1)$ possible destinations for a one-step diffusion (including virtual diffusions), so there are obviously ω^L destinations (not necessary distinct) for a L-step diffusion. Thus, one gets

$$\mathcal{N}(C) \ = \ \sum_{C'} < C'|e^{-\Delta t\ H^{2-b}}|C >$$

$$
\begin{aligned}
&= \sum_{L=0}^{\infty} \sum_{\lambda=1}^{\omega^L} \frac{(G\Delta t)^L}{L!} \\
&= \exp(\nu) \ , \qquad (19)
\end{aligned}
$$

where we define $\nu = \omega\ G\ \Delta t$. Note that $\mathcal{N}(C)$ is independent of $|C>$ for a constant strength pairing force, but this will not be the case for a general interaction $G_{i,j}$ (see Section 2.2). Thus, it appears that the probability distribution of the number of steps L (between $|C>$ and $|C'>$) is a Poisson distribution of parameter ν,

$$
\mathcal{P}(L) = \frac{\nu^L \exp(-\nu)}{L!} \qquad \text{where} \quad \nu = E_{sen}\ \Delta t\ . \qquad (20)
$$

The parameter ν simply represents the average number of steps per time interval Δt, and can also be written using the expression (3) of the energy in the seniority scheme (i.e., $E_{sen} = \omega\ G$).

Defining the probability of going from $|C>$ to $|C'>$ as $P(C',C) =< C'| \cdot |C> / \mathcal{N}(C)$, the stochastic process associated to the probability $P(C',C)$ is thus the following : firstly, the number of steps L is chosen according to a Poisson law of parameter ν; secondly, each effective step is chosen randomly among the $\omega = n(\Omega - n + 1)$ possible pair diffusions. This random process exactly simulates the evolution operator associated with the 2-body part of the Hamiltonian, i.e. pair diffusion, up to the multiplicative factor $\exp(\nu)$.

Now, the matrix elements of the complete time evolution operator can be written as

$$
\begin{aligned}
< C'|e^{-\Delta t(H-E)}|C> &\simeq e^{-\Delta t(E^{1-b}_{C'}-E)} \cdot e^{\nu} \cdot P(C',C) \\
&\simeq w(C') \cdot P(C',C)\ , \qquad (21)
\end{aligned}
$$

where we have defined $w(C) = e^{-\Delta t(E^{1-b}_{C}-E_{sen}-E)}$. Thus applying $e^{-\Delta t(H-E)}$ to a given $|C>$ is equivalent to a random diffusion according to $P(C',C)$, followed by a multiplication by the weight $w(C')$ depending on the one-body energy of the destination configuration $|C'>$. The evolution operator associated with H^{2-b} acts as if all the single-particle levels were degenerate, and diffuses the pairs in the available orbits (according to the Poisson distribution). Then, the evolution operator associated with H^{1-b} corrects for the real single-particle spectrum by taking into account the weights $w(C)$. These weights become small when a diffusion leads to a large increase of the energy E^{1-b}.

The above is analogous to the well-known Feynman procedure [31] related to the separation of H into a kinetic and a potential part, yielding two separate propagators. Here, H^{2-b} plays the role of a kinetic energy by spreading out $|\Psi(t)>$ in the configuration space, whereas H^{1-b} plays the role of a potential energy and concentrates $|\Psi(t)>$ in its components with little one-body energy E^{1-b}. The balance between these two competing tendencies determines the exact ground state $|\Psi_0>$.

It is interesting to note that, in the case of a single-level system, all the configurations $|C>$ are degenerate ($E^{1-b}_C = 0$) and play the same role, so that we must have $w(C) = 1$ for all C in

order to keep constant the norm of $|\Psi(t)>$ during the time evolution. Thus, the normalization energy must be $E = -E_{sen}$ (i.e., that of the seniority scheme) as expected.

2.2 GENERAL PAIRING INTERACTION

We consider now the case of a many-body system described by the Hamiltonian

$$H = \sum_{k>0}^{\Omega} \epsilon_k (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - \sum_{k,k'>0}^{\Omega} G_{k,k'}\ a_{k'}^\dagger a_{\bar{k}'}^\dagger a_{\bar{k}} a_k \ , \tag{22}$$

where the $G_{k,k'}$ are the interaction matrix elements ($G_{k,k'} > 0$). It is easy to show that the components α_C of the ground state must also be positive in this case, so that it is also appropriate to consider a Monte Carlo procedure (as in Section 2.1).

The only difference here is the expression of two-body matrix elements of H, that is

$$< C'|H^{2-b}|C >= \begin{cases} -G_{i,j} & \text{if } C \text{ and } C' \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases} \tag{23}$$

where we consider C and C' as connected if they differ by the position of one pair (which is diffused from state i to state j). Note that virtual diffusions are also included. Thus, using the same breakup as in Section 2.1, we have to generate stochastically the imaginary time evolution operator associated with the two-body part of this Hamiltonian. Let us evolve a given $|C>$ with this operator, as in equation (18),

$$e^{-\Delta t\ H^{2-b}}|C >= \sum_{L=0}^{\infty} \sum_{\lambda=1}^{\omega^L} \underbrace{\cdots G_{i,j} \cdots}_{L \text{ terms}} \frac{\Delta t^L}{L!}\ |C_L^\lambda > \ , \tag{24}$$

where the product of L terms $G_{i,j}$ corresponds to the L successive diffusions from $|C>$ to $|C_L^\lambda>$. It is impossible here to directly simulate this diffusion process, as in Section 2.1. However, it is possible to apply an importance sampling procedure [32] for the stochastic evaluation of the two-body evolution operator matrix elements. Let us consider the matrix element

$$< C'|e^{-\Delta t\ H^{2-b}}|C >= \sum_{L=0}^{\infty} \sum_{\lambda=1}^{\omega^L} F(C_L^\lambda) \qquad \text{where } F(C_L^\lambda) = \underbrace{\cdots G_{i,j} \cdots}_{L \text{ terms}} \frac{\Delta t^L}{L!}\ \delta_{C',C_L^\lambda} \ . \tag{25}$$

If we proceed to a random sampling of the configurations $|C_L^\lambda>$ according to the distribution corresponding to a constant G (arbitrary chosen for the moment), that is

$$\mathcal{P}(C_L^\lambda) = \exp(-\nu)\ \frac{(G\Delta t)^L}{L!} \ , \tag{26}$$

with the normalization condition

$$\sum_{L=0}^{\infty} \sum_{\lambda=1}^{\omega^L} \mathcal{P}(C_L^\lambda) = 1 \ , \tag{27}$$

we may evaluate our matrix element by importance sampling, using

$$< C'|e^{-\Delta t\ H^{2-b}}|C > \ = \ \mathrm{E}\left[\frac{F(C_L^\lambda)}{\mathcal{P}(C_L^\lambda)}\right]_{C_L^\lambda} \tag{28}$$

$$= \ \exp(\nu)\ \cdot\ \mathrm{E}\left[\underbrace{\cdots\left(\frac{G_{i,j}}{G}\right)\cdots}_{L\ \text{terms}}\ \delta_{C',C_L^\lambda}\right]_{C_L^\lambda} \ . \tag{29}$$

Here E means the expectation value for a random sampling of the C_L^λ according to the probability distribution $\mathcal{P}(C_L^\lambda)$.

Thus, the two-body part of the evolution operator is obtained *exactly* by applying the random process corresponding to the constant G case, and then weighting each effective one-step diffusion by the factor $G_{i,j}/G$. In order to make this procedure efficient, it is clear that we have to choose for G a value of the order of the $G_{i,j}$. For simplicity, we arbitrary take the average value $G = \sum_{i,j} G_{i,j}/\Omega^2$. Thus, we simulate the diffusion process as if the matrix was constant (with $G_{i,j} = G$), and then we correct for the differences by taking into account the factors $G_{i,j}/G$.

The matrix elements of the complete time evolution operator are then given by

$$< C'|e^{-\Delta t(H-E)}|C > \simeq\ w(C')\cdot W(C',C)\cdot P(C',C)\ , \tag{30}$$

where $W(C',C)$ is defined as the product of the factors $G_{i,j}/G$ corresponding to the diffusion path from $|C>$ to $|C'>$. Thus, the only difference when treating the case of a general interaction $G_{i,j}$ consists in multiplying by a supplementary weight $W(C',C)$ in equation (21).

