Monte Carlo calculations of energies in the erbium region

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We investigate the validity of the method of computing ground-state energies, at a given angular momentum, with Monte Carlo methods applied to the functional integral formulation containing pairing fields. Calculations have been performed for several erbium isotopes and a few dysprosium isotopes. It is found that some residual sign fluctuations, which seem to be associated with a small neutron number above the $N = 82$ shell closure, are present, but that they do not affect the feasibility of the calculations. Such sign fluctuations disappear as the neutron number is increased. Also, an efficient improved method for the computation of the functional integral in the case of an odd number of particles is presented. The Monte Carlo method of Metropolis *et al.* [J. Chem. Phys. **21**, 1087 (1953)] is used in the evaluation of expectation values.

I. INTRODUCTION

The problem of understanding the low-energy collective behavior of heavy nuclei has always been a central problem since the early days of nuclear physics. With a large number of active nucleons and available many-body states, it is far beyond the capabilities of nuclear shell model diagonalization approaches. Functional integral methods [1], implemented with Monte Carlo integration techniques, seem to be so far a promising method to tackle the problem.

Recently, we presented a method to evaluate the particle number, angular momentum, and parity projected many-body matrix elements of the form

$$\mathcal{B} = \langle \psi, J, M, \pi, N, Z | e^{-\beta \hat{H}} | \psi, J, M, \pi, N, Z \rangle, \qquad (1)$$

using functional integrals containing pairing fields [2]. In the above expression the trial state not orthogonal to the ground state, $|\psi, J, M, \pi, N, Z\rangle$, has definite angular momentum J, M, good parity π, and neutron and proton number, respectively, N and Z. This technique was applied to few cases, with the pairing plus quadrupole Hamiltonian and with the schematic pairing Hamiltonian [3]. It seems appropriate to investigate systematically the applicability of these techniques to several nuclei. In this work we do so and discuss improvements on the method presented in Ref. [2] for the case of an odd number of particles. Moreover, while in Ref. [2] the matrix elements in Eq. (1) were computed directly using the Gaussian path method, here we evaluate the energies of the many-body Hamiltonian as expectation values using the sampling method of Metropolis *et al.* [4].

We consider several erbium isotopes and a few dysprosium isotopes in the pairing plus quadrupole model. We use the restricted single-particle basis in the $N = 82$, $N = 126$ neutron major shell and in the $Z = 50$, $Z = 82$ proton major shell. We consider several isotopes with neutron number ranging from few to about 20 above the $N = 82$ shell closure. In Refs. [2,3], the sign fluctuations were suppressed by properly adjusting the chemical potentials. A question remains whether, with this method, the sign fluctuations in the functional integral can be eliminated entirely. We found that residual sign fluctuations remain for neutron numbers in the vicinity of the

$N = 82$ closure, but they disappear as the neutron number is increased. It should be mentioned, although we shall not dwell on it, that these sign fluctuations are also present if we switch off the quadrupole force in the model Hamiltonian and that with such a simplified model these fluctuations are completely absent in the vicinity of the $N = 126$ shell closure, below and above (in this latter case the single-particle space was increased).

In the rare earth region, other systematic Monte Carlo calculations have been performed by White, Koonin, and Dean [5]. In these calculations a different functional integral (that preserves the number of particles) was applied to the canonical ensemble unprojected partition function. It is straightforward to apply the projection methods of Ref. [2] to the type of functional integrals used in Ref. [5] as done in Ref. [6]. We found that these functional integrals are most useful in the case of an even number of particles, where the functional integral is free of sign oscillations in the case of zero angular momentum. However, in a trial case of an odd number of particles in the middle of neutron major shell, using the pairing plus quadrupole model, sign oscillations remained. In the formulation we use, instead, sign fluctuations disappear as we increase the particle number, as we shall see later.

Despite positivity of the functional integrals used in Ref. [5] in the case of $J^\pi = 0^+$, the number of integration variables is large (since it depends on the square of the number of the single-particle states in the basis), and if we were to extend the single-particle basis to the full basis employed by Kumar and Baranger [7], the number of integration variables would make practical calculations much more expensive precisely because of the large number of integration variables that have to be updated in the Monte Carlo calculation. On the other hand, the formulation that we discussed in Refs. [2,3] and that we use in this work does not change the dimensionality of the functional integral as we increase the size of the single-particle basis.