2.3 EXPECTATION VALUE OF OBSERVABLES

Let us consider now the stochastical evaluation of the multiple integral appearing when calculating the ground state wave function (see [27]). We have, using expression (12),

$$\begin{aligned}|\Psi_0 > \simeq\ e^{-t(H-E)}|\Phi > = \sum_{C_N}\cdots\sum_{C_0}|C_N >\ w(C_N)\ W(C_N,C_{N-1})\ P(C_N,C_{N-1})\\ \cdots w(C_1)\ W(C_1,C_0)\ P(C_1,C_0)\ < C_0|\Phi >\ ,\end{aligned} \tag{31}$$

where we take the weights $W(C_N,C_{N-1}) = 1$ when treating the case of G constant. Let us take an ensemble of N_{ens} initial configurations $\{C_0^i\}$ selected according to $\Phi(C_0) = < C_0|\Phi >$ taken here as a probability distribution. The algorithm consists in evolving stochastically the configurations C_s^i (with $i = 1,\cdots N_{ens}$) according to the matrix elements $w(C_{s+1}^i)\ W(C_{s+1}^i, C_s^i)$ $\times\ P(C_{s+1}^i, C_s^i)$ so that a new ensemble $\{C_{s+1}^i\}$ is generated. Each C_{s+1}^i is chosen randomly with the probability distribution $P(C_{s+1}^i, C_s^i)$, and replicated stochastically by a factor $w(C_{s+1}^i)$ $\times\ W(C_{s+1}^i, C_s^i)$. This is done (see [15]) by choosing a random number ξ uniformly distributed

in the interval [0,1], and taking N_{repl} replicates for each C^i_{s+1}. The number of replicates N_{repl} is written as

$$N_{repl} = [w(C^i_{s+1})\ W(C^i_{s+1}, C^i_s) + \xi]\ , \tag{32}$$

where $[x]$ stands for the greatest integer in x. In the limit of a large ensemble, the average number of replicates will be $w(C^i_{s+1})\ W(C^i_{s+1}, C^i_s)$, so that the evolution of the ensemble $\{C^i_s\}$ is produced stochastically.

After this random walk process, the final ensemble $\{C^i_N\}$ will be distributed according to $\prod_{s=1}^{N} w(C^i_s)\ W(C^i_s, C^i_{s-1})\ P(C^i_s, C^i_{s-1})\ \Phi(C_0)$, and we will have

$$|\Psi_0 > \simeq \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} |C^i_N >\ . \tag{33}$$

Hence, this stochastic method allows the evaluation of matrix elements of any operator as an average on the final ensemble of configurations. This ensemble $\{C^i_N\}$ represents a sample of the α_C of the exact solution $|\Psi_0 >$, so that each configuration $|C >$ appears with the probability α_C in the Monte Carlo simulation. Indeed, we have

$$\alpha_C =< C|\Psi_0 > \simeq \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} \delta_{C,C^i_N}\ . \tag{34}$$

In particular, we may evaluate the ground state energy from its wave function $|\Psi_0 >$. Using the normalization condition $\sum_C \alpha_C = 1$, we can write

$$\begin{aligned} E_0 &= \sum_{C'} < C'|H|\Psi_0 > \\ &= \sum_{C,C'} \alpha_C\ \ < C'|H|C > \\ &= \sum_{C} \alpha_C\ (E^{1-b}_C + E^{2-b}_C)\ , \end{aligned} \tag{35}$$

where we have defined

$$E^{2-b}_C = \sum_{C'} < C'|H^{2-b}|C > = -\sum_{\lambda=1}^{\omega} G_{i,j}\ . \tag{36}$$

This corresponds to a summation over the ω possible one-step diffusions from the configuration $|C >$ (the pair being diffused from state i to j). Note that, in the case of a constant G, it is simply given by $E^{2-b}_C = -E_{sen}$, and is thus independent of the configuration $|C >$. Thus the energy E_0 is given by the average of the $(E^{1-b}_C + E^{2-b}_C)$ weighted by the Monte Carlo sampling probabilities α_C. The Monte Carlo estimator for the energy is

$$E_0 \simeq \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} \begin{cases} E^{1-b}_{C^i_N} - E_{sen} & \text{for a constant } G\ , \\ E^{1-b}_{C^i_N} + E^{2-b}_{C^i_N} & \text{for a general interaction } G_{i,j}\ . \end{cases} \tag{37}$$

Note that, in the case of a single-level system with a constant G for which all the configurations $|C>$ are degenerate ($E_C^{1-b}=0$), this estimator clearly yields $E_0=-E_{sen}$ as expected.

The value of the energy can also be determined from the normalization energy which appears in the time evolution operator. Indeed, if E_N is defined as the value of E which keeps the size of the ensemble of configurations stable, it is clearly another estimation of E_0. The agreement between these two methods constitutes a nontrivial consistency test of the Monte Carlo algorithm (see [27]). A particular example is the case of a single-level system with a constant G, where both Monte Carlo energy estimators yield $E_0=E_N=-E_{sen}$, that is the exact solution with no statistical noise.

The Monte Carlo algorithm also makes possible the calculation of the exact pair occupation probabilities. Indeed, the expectation value of the pair number operator n_k is given by

$$< n_k >= \frac{< \Psi_0|a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{k}} a_k|\Psi_0 >}{< \Psi_0|\Psi_0 >} = \frac{< \zeta|e^{-t(H-E)}|a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{k}} a_k|\Psi_0 >}{< \zeta|e^{-t(H-E)}|\Psi_0 >} , \tag{38}$$

where $|\zeta>$ is an arbitrary state, and t should be taken large enough to eliminate contributions from excited states. Using the fact that the n_k operator is local in our configuration space and taking $<C|\zeta>=1$ for all $|C>$, we have

$$< n_k >= \frac{\sum_{C,C'} < C'|e^{-t(H-E)}|C > \; n_k(C)\; \alpha_C}{\sum_{C,C'} < C'|e^{-t(H-E)}|C > \alpha_C} . \tag{39}$$

This clearly requires further evolution of the random walk, in order to filter the ground state from the state $|n_k\ \Psi_0>$. Expression (39) can be used as follows. Starting at time t_I with an ensemble of configurations distributed according to $|\Psi_0>$, apply the local operator n_k to the ensemble, i.e. weight each $|C>$ by its occupation number $n_k(C)$. Then evolve the ensemble to the time t_{II}. We take as estimator for the occupation probability:

$$< n_k > \simeq \frac{1}{N_{ens}} \sum_{j=1}^{N_{ens}} n_k(C_I^{i(j)}) , \tag{40}$$

where $n_k(C_I^{i(j)})$ is the kth occupation number of the configuration C_I^i, progenitor of C_{II}^j. Thus, it is necessary to keep track of each ensemble member's history in order to calculate the occupation probabilities.

The exact expectation value of other local observables could be obtained in principle with this Monte Carlo method, even if their calculations may be tedious. The case of non-local observables is still more complicated, since their expectation value can only be obtained approximately by a perturbation method (see [27]). We have not considered this problem here.

2.4 SYMMETRIZED BREAKUP OF THE EVOLUTION OPERATOR

As already mentioned, it is possible to replace the breakup of the evolution operator (equation 14) by the symmetrized form [30].

$$e^{-\Delta t\ H} = e^{-\frac{\Delta t}{2}\ H^{1-b}} \cdot e^{-\Delta t\ H^{2-b}} \cdot e^{-\frac{\Delta t}{2}\ H^{1-b}} + \mathcal{O}(\Delta t^3) . \tag{41}$$

It is obvious to show, by expanding both l.h.s and r.h.s. of this equation, that it is exact to the 2nd order in Δt, so that one order is gained compared to the more common breakup (14). When using this breakup, the matrix elements of the complete time evolution operator become

$$< C'|e^{-\Delta t(H-E)}|C > \simeq \tilde{w}(C',C) \cdot W(C',C) \cdot P(C',C) \ , \tag{42}$$

where we have defined $\tilde{w}(C',C) = [w(C') \cdot w(C)]^{1/2}$. Thus the same stochastic procedure can be applied here, if we replace the weights $w(C')$ by $\tilde{w}(C',C)$ in equations (31) and (32). In fact, the decomposition of exponential operators may be generalized [33] to get an exact expression up to any order in Δt. However, in general it cannot be applied in a quantum Monte Carlo simulation because it calls for the existence of an inverse exponential diffusion operator.

As an illustration, we have investigated the convergence of our estimate for the ground state energy E_0 as a function of Δt (or ν). We define here the pairing energy as $E_P = |E_0 - E_0^{1-b}|$, where E_0^{1-b} is the one-body energy of the unperturbed ground state $|\Psi_0^{1-b} >$. Figure 1 shows the dependence of the measured E_P on ν for a test case of 8 particles in 8 equispaced doubly-degenerate single-particle levels (i.e., $N = \Omega = 8$) with $G = 1.0$. Note that we express energies and the pairing strength G in units of the single-particle level spacing. We show: (a) the case for the symmetrized operator (i.e., Δt^3 breakup); (b) the case of the non-symmetrized operator (i.e., Δt^2 breakup). The runs were such that statistical errors are of the same size as the symbols. When going from the infinitesimal evolution operator to the finite time evolution operator, on the order of $1/\Delta t$ steps are required, so that the accuracy is reduced by one order in Δt. Thus, as confirmed by the numerics, the systematic error (due to $\Delta t \neq 0$) in the estimator of E_0 is proportional to Δt^2 in the case of the symmetrized operator while it is proportional to Δt for the non-symmetrized case. This clearly exhibits the accuracy gained when using the Δt^3 breakup, while the extra cpu cost is negligible. We have also numerically checked that, when suppressing the terms of order $L > 1$ in the Poisson distribution, the convergence still goes like Δt, so that one order is lost. This shows that the Poisson distribution allows to gain the supplementary order in Δt.

The detailed discussion of the different sources of errors (statistical and systematic) is reported in Appendix A.

3. Results

In order to get good statistics for the ground state energy and pair occupation probabilities, we have to average our estimates of E_0 and n_k over time, after removing the initial transients so that the excited states have decayed away from the initial state $|\Phi >$. We arbitrary choose for $|\Phi >$ the ground state wave function $|\Psi_0^{1-b} >= |C^{1-b} >$ of the unperturbed one-body Hamiltonian, where $|C^{1-b} >$ is simply the configuration obtained by putting the pairs into the lowest available orbits. Thus we take $\Phi(C_0) =< C_0|\Phi >= \delta_{C_0,C^{1-b}}$, that is the initial configurations $\{C_0^i\}$ for the whole ensemble are always taken equal to C^{1-b}.

It is convenient to define a reduced time $\tau = \omega G t = n(\Omega - n + 1)Gt$ which has the advantage of corresponding to the average expected number of steps (pair diffusions) along the random

walk of length t. Thus we average our estimators from $\tau_i = N\ \Delta t$ (where N is the number of terms in expression (31) needed to have negligible contribution from the excited states) to $\tau_f = \tau_i + T$ using steps of $\nu = \omega G\ \Delta t$. Note that we use the symmetrized breakup (see Section 2.4) for all our calculations since it permits to gain accuracy at essentially no computation cost.

3.1 THE SYMMETRIC TWO-LEVEL MODEL

We study here the case of an exactly solvable symmetric two-level model, with the number of particles N equal to the degeneracy $\Omega = 2j + 1$ of each level (i.e., $n = \Omega/2$). This model has been first examined in ref. [34], and its exact solution was studied in details by Rho and Rasmussen [35]. Then, it has been extensively used to validate various approximation methods (see e.g. [36, 37, 38]). More recently, the general case of a two-level model with $N \neq \Omega$ has been discussed in ref. [39].

The pairing Hamiltonian for this model can be written as

$$H = -\epsilon \sum_{k=1}^{\Omega/2} (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) + \epsilon \sum_{k=\Omega/2+1}^{\Omega} (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) - G \sum_{k,k'=1}^{\Omega} a_{k'}^\dagger a_{\bar{k}'}^\dagger a_{\bar{k}} a_k \ , \tag{43}$$

the energy gap between the two levels being thus 2ϵ. In the following, we will be interested in the two-body pairing energy $\mathcal{E}_P$ which we define as $\mathcal{E}_P = |E_0 - E_{MF}|$, where E_0 is the total ground state energy of the system, and $E_{MF} =< \Psi_0^{1-b}|H|\Psi_0^{1-b} >= -N\epsilon - nG$ is the mean field energy (corresponding to the solution $|\Psi_0^{1-b}>$ of the unperturbed one-body Hamiltonian). Note that the term nG is the pairing energy in the case $G \simeq 0$, and corresponds to the part of the pairing energy which can be incorporated into the one-body energy (i.e. the virtual diffusions).

The exact solution $\mathcal{E}_P^{exact}$ is obtained by introducing two sets of quasispin operators, and the problem finally reduces to the diagonalization of a tri-diagonal matrix of dimension $n + 1$ (see [35]). The BCS energy for this model can be easily computed (see e.g. [39]), and it appears that there is a critical value of the pairing strength $G_c = 2\epsilon/(\Omega - 1)$ below which there is no non-trivial solution. Thus we define for convenience a reduced pairing strength $x = G/G_c$.

In Figure 2, we plot the pairing energy as a function of x for the case $N = \Omega = 24$. It is useful to define here a dimensionless pairing energy $P = \mathcal{E}_P/N\epsilon$, with $N\epsilon$ being the unperturbed one-body energy (i.e., $< \Psi_0^{1-b}|H^{1-b}|\Psi_0^{1-b} >$). The solid line stands for the exact energy P_{exact}, whereas the symbols correspond to our computed energies P_{MC} obtained by a Monte Carlo simulation with the parameters: $\nu = 0.5$, $\tau_i = 100$, $T = 3000$, and $N_{ens} = 10000$. The two different Monte Carlo estimations E_0 and E_N of the energy agree very well (i.e., their difference is smaller than the statistical errors of either). They are consistent with the exact solution (within statistical errors) in the whole range of x (or G) values. Note that, for $x \lesssim 0.5$ (i.e., at the limit of weak pairing), the Monte Carlo estimation of E_P becomes difficult because E is very close to E_{MF}, and thus E_P is dominated by statistical noise. However, it has no practical importance since the pairing energy becomes very small compared to the one-body energy. Also, perturbation methods apply very well in this low pairing regime.

In Figure 3, we compare our computed energies with the energies resulting from different approximation methods. We are interested in the quantities $Q = E_P/E_P^{exact}$, that is in the ratios of the pairing energy (in various approximations) to the exact result. We show for reference the solution of BCS equations without particle number projection and with exact projection (variation after projection), and the solutions of the Kamlah and the Lipkin-Nogami methods from [40]. It is well known that BCS method accounts only for part of the two-body pairing energy E_P since it is a variational method, and thus $Q_{BCS} < 1$ especially for low x. Note that it has two major problems: firstly it yields $Q = 0$ for $x \leq 1$, and secondly it tends to give $Q = (\Omega - 1)/\Omega$ in the strong pairing limit (i.e., $x \gg 1$). The exact particle number projection method is very accurate in both small x and large x limits, but it introduces an error (less than 10%) to the pairing energy when x is close to 1. The Kamlah and Lipkin-Nogami methods give very accurate energies for $x \gtrsim 1$, but the ratio Q becomes very low for small x with both methods. However, we should mention that the predicted energies become much more accurate in the case $N \neq \Omega$ for both methods (see [39]). The symbols in Figure 3 represent the results of our Monte Carlo simulation. In order to reduce the statistical noise, we had to increase the integration time T and the ensemble size N_{ens} compared to Figure 2 (we took $T = 6000$, and $N_{ens} = 20000$). It clearly appears that the Monte Carlo method gives a very good agreement with the exact result (i.e., $Q_{MC} \simeq 1$ within statistical errors) in the considered range of x (or G) values, better than with any approximation method. Such an accuracy could not be useful for practical applications of the method, but what we intended here was just to show that the result is asymptotically exact. Note that the critical value $x = 1$ does not play a particular role in the Monte Carlo method, since no assumption is made concerning the functional form of the ground state wave function. The spurious critical behaviour at $x = 1$, originating in BCS method itself, is thus absent in the Monte Carlo results.

3.2 EQUIDISTANT DOUBLY-DEGENERATE LEVELS

We study now the case of equispaced doubly-degenerate single-particle levels. This problem has been solved exactly [8] for some model spaces with different values of the interaction strength reproducing typical values of the nuclear pairing energy. We only consider here the calculation of the pair occupation probabilities; the corresponding pairing energies can be found in ref. [9].