The outline of this paper is the following. In Sec. II we briefly review the method of evaluation of the matrix elements of Eq. (1) (Sec. II A) and discuss an improved method in the case of an odd number of particles, which greatly increases the speed of the calculation (Sec. II B), and the

method currently used to determine the chemical potentials (Sec. II C). In Sec. III we discuss the numerical calculations in the erbium region.

II. EVALUATION OF THE FUNCTIONAL INTEGRAL EXPRESSION OF MATRIX ELEMENTS $\mathcal{B}$

A. The functional integral

In order to shorten the equations, let us consider one kind of particle. The pairing + quadrupole Hamiltonian is defined as

$$\hat{H}=\hat{H}_0-\frac{k}{2}\sum_{a=-2}^{2}(-1)^a\hat{Q}_{-a}^{(2)}\hat{Q}_a^{(2)}-G\hat{P}^\dagger\hat{P}, \quad (2)$$

where $\hat{H}_0=\Sigma_{i=1}^{N_s}E_ia_i^\dagger a_i$ is the single-particle Hamiltonian for N_s single-particle levels. The second quantized operators $\hat{Q}_a^{(2)}=\Sigma_{i,j}(q_a^{(2)})_{ij}a_i^\dagger a_j$ (for $a=-2,\ldots,2$) are the spherical components of the quadrupole operator, and $\hat{P}=\Sigma_{i>0}a_{\bar{i}}a_i$ is the monopole pairing operator. Time reversal states are defined as $|i\rangle=|njm\rangle$ and $|\bar{i}\rangle=(-1)^{j+1/2}|nj-m\rangle$. The pairing operator is recast in the form

$$\hat{P}^\dagger=\frac{1}{2}a^\dagger\mathcal{P}a^\dagger, \quad (3)$$

where $\mathcal{P}$ is an antisymmetric matrix in the single-particle indices. Instead of using the spherical tensors $\hat{Q}_a^{(2)}$, we find it more convenient to work with their corresponding Cartesian components denoted as $\hat{Q}_a$ ($a=-2,-1,0,1,2$) (which are their real and imaginary parts). From Ref. [2], the functional integral expression for $e^{-\beta\hat{H}+\alpha\hat{N}}$ for any α is

$$e^{-\beta\hat{H}+\alpha\hat{N}}=e^{-\beta G\Omega/2}\mathcal{N}\int\prod_{n=1}^{N_t}\left(d\phi_{xn}d\phi_{yn}\prod_{a=-2}^{2}d\sigma_{an}\right)$$
$$\times\exp\left(-\frac{1}{2}\sum_{an}\sigma_{an}^2-\frac{1}{2}\sum_n(\phi_{xn}^2+\phi_{yn}^2)\right)\hat{U}, \quad (4)$$

where $\hat{U}$ is the evolution operator

$$\hat{U}=\hat{U}_{N_t}\hat{U}_{N_t-1}\cdots\hat{U}_1, \quad (5)$$

$$\hat{U}_n=\exp\left(-\epsilon\left[\hat{H}_0'-\sqrt{\epsilon k}\sum_a\sigma_{an}\hat{Q}_a\right.\right.$$
$$\left.\left.-\sqrt{\epsilon G/2}(\phi_n\hat{P}+\phi_n^\star\hat{P}^\dagger)\right]\right) \quad (6)$$

and $\phi_n=(\phi_{xn}+i\phi_{yn})$. In Eq. (6), $\hat{H}_0'=\hat{H}_0-\mu'\hat{N}$ and $\mu'=\mu-G/2$ ($\mu=\alpha/\beta$). $\mathcal{N}$ is the normalization constant

$$\mathcal{N}=\left(\frac{1}{2\pi}\right)^{7N_t/2}.$$

We write the functional integral using this form for the integration variables because it is the most appropriate to perform numerical calculations, regardless of the integration method. Second-quantized operators are denoted by capital letters with a caret and their corresponding first-quantized operators by lowercase letters.