We chose the problem of 16 particles placed in 16 equispaced single-particle levels (i.e., $N = \Omega = 16$) with a pairing strength $G = 0.48$ (expressed in units of the single-particle level spacing). In Table 1, we show the occupation probabilities for three levels above and below the Fermi level. For comparison, we indicate the result of our Monte Carlo computation, the exact values [8], and the predictions of BCS equations (i.e., v_k^2). We made the Monte Carlo simulation with the parameters $\nu = 0.2$, $\tau_i = 300$, $T = 16000$, and $N_{ens} = 20000$, in order to get very good statistics (the pair occupation probabilities are more subject to statistical noise than the pairing energy). Note that in order to implement our time averaging for the n_k, we have to keep in memory an associated n_k for each configuration of the ensemble during a given time (long enough to get relaxation). We calculate a running average of the n_k from the ensemble, using a time difference $\tau_{II} - \tau_I$ of 100 steps. This choice results from a compromise.

For small values of $\tau_{II} - \tau_I$, the contributions from excited states have not sufficiently decayed, whereas for large values the statistical errors in the estimator for $< n_k >$ become important. This behavior was worsened when studying larger model spaces (in particular, we considered the case $N = \Omega = 24$ where no good compromise was found).

3.3 THE CASE OF ^{208}Pb AND ^{116}Sn

For illustrative purposes, we have applied our Monte Carlo method to the case of two nuclei, ^{208}Pb and ^{116}Sn, because they essentially correspond to two extreme cases. For the doubly-magic nucleus ^{208}Pb, the effect of the pairing correlations is considered as very weak (the pairing never switches on with a reasonable strength within BCS). On the contrary, the neutrons in ^{116}Sn (midway between two shell closures) pair strongly, so that the calculations using variation after projection are expected to be accurate. We have thus calculated the pairing energy for these two nuclei using realistic single-particle energies ϵ_k and pairing matrix elements $G_{k,k'}$ from [41]. These come from a self-consistent Hartree-Fock plus BCS (HFBCS) calculation [42], with the Skyrme SkM* [43] effective interaction for the mean-field. For the pairing interaction, a zero-range force [44] is used,

$$V^\tau(\vec{r}_1, \sigma_1; \vec{r}_2, \sigma_2) = V_0^\tau \, \frac{1 - \vec{\sigma}_1 \cdot \vec{\sigma}_2}{4} \, \delta(\vec{r}_1 - \vec{r}_2) \, , \tag{44}$$

where $\vec{r}$ and $\vec{\sigma}$ are the space and spin variable respectively. Here, V_0^τ is the strength for the neutrons ($\tau = n$) or the protons ($\tau = p$). Thus, the derived wave functions from HFBCS calculation are used to determine the matrix elements $G_{k,k'}$ of this two-body interaction. Then, the variation after projection equations are solved in order to yield the pairing energy and occupation probabilities.

In Table 2, we compare the pairing energy predicted by our Monte Carlo method for both neutrons and protons in ^{208}Pb and ^{116}Sn to the result of a variation after projection calculation. This energy represents thus the energy gained by switching on the delta-force for the pairing interaction. The strength was taken to be $V_0 = -240$ MeV Fm^3 for both neutrons and protons. Note that we took for the cut-off a Fermi factor with a range near 5 MeV. We ran the Monte Carlo simulations with the parameters $\nu = 0.5$, $T = 500$, and $N_{cns} = 20000$, which took a reasonable computation time (e.g. 10 min. on a Vax Station 4000). From Table 2, it clearly appears that the variation after projection calculation cannot account for the totality of the pairing energy, especially in the weak pairing regime (i.e., near shell closures). On the contrary, in the case of the neutrons in ^{116}Sn, one notices that the variation after projection predictions are much closer to the exact result, as expected. Thus, our Monte Carlo procedure proves to be appropriate for calculating realistic pairing energies in nuclei, yielding a better accuracy than the available approximation methods.

4. Conclusion

We presented a novel quantum Monte Carlo approach, and successfully applied it to nuclear systems with a pairing interaction. Our Monte Carlo algorithm is very efficient from the

computational point of view, and is also very appealing for its conceptual simplicity. Pair diffusion is simulated stochastically in order to calculate interesting quantities such as the pairing energy or the pair occupation probabilities. The sequence of random walk processes followed by replications corresponds to one's intuitive view of pair diffusion.

Comparison of our results with exact calculations for the simple models presented in Section 3.1 and 3.2 show that the method is reliable. Moreover, it leads to a better agreement with the exact solution than the standard approximation methods such as the Kamlah method, the Lipkin-Nogami method, or the exact particle number projection method. It is the only method able to give, at least in principle, an exact solution when treating a general pairing interaction (i.e., G not constant). Thus, it is very promising for treating realistic pairing correlations in nuclei.

Acknowledgments

We are especially grateful to O. Martin for many stimulating discussions and his constant enthusiasm for the topic. This work has been possible thanks to his collaboration. We would like to thank H. Flocard and P. H. Heenen for providing us with helpful results, and for useful comments. We also express our gratitude to M. Arnould, O. Bohigas, M. Rayet, and J. Treiner for their encouragement. We acknowledge O. Martin for a careful reading of the manuscript. This work has been partially supported by the Science Program of the Commission of the European Communities SC1-0065.

Appendix A : Statistical and systematic errors

The Monte Carlo estimators for the ground state energy and the pair occupation probabilities are subject to both statistical and systematic errors.

i) Systematic error : The first source of systematic error is trivially due to the fact that the exact evolution operator in configuration space is not simulated, as mentioned in Section 2.1. In particular, the breakup of the evolution operator leads to an error quadratic in Δt (in the case of the symmetrized breakup) as explained in Section 2.4. Besides this, there exist a more subtle bias in the Monte Carlo estimation of the energy (and other observables) related to the finite size of the ensemble (N_{ens} is finite). This bias is specific to projection Monte Carlo methods (i.e., Green Function and Path Integral Monte Carlo calculations) [10]. Generally, it is not recognized that this bias exists, or at best it is believed to be negligible, but we have found that it is important in some cases. (For instance, a size of about ten thousand configurations is required to make this error negligible for reasonable model spaces.) The main purpose of this Appendix is to quantify this systematic error. In particular, we will show that it scales like $1/N_{ens}$ for all estimators.

Firstly, we have numerically checked the existence of this bias for our estimates of the energy in the case treated in Section 2.4 (i.e., equidistant doubly-degenerate levels with $N = \Omega = 8$ and $G = 1.0$). We have chosen for ν the value 0.5 so that the systematic error due to $\Delta t \neq 0$ is small (see Figure 1). In Figure 4, we plot the measured pairing energy E_P as a function of N_{ens}^{-1}. The existence of a bias inversely proportional to N_{ens} is thus confirmed in this case. Note that this bias leads to underestimating the pairing energy, so that the estimated ground state energy is too high. This behaviour will be explained in what follows.

Let us show how N_{ens} finite introduces a bias. It is the fact that the weights (after time evolution) are distributed with a non-zero variance which is at the origin of the bias. The estimator for an observable consists in an average over the ensemble of size N_{ens}, and is thus expressed as a ratio, the denominator of which being the sum of the weights of the configurations (i.e., the normalization factor). Then the bias originates from the fact that the expectation value for a ratio is not the ratio of the expectation values, if the denominator is a fluctuating quantity. Here, the denominator is the normalization factor, and fluctuates because of the variation of the weights. In order to simplify the discussion, we will limit ourselves to showing that the application of the time evolution operator to an ensemble of configurations distributed according to the exact ground state yields a new ensemble with a biased distribution. This will demonstrate that our stochastic procedure tends to a steady-state distribution which does not exactly correspond to the exact ground state when N_{ens} is finite. (The determination of the actual steady-state distribution is beyond the scope of the present paper.) For convenience, we will also neglect the replication procedure in the following, because it seems difficult to precisely account for the error which it introduces. Also, the purpose of the replication is to make the Monte Carlo procedure efficient (that is to significantly reduce the statistical error), and one may reasonably assume that the replication will not suppress the systematic error. Thus, we also neglect the fact that the ensemble size is not constant in practice (in fact the normalization

energy E_N is constantly adjusted in order to compensate for deviations from N_{ens}), but this does not change our conclusions.

Let us follow the time evolution of an ensemble of finite size from an initial ensemble of configurations $\{C_i\}$ (with $i = 1, \cdots N_{ens}$) randomly chosen according to the exact distribution of the ground state, i.e., α_C. For the time being, we assume that the exact time evolution operator is used, so that we can ignore the trivial bias due to the breakup. We will show that the estimators for observables are sensibly biased when one uses the new distribution obtained by evolving the initial one for a time t. We define here the exact evolution operator by

$$U_t = e^{-(H-E_0)t} \ , \tag{45}$$

where E_0 stands for the exact ground state energy. Of course, this expression depends on an a priori knowing of E_0, but it is just a way to normalize the weights, and it has no importance in the following. The matrix elements of U_t are given by

$$U_t(C', C) =< C'|U_t|C >= P(C', C) \cdot w(C) \ , \tag{46}$$

where the weights are defined as $w(C) = \sum_{C'} U_t(C', C)$, in order to normalize the transition probabilities $P(C', C)$. (Note that $w(C)$ has an implicit dependence on t.) It is clear that

$$U_t|\Psi_0 >= \sum_C \sum_{C'} U(C', C)\alpha_C|C' >= \sum_{C'} \alpha_{C'}|C' > \ , \tag{47}$$

so that we have the following equation for U_t

$$\sum_C \alpha_C U_t(C', C) = \alpha_{C'} \ . \tag{48}$$

In the following, we will apply estimators acting on the initial ensemble of configurations $\{C_i\}$ and the corresponding ensemble of configurations $\{C_i'\}$ (after the evolution for a time t), in order to measure the energy E_0 and the probabilities α_C. We introduce the quantities

$$W_{ens} = \sum_{i=1}^{N_{ens}} w(C_i) \ , \tag{49}$$

$$E_{ens} = \sum_{i=1}^{N_{ens}} w(C_i)E(C_i') \ , \tag{50}$$

$$A_{ens}(\tilde{C}) = \sum_{i=1}^{N_{ens}} w(C_i)\delta_{C_i',\tilde{C}} \ , \tag{51}$$

where the $w(C_i)$ are the weights of the configurations (before the time evolution), and the $E(C_i')$ are the energies of the corresponding configurations after time evolution with the definition $E(C) = E_C^{1-b} + E_C^{2-b}$. Here, E_C^{1-b} and E_C^{2-b} are defined as in Section 2. Note that, with this definition we have $E_0 = \sum_C \alpha_C E(C)$. Thus we clearly see that E_{ens}/W_{ens} yields an estimator for the ground state energy E_0, while $A_{ens}(\tilde{C})/W_{ens}$ is an estimator for the probability $\alpha_{\tilde{C}}$.

Now we are interested in the distribution (in fact, the first moments) of these estimators. Let us consider first the estimator for the ground state energy. We have respectively for its expectation value and its variance

$$\frac{\mathrm{E}[E_{ens}/W_{ens}]}{\mathrm{E}[E_{ens}]/\mathrm{E}[W_{ens}]} \simeq 1 - \frac{\mathrm{Cov}[E_{ens}, W_{ens}]}{\mathrm{E}[E_{ens}]\mathrm{E}[W_{ens}]} + \frac{\mathrm{Var}[W_{ens}]}{\mathrm{E}[W_{ens}]^2} , \tag{52}$$

$$\frac{\mathrm{Var}[E_{ens}/W_{ens}]}{(\mathrm{E}[E_{ens}]/\mathrm{E}[W_{ens}])^2} \simeq \frac{\mathrm{Var}[E_{ens}]}{\mathrm{E}[E_{ens}]^2} + \frac{\mathrm{Var}[W_{ens}]}{\mathrm{E}[W_{ens}]^2} - 2\frac{\mathrm{Cov}[E_{ens}, W_{ens}]}{\mathrm{E}[E_{ens}]\mathrm{E}[W_{ens}]} . \tag{53}$$

We thus need the expectation value, variance, and covariance of the quantities introduced in equations (49), (50), and (51). Since the configurations C_i of the ensemble are independent (only the replication process introduces a correlation between the configurations), these quantities can be simply expressed with the help of the corresponding one-configuration quantities (acting on one individual configuration C and the corresponding one C' after time evolution) as

$$W_{ens} = \sum_{i=1}^{N_{ens}} W_1(C_i) \qquad \text{with} \quad W_1(C_i) = w(C_i) , \tag{54}$$

$$E_{ens} = \sum_{i=1}^{N_{ens}} E_1(C_i) \qquad \text{with} \quad E_1(C_i) = w(C_i)E(C_i') . \tag{55}$$

The expectation value for these one-configuration quantities, when beginning with a configuration distributed according to α_C (the exact ground state distribution) can be easily obtained as

$$\mathrm{E}[W_1] = \sum_C \alpha_C w(C) = \sum_C \sum_{C'} \alpha_C U_t(C', C) = 1 , \tag{56}$$

$$\mathrm{E}[E_1] = \sum_C \sum_{C'} \alpha_C P(C', C) w(C) E(C') = E_0 , \tag{57}$$

where we have used equations (46) and (48), and the definition of $w(C)$. In order to express their second-order moments (variance and covariance), we must find an approximate expression for the weights $w(C)$. It is easy to show that, for small values of t,

$$w(C) \simeq e^{-t[E_C^{1-b} + E_C^{2-b} - E_0]} = e^{-t[E(C) - E_0]} , \tag{58}$$

so that we have

$$\begin{aligned} \mathrm{Var}[W_1] &= \sum_C \alpha_C [w(C) - 1]^2 \\ &\simeq t^2 \cdot \sum_C \alpha_C [E(C) - E_0]^2 . \end{aligned} \tag{59}$$

We can also express

$$\begin{aligned} \mathrm{Var}[E_1] &= \sum_C \sum_{C'} \alpha_C P(C', C)[w(C)E(C') - E_0]^2 \\ &\simeq \sum_C \alpha_C [E(C) - E_0]^2 , \end{aligned} \tag{60}$$

using the fact that $P(C',C) \simeq \delta_{C',C}$ and $w(C) \simeq 1$ at the lowest order in t. Finally, we calculate the covariance

$$\begin{aligned} \mathrm{Cov}[E_1, W_1] &= \sum_C \sum_{C'} \alpha_C P(C',C)[w(C)-1]\,[w(C)E(C') - E_0] \\ &\simeq -t \cdot \sum_C \alpha_C [E(C) - E_0]^2 \ , \end{aligned} \tag{61}$$

showing that E_1 and W_1 are perfectly anticorrelated (at the lowest order in t).

Now, we may calculate the corresponding quantities for E_{ens} and W_{ens}, using equations (56), (57),(59),(60), and (61), and using the fact that the configurations are independent:

$$\mathrm{E}[W_{ens}] = N_{ens} \ , \tag{62}$$

$$\mathrm{Var}[W_{ens}] \simeq N_{ens}\, t^2\, \sigma^2 \ , \tag{63}$$

$$\mathrm{E}[E_{ens}] = N_{ens}\, E_0 \ , \tag{64}$$

$$\mathrm{Var}[E_{ens}] \simeq N_{ens}\, \sigma^2 \ , \tag{65}$$

$$\mathrm{Cov}[E_{ens}, W_{ens}] \simeq -N_{ens}\, t\, \sigma^2 \ , \tag{66}$$

where we have defined $\sigma^2 = \sum_C \alpha_c [E(C) - E_0]^2$. Thus it appears naturally that the expectation value for our energy estimator is biased since one has, using expression (52),

$$\frac{\mathrm{E}[E_{ens}/W_{ens}]}{E_0} \simeq 1 + \frac{\sigma^2}{N_{ens} E_0^2}(tE_0 + t^2 E_0^2) \ . \tag{67}$$

This leads (at the lowest order in t) to a bias equal to $t\sigma^2/N_{ens}$, thus scaling like $1/N_{ens}$. The Monte Carlo method provides thus a zero bias only in the limit of N_{ens} infinite. This bias is also proportional to the quantity σ^2, depending on the exact ground state of the considered system. Note that in both the weak and strong coupling limits, σ^2 tends to zero. Indeed, when G tends to zero, only one configuration (i.e., C^{1-b}) contributes to the ground state, and one has $\alpha_C = \delta_{C,C^{1-b}}$, so that $\sigma^2 = 0$. When G tends to infinity, all the configurations play the same role and the $E(C)$ are degenerate, so that one has also $\sigma^2 = 0$. This explains why the Monte Carlo method tends to give the exact result in these limiting cases. It is also interesting to note that the predicted bias is always positive, so that the ground state energy is overestimated, which is exactly what appeared in the numerical simulations (see Figure 4).