Inserting Eq. (4) in Eq. (1), one has, for A particles,

$$\mathcal{B}=e^{-\beta G\Omega/2}\mathcal{N}\int\prod_{n=1}^{N_t}\left(d\phi_{xn}d\phi_{yn}\prod_{a=-2}^{2}d\sigma_{an}\right)$$
$$\times\exp\left(-\frac{1}{2}\sum_{an}\sigma_{an}^2-\frac{1}{2}\sum_n(\phi_{xn}^2+\phi_{yn}^2)\right)e^{-\alpha A}$$
$$\times\langle\psi,J,M,\pi,A|\hat{U}|\psi,J,M,\pi,A\rangle. \quad (7)$$

Since only the scalar part of $\hat{U}$ matters, we are allowed to replace the matrix elements of Eq. (7) with

$$B=\sum_M\frac{1}{2J+1}\langle\psi J,M,\pi,A|\hat{U}|\psi,J,M,\pi,A\rangle. \quad (8)$$

As in Ref. [2], we take trial states of a very simple form. For the case of an even number of particles and angular momentum and parity $J^\pi=0^+$, we take

$$|J^\pi=0^+\rangle=\hat{C}|0\rangle=e^{a^\dagger Xa^\dagger/2}|0\rangle\equiv\hat{V}|0\rangle, \quad (9)$$

where $|0\rangle$ is the particle vacuum and X is an antisymmetric matrix of the Clebsh-Gordan coefficients that couple the particle operators to zero angular momentum:

$$a^\dagger Xa^\dagger=\sum_i f_i[a_{j_i}^\dagger\times a_{j_i}^\dagger]^{(0)}. \quad (10)$$

For simplicity we take all $f_i=1$. For an odd particle number we take

$$|0^+,jm\rangle=a_{jm}^\dagger|0^+\rangle. \quad (11)$$

We stress that the essential requirements for these trial states are their angular momentum and parity content. Since we shall perform the exact calculation of the full functional integral using Monte Carlo methods, the details and the accuracy of these trial functions do not determine the final result, provided they are not orthogonal to the ground state; however, they might affect the temperatures at which the ground state dominates the matrix elements of Eq. (1).

To ensure proper particle number, the matrix elements B of Eq. (8) must be projected by a particle number operator. If we call $\wp_A$ the particle-number projector for A particles

$$\wp=\frac{1}{2\pi}\int_0^{2\pi}d\alpha\,e^{i\alpha(\hat{N}-A)} \quad (12)$$

and we denote

$$B'(z_p,z_q)=\frac{1}{2J+1}\sum_M\langle\psi,J,M,\pi|e^{i\alpha_p\hat{N}}\hat{U}e^{i\alpha_q\hat{N}}|\psi,J,M,\pi\rangle, \quad (13)$$

where

$$z_p=e^{i\alpha_p}, \quad z_q=e^{i\alpha_q}, \quad (14)$$

then Eq. (8) becomes

$$B = (2\pi)^{-2} \int_0^{2\pi} d\alpha_p d\alpha_q B'(z_p, z_q) e^{-i(\alpha_p + \alpha_q)A}. \quad (15)$$

Since the evaluation of B' in Eq. (15) requires a double particle-number projection, some manipulations are necessary in order to perform the calculation efficiently. This is the goal of the next subsection.

B. Evaluation of B' and B

The evaluation of Eq. (13) makes use of the quasiparticle formalism of Ref. [8] and follows the analysis done in Ref. [2]. The difference between the method illustrated here and the method used in Ref. [2] is that the method we discuss here is several times faster then that implemented in Ref. [2] for odd nuclei. In some of the calculations, discussed in Ref.

[2], we obtained an increase in the computational speed by about a factor of 7. To describe the method, let us give some definitions and let us rewrite the evolution operator of Eq. (5) as

$$\hat{U} = \mathcal{C}\hat{W}_{N_t}\hat{W}_{N_t-1}\cdots\hat{W}_1, \quad (16)$$

with

$$\mathcal{C} = \exp\left[-\frac{1}{2}\sum_{n=1}^{N_t} \mathrm{tr}\left(\epsilon h_0 - \epsilon\mu' - \sqrt{\epsilon k}\sum_{a=-2}^{2} \sigma_{an}q_a \right) \right], \quad (17)$$

where q_a is the single-particle quadrupole matrix and the trace is over the single-particle indices. In Eq. (6) the modified propagators $\hat{W}_n$ are given by

$$\hat{W}_n = \exp\left[\frac{1}{2}(a^\dagger, a) \begin{pmatrix} -(\epsilon h_0 - \epsilon\mu' - \sqrt{\epsilon k}\sigma_{an}q_a) & -\sqrt{\epsilon G/2}\phi_n^\star\mathcal{P} \\ \sqrt{\epsilon G/2}\phi_n\mathcal{P} & \epsilon h_0 - \epsilon\mu' - \sqrt{\epsilon k}\sigma_{an}\tilde{q}_a \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right]. \quad (18)$$

Exponential operators of a quadratic form in the creation and annihilation operators, such as

$$\hat{W} = \exp\left[\frac{1}{2}(a^\dagger, a)R\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right], \quad (19)$$

provided $R_{11} = -\tilde{R}_{22}$, and $R_{12} = -\tilde{R}_{21}$, form a group; more precisely

$$\exp\left[\frac{1}{2}(a^\dagger, a)R_1\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right]\exp\left[\frac{1}{2}(a^\dagger, a)R_2\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right] = \exp\left[\frac{1}{2}(a^\dagger, a)R\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right], \quad (20)$$

with the matrix R determined by

$$e^{R_1}e^{R_2} = e^R. \quad (21)$$

The matrices W_n associated with $\hat{W}_n$ are given by

$$W_n = \exp\left[\begin{pmatrix} -(\epsilon h_0 - \epsilon\mu' - \sqrt{\epsilon k}\sigma_{an}q_a) & -\sqrt{\epsilon G/2}\phi_n^\star\mathcal{P} \\ \sqrt{\epsilon G/2}\phi_n\mathcal{P} & \epsilon h_0 - \epsilon\mu' - \sqrt{\epsilon k}\sigma_{an}\tilde{q}_a \end{pmatrix} \right]. \quad (22)$$

The matrix $\mathcal{P}$ in Eq. (18) is the same as that appearing in the definition of the pairing operator [Eq. (3)]. Moreover, if we set $z = e^{i\alpha}$, the operator $e^{i\alpha\hat{N}}$ is rewritten as

$$e^{i\alpha\hat{N}} = z^{N_s}\hat{P}_N = z^{N_s}\exp\left[\frac{1}{2}(a^\dagger, a)\begin{pmatrix} i\alpha & 0 \\ 0 & -i\alpha \end{pmatrix}\begin{pmatrix} a \\ a^\dagger \end{pmatrix} \right] \quad (23)$$

and therefore its representation matrix is

$$\begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix}.$$

The operator $\hat{V}$, defined in Eq. (9), is represented in the same way. The quantities to be evaluated, for the cases of even and odd numbers of particles, are, respectively,

$$B'_e = (z_p z_q)^{N_s}\mathcal{C}\langle 0|\hat{V}^\dagger \hat{P}_N(z_p)\hat{W}\hat{P}_N(z_q)\hat{V}|0\rangle, \quad (24)$$

$$B'_o = (z_p z_q)^{N_s}\mathcal{C}\langle 0|a_k\hat{V}^\dagger \hat{P}_N(z_p)\hat{W}\hat{P}_N(z_q)\hat{V}a_k^\dagger|0\rangle, \quad (25)$$

with k being a single-particle index. Respectively, they are the vacuum matrix elements and one-particle matrix elements of the modified propagator

$$\hat{W}' = \hat{V}^\dagger \hat{P}_N(z_p)\hat{W}\hat{P}_N(z_q)\hat{V}. \quad (26)$$

The vacuum expectation value of this propagator is given by

$$\langle 0|\hat{W}'|0\rangle = [\det(W'_{22})]^{1/2}, \tag{27}$$

where W'_{22} is the 2×2 submatrix of the matrix W' associated with $\hat{W}'$. Similarly, the one-particle expectation value of $\hat{W}'$ is given by

$$\langle 0|a_k\hat{W}'a_k^\dagger|0\rangle = (W'_{22})_{kk}^{-1}[\det W'_{22}]^{1/2}. \tag{28}$$

Since W'_{22} depends in a nontrivial way on z_p and z_q, optimal ways of evaluating both the determinant and the inverse in the above expressions have to be found in order to avoid the costly evaluation for all z_p and z_q. In Ref. [2], we discussed how this can be done for Eq. (27) (even systems), where we reduced the evaluation of such determinants to the evaluation of determinants of a matrix that depends on only one of the variables z_p or z_q. Here we discuss how a similar technique can be implemented for the case of an odd particle number, instead of evaluating the inverse and the determinant in Eq. (28) for all values of the fugacities z_p and z_q, as previously done for numerical stability.