The reduced variance of the estimator for the energy can also be expressed, using (53), as

$$\frac{\mathrm{Var}[E_{ens}/W_{ens}]}{E_0^2} \simeq \frac{\sigma^2}{N_{ens} E_0^2}(1 + 2tE_0 + t^2 E_0^2) \ , \tag{68}$$

so that the (squared) relative statistical error on E_0 is approximately given by $\sigma^2/(N_{ens}E_0^2)$, with the same dependence in N_{ens} and σ^2 as the bias. Note that, up to now, we have not specified the time t. If one followed the evolution during a long time interval (taking into account the exact dependence in t, and not only the lowest order terms of the expansion in

t), one would tend to a steady-state situation and the corresponding bias and statistical error would then saturate. Thus, the value of t has no real significance here, except for describing the short time behaviour (and in particular, times shorter than the replication time). However, our analysis has already the merit of clearly exhibiting the existence of a bias and its dependence on N_{ens} and σ/E_0.

Let us consider now the estimator for the probability $\alpha_{\tilde{C}}$, that is $A_{ens}(\tilde{C})/W_{ens}$, where we define

$$A_{ens}(\tilde{C}) = \sum_{i=1}^{N_{ens}} A_1(C_i) \qquad \text{with} \quad A_1(C_i) = w(C_i)\delta_{C_i',\tilde{C}} \ . \tag{69}$$

In order to determine its expectation value and variance, we have to calculate the corresponding moments for the one-configuration quantity A_1. We have for its expectation value

$$\mathrm{E}[A_1] = \sum_C \sum_{C'} \alpha_C P(C',C) w(C) \delta_{C',\tilde{C}} = \alpha_{\tilde{C}} \ , \tag{70}$$

and for its variance

$$\begin{aligned} \mathrm{Var}[A_1] &= \sum_C \sum_{C'} \alpha_C P(C',C)[w(C)\delta_{C',\tilde{C}} - \alpha_{\tilde{C}}]^2 \\ &\simeq \sum_C \alpha_C [\delta_{C,\tilde{C}} - \alpha_{\tilde{C}}]^2 \\ &\simeq \alpha_{\tilde{C}}(1-\alpha_{\tilde{C}}) \ , \end{aligned} \tag{71}$$

where we used the same approximation as previously. For the covariance between the quantities A_1 and W_1, we have

$$\begin{aligned} \mathrm{Cov}[A_1, W_1] &= \sum_C \sum_{C'} \alpha_C P(C',C)[w(C)-1][w(C)\delta_{C',\tilde{C}} - \alpha_{\tilde{C}}] \\ &\simeq -t \cdot \alpha_{\tilde{C}}(E_{\tilde{C}} - E_0) \ . \end{aligned} \tag{72}$$

Using relations analogous to expressions (52) and (53), one gets the following expressions for the expectation value and variance of the estimator $A_{ens}(\tilde{C})/W_{ens}$ for the probability $\alpha_{\tilde{C}}$:

$$\frac{\mathrm{E}[A_{ens}(\tilde{C})/W_{ens}]}{\alpha_{\tilde{C}}} \simeq 1 + \frac{1}{N_{ens}}\left(t(E_{\tilde{C}} - E_0) + t^2\sigma^2\right) \ , \tag{73}$$

$$\frac{\mathrm{Var}[A_{ens}(\tilde{C})/W_{ens}]}{\alpha_{\tilde{C}}^2} \simeq \frac{1}{N_{ens}}\left(\sigma_{\tilde{C}}^2/\alpha_{\tilde{C}}^2 + 2t(E_{\tilde{C}} - E_0) + t^2\sigma^2\right) \ , \tag{74}$$

where we have defined $\sigma_{\tilde{C}}^2 = \alpha_{\tilde{C}}(1-\alpha_{\tilde{C}})$. The bias is approximately (at the lowest order in t) equal to $t\alpha_{\tilde{C}}(E_{\tilde{C}} - E_0)/N_{ens}$, whereas the (squared) absolute statistical error is about $\sigma_{\tilde{C}}^2/N_{ens}$. Thus, both the bias and the (squared) statistical error on the α_C scale like $1/N_{ens}$, as in the case of the energy estimator. Expression (72) shows that, for all the configurations $\tilde{C}$ such that $E_{\tilde{C}} < E_0$, the estimators A_1 and W_1 are (positively) correlated, whereas they are anticorrelated

when $E_C > E_0$. Thus, the Monte Carlo estimator underestimates the components of the low energy configurations and overestimates those of the highly excited configurations. The consequence is a bias in the occupation probabilities n_k; they are underestimated below the Fermi level and overestimated above this level. We have numerically checked the existence of this bias in the case $N = \Omega = 16$ and $G = 0.48$ presented in Section 3.2. Also, since the statistical error is principally related to the variance on A_1, expression (71) implies that this error is maximum for the configurations having a component close to 0.5, and tends to zero for the configurations with a component close to zero or when only one configuration significantly contributes to the ground state (i.e., when $G \simeq 0$). This results in a statistical error on the occupation probabilities n_k which is important in the region of the Fermi level principally.

ii) Statistical error : It is clear that a statistical noise is superimposed on the (biased) value of the observables, due to the principle of the Monte Carlo method (i.e., the sampling of a finite number of configurations). We have already calculated the statistical error on the observables for each ensemble (see equations 68 and 74). However, another fact has to be taken into account when calculating the total statistical error on the estimators averaged along the time evolution as described in Section 3. After the ensemble has relaxed to its steady-state situation (after N applications of the infinitesimal evolution operator $e^{-\Delta t\ H}$), the continued evolution yields successive ensembles of N_{ens} configurations distributed according to the ground state wave function α_C (except for the above mentioned bias). This distribution is then sampled by repeated applications of the infinitesimal evolution operator, each sample of N_{ens} configurations yielding an energy estimate E_{ens}/W_{ens} as explained above. However, the successive ensembles are clearly correlated, since each one is obtained by diffusing generally one pair at most (ν pairs on average) from the previous one. This fact has to be taken into account in the estimation of the statistical error. It is necessary to compute the autocorrelation function in order to determine the number of time steps Δt required to yield statistically independent samples. In fact, it is clear that an average number of random pair diffusions of the order of the number of pairs $n = N/2$ is needed to yield a completely random configuration from a given one, so that about n/ν time steps Δt are necessary. Thus, if the total number of sampled ensembles (after relaxation) is called $\mathcal{N}$, the relative statistical error will be $(\mathcal{N}\nu/n)^{-1/2} \cdot \epsilon_{ens}$, where $\epsilon_{ens} = (\sigma/E_0) \cdot N_{ens}^{-1/2}$ is the statistical error on the energy for each sample (see 68). Of course, the same reasoning is also valid for the calculation of the statistical error on other observables such as the occupation probabilities.

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Table captions

Table 1:

Pair occupation probabilities of the 3 levels above and below the Fermi level for the case of equispaced doubly-degenerate levels with $N = \Omega = 16$, and $G = 0.48$.

Table 2:

Pairing energy for both neutrons and protons in ^{208}Pb and ^{116}Sn. The result of our Monte Carlo simulation is compared to the prediction of a variation after projection calculation.

Figure captions

Figure 1:

Systematic error in the pairing energy estimate E_P due to a finite Δt, as a function of ν for the case of equispaced doubly-degenerate levels with $N = \Omega = 8$, and $G = 1.0$. (The exact value is 9.513)

Figure 2:

Dimensionless pairing energy P as a function of the reduced pairing strength x for the symmetric two-level case with $N = \Omega = 24$. The solid line stands for the exact energy, whereas the symbols correspond to the values computed by the Monte Carlo simulation.

Figure 3:

Ratio Q of the pairing energy (in various approximations) to the exact result for the symmetric two-level case with $N = \Omega = 24$. The symbols correspond to the values computed by the Monte Carlo simulation, while the different lines represent the predictions of various approximation methods: (a) exact projection; (b) Kamlah method; (c) Lipkin-Nogami method; (d) BCS without projection.