As done in Ref. [2], the matrix W' can be obtained from the multiplication law of the matrices associated with the factors in Eq. (26). The result for W_{22} is

$$W'_{22}=(z_pz_q)^{-1}[W_{22}+z_q^2W_{21}X-z_p^2X(z_q^2W_{11}X+W_{12})], \tag{29}$$

where the matrix X is given by Eq. (10). In the Appendix we show that this matrix can be rewritten as

$$W'_{22}=(z_pz_q)^{-1}(1+z_p^2XG_q)W_{22}(1+z_q^2DX), \tag{30}$$

where the matrices D and G_q are antisymmetric and given by

$$D=W_{22}^{-1}W_{21}, \tag{31}$$

$$G_q=-[C+z_q^2\widetilde{W}_{22}^{-1}X(1+z_q^2DX)^{-1}W_{22}^{-1}], \tag{32}$$

with $C=W_{12}W_{22}^{-1}$. These expressions show that the calculation of the determinant and of the inverse of W'_{22} can be carried out efficiently because of the simple dependence on z_q and z_p of the factors in Eq. (30). A single diagonalization is sufficient to obtain the determinant and the inverse of $1+z_q^2DX$, and the eigenvalues and eigenvectors of G_q depend only on z_q. Using these expressions, Eqs. (25) and (26) become

$$B'_e(z_p^2,z_q^2)=\mathcal{C}|W_{22}|^{1/2}|1+z_q^2DX|^{1/2}|1+z_p^2XG_q|^{1/2} \tag{33}$$

and

$$B'_o=\mathcal{C}z_pz_q[(1+z_q^2DX)^{-1}W_{22}^{-1}(1+z_p^2XG_q)^{-1}]_{kk}$$
$$\times|W_{22}|^{1/2}|1+z_q^2DX|^{1/2}|1+z_p^2XG_q|^{1/2}. \tag{34}$$

Some observations are in order about the structure of Eqs. (33) and (34). Let us consider first Eq. (33). In Eq. (33) the dependence on the variables is only quadratic, so rather than project to a given particle number, we can most simply

project to a given number of pairs. The double particle-number projection can be achieved by simply replacing the integrals over z_p and z_q in Eq. (14) by the double sum

$$B_e(A)=\frac{1}{(N_p+1)^2}\sum_{l,m=0}^{N_p}B'(l,m)\exp\left(-i\frac{2\pi}{N_p+1}(1+m)\nu\right), \tag{35}$$

where $\nu=A/2$ is the number of pairs, N_p is the maximum number of pairs, and $B'(l,m)$ is $B'(z_p,z_q)$ evaluated at $z_q^2=e^{i2\pi l/(N_p+1)}$ and $z_q^2=e^{i2\pi m/(N_p+1)}$. The projection over A particles of the sum over l can be carried out very simply using the recursion relations of Ref. [9] [cf. Eqs. (41)–(44) of Ref. [9]]. First, the matrix XG_q is diagonalized for all values of $z_q^2=e^{i2\pi m/(N_p+1)}$. Since XG_q is the product of two antisymmetric matrices, its spectrum has a double degeneracy [2], and this allows a simple evaluation of the square root of $|1+z_p^2XG_q|$. Then, the coefficient of the power z_p^A in B' can be evaluated with the aforementioned recursion relations. We are then left with only one sum over z_q^2. The square root of $|1+z_q^2DX|$ is simply $\Pi(1+z_q^2\lambda)$, where the λ's are the eigenvalues of DX (one per degenerate pair).