Figure 4:

Systematic error due to a finite N_{ens} for the pairing energy estimate E_P as a function of $1/N_{ens}$ for the case of equispaced doubly-degenerate levels with $N = \Omega = 8$, and $G = 1.0$. Note that the extrapolated (for an infinite N_{ens}) pairing energy is about 9.52, which is still weakly biased compared to the exact value 9.513 because of $\Delta t \neq 0$.

Table 1

k	$< n_k >_{exact}$	$< n_k >_{MC}$	v_k^2
+3	0.0929	0.0926 ± 0.0010	0.0899
+2	0.1570	0.1598 ± 0.0010	0.1693
+1	0.3056	0.3050 ± 0.0010	0.3551
-1	0.6944	0.6952 ± 0.0010	0.6449
-2	0.8430	0.8430 ± 0.0010	0.8307
-3	0.9071	0.9068 ± 0.0010	0.9101

Table 2

		E_{VAP} [MeV]	E_{MC} [MeV]
^{208}Pb	ν	0.22	2.06
	π	0.17	2.21
^{116}Sn	ν	2.18	2.49
	π	0.10	2.01

Fig. 1

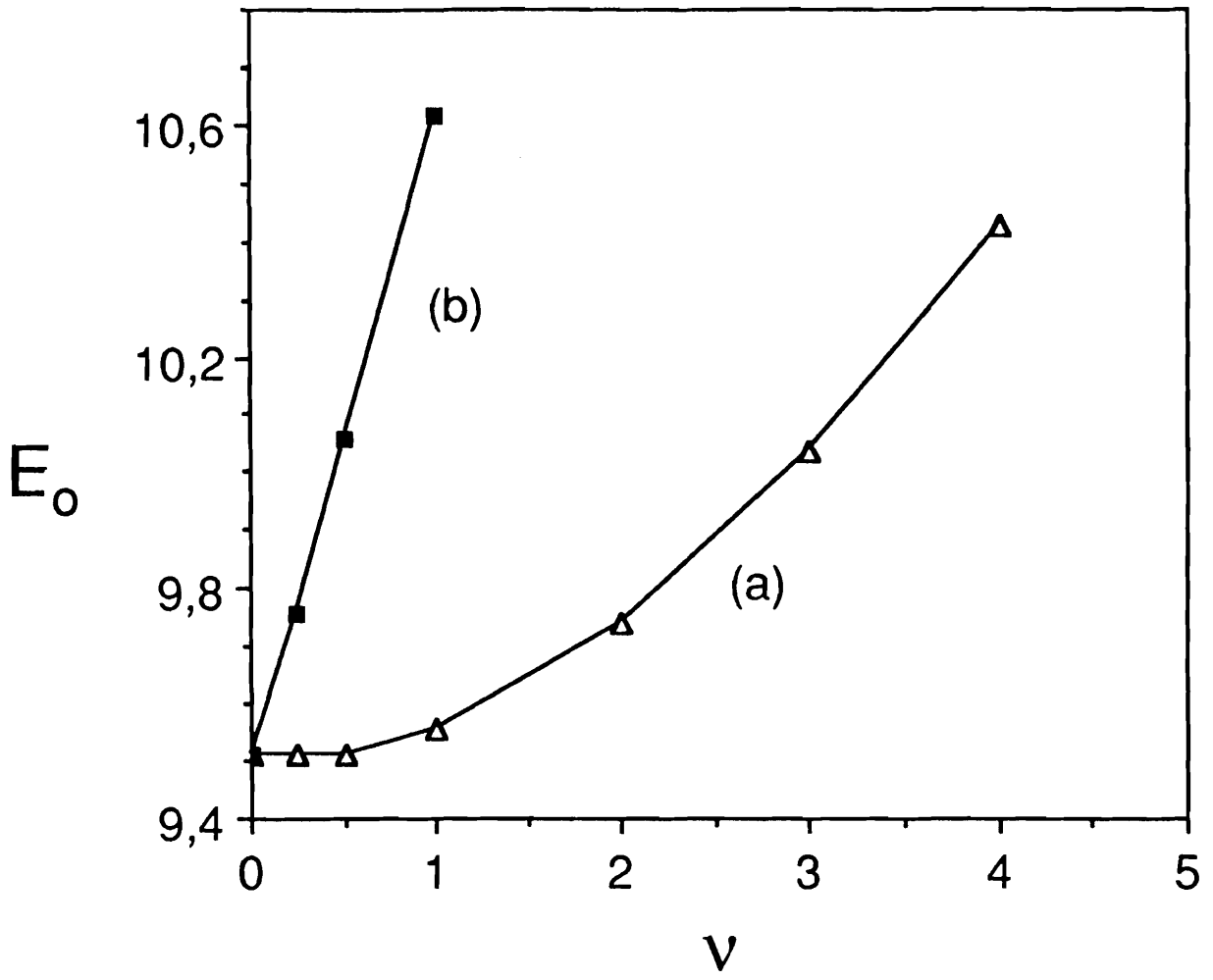

Fig. 2

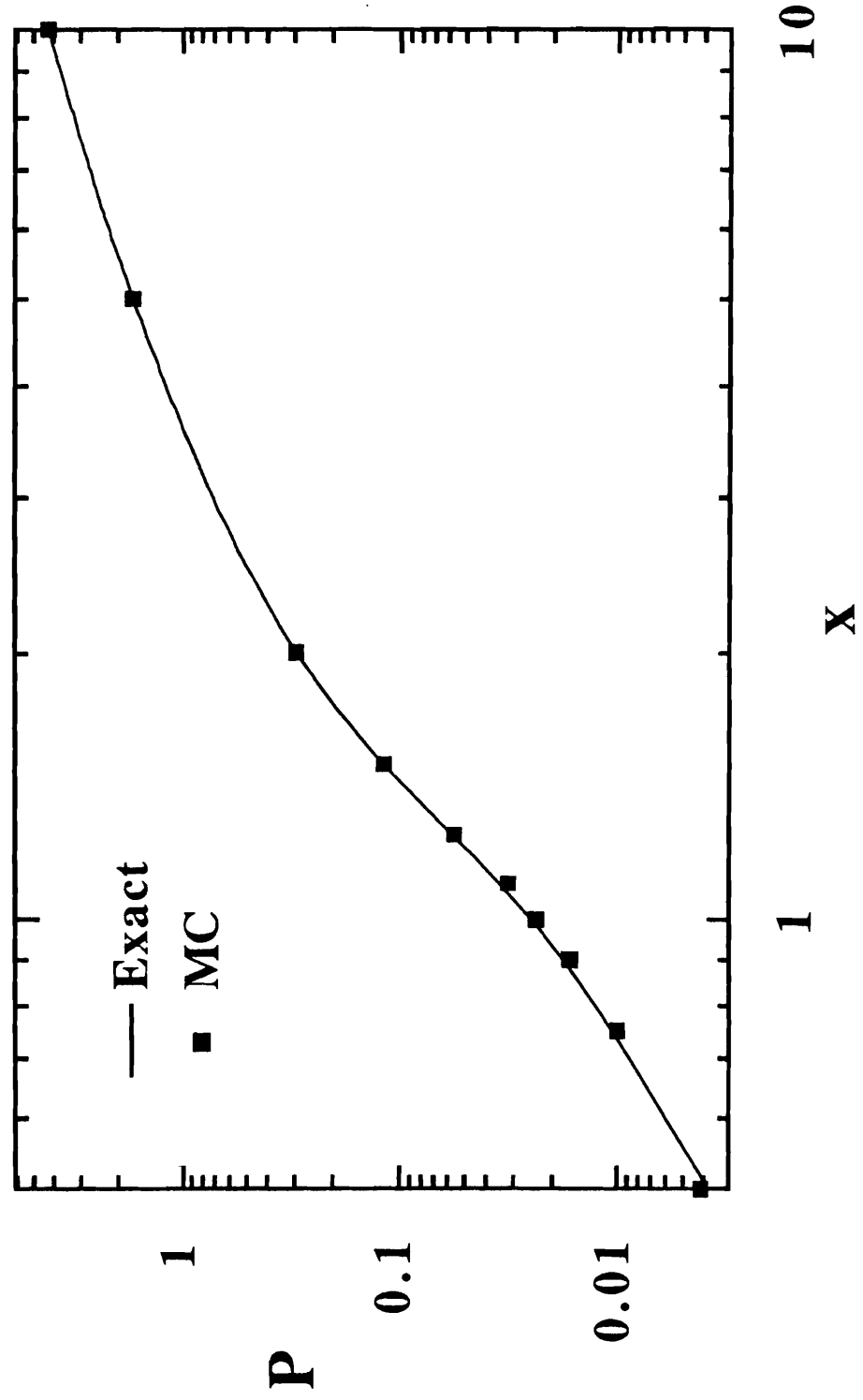

Fig. 3

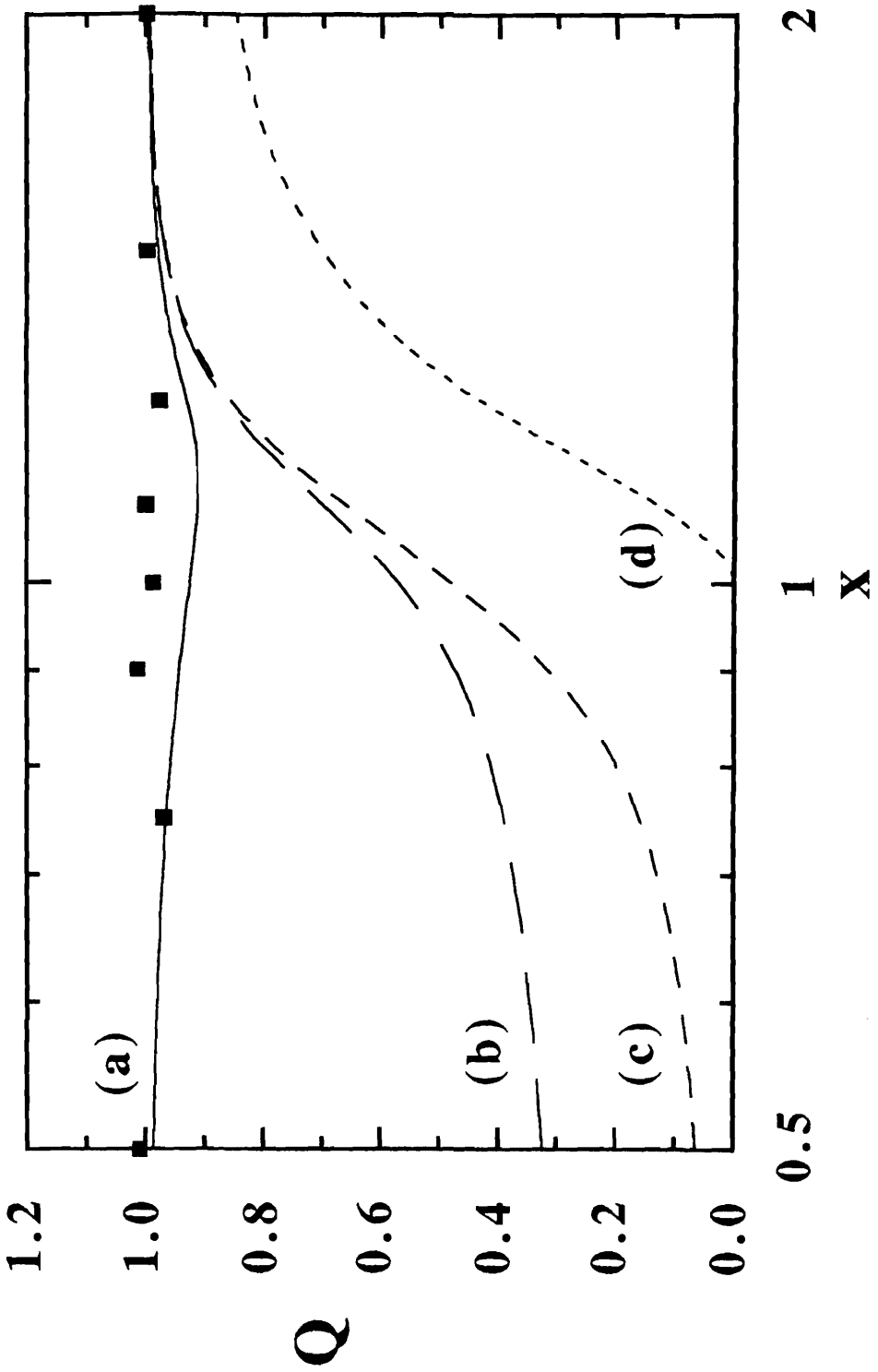
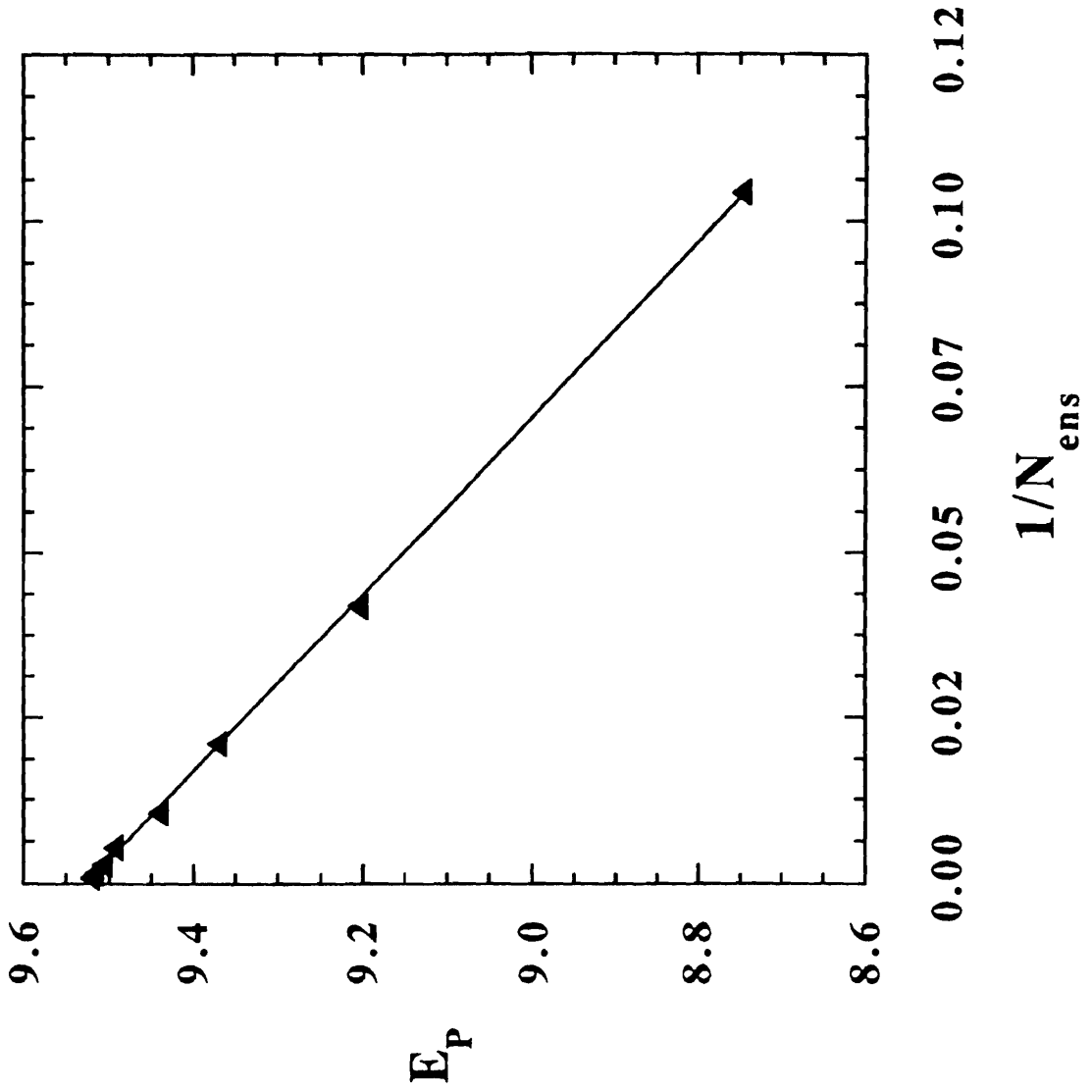
Fig. 4