The square root of $\det W_{22}$ (the vacuum contribution), as well as its sign, can be evaluated by factorizing the matrix W_{22} into a product of vacuum matrices at a higher temperature, as discussed in Ref. [2], to which we refer. In the calculation discussed here, we factorized the vacuum contribution with a product of vacuum terms at a temperature equal to $4/\beta$.

Let us discuss now the structure of Eq. (34) relative to the odd-number case. Because of the presence of the factor z_pz_q, B'_o contains only an odd number of particles. Since the remaining dependence on the fugacities contains only an even power, the remaining part of B'_o has to be projected to the number pairs $(A-1)/2$. To understand the structure of contributions to the particle-number projected B_o, consider, in Eq. (34), a fixed value of z_q^2. The z_p dependence in $B'_o(z_p)$ is determined by the matrix

$$(1+z_p^2XG_q)^{-1}|1+z_p^2XG_q|^{1/2}.$$

If λ_k are the eigenvalues of XG_q with eigenvectors V_{ik} and if we call λ_{-k} the degenerate partner of λ_k, one has

$$(1+z_p^2XG_q)_{ij}^{-1}|1+z_p^2XG_q|^{1/2}$$

$$=\sum_{k>0}[V_{ik}V_{kj}^{-1}+V_{i-k}V_{-kj}^{-1}]\prod_{k'>0,\ k'\neq k}(1+z_p^2\lambda'_k), \tag{36}$$

so the term in square brackets plays the role of a density (although in a generalized sense), and the product over the eigenvalues gives the contribution of the remaining $(A-1)/2$ pairs.

C. The determination of the chemical potentials

From the structure of the propagator appearing in Eq. (6), it is seen that the values of the integrand depend on the

selected values of the chemical potential. Here we discuss how such a determination is made in practice. As pointed out in previous works that use this functional integral formulation, the value of the chemical potential affects the amount of sign fluctuations in a Monte Carlo calculation. In fact, although we work exclusively with canonical quantities (i.e., pertaining to a fixed value of the particle number), the propagator, appearing in the functional integral, contains several particle-number components (since it does not conserve particle number), and the chemical potential fixes the average particle number. Differently stated, each evolution operator $\hat{U}_n$ in Eq. (5), acting on a state of exactly A particles, will generate components with several particle numbers. These spurious particle-number components are suppressed by an appropriate choice of the chemical potential only in an average sense. If we do not fix optimally the chemical potential, these spurious particle-number components would be cancelled only upon integration, and this could cause sign fluctuations. An obvious limitation of this method is that in some cases the chemical potential might not suppress entirely spurious particle-number components. However, as discussed in the next section, they do so especially as we increase the number of particles.

In practice, we determine the chemical potential by minimizing the matrix elements, in the integrand of Eq. (9), as a function of the chemical potential, only at the mean field. The mean field is the integration point at which the integrand reaches its maximum. This mean field is time dependent and the mean-field variables (both deformation and pairing variables) turned out to be even in time, in the interval $[0, \beta]$ around $\beta/2$, in a few cases where the variation of the variables was left unconstrained. Because of this, we implement this time-even feature as a constraint in the determination of the solution of the mean-field equations; this time-even constraint considerably reduces the computational effort. The mean-field equations are obtained by maximizing the effective action

$$S_{\text{eff}} = -\tfrac{1}{2} \sum_{an} \sigma_{an}^2 - \tfrac{1}{2} \sum_n (\phi_{xn}^2 + \phi_{yn}^2)$$

$$+ \ln[\langle \psi, J, M, \pi, A | \hat{U} | \psi, J, M, \pi, A \rangle], \qquad (37)$$

as a function of the time-dependent variables σ_{an}, ϕ_{xn}, and ϕ_{yn}. If we denote by x_n any of these variables, the mean-field equations are

$$x_n = \partial_{x_n} \ln[\langle \psi, J, M, \pi, A | \hat{U} | \psi, J, M, \pi, A \rangle], \qquad (38)$$

with periodic boundary conditions in the interval $[0, \beta]$. Numerically these equations are solved by inserting some initial starting values in the right-hand side of the above equation and taking the left-hand side as new values. Typically, if we take the static mean-field solutions as starting values, convergence is quickly achieved. However, if the particle number is small, convergence can be slow. The mean-field equations are solved for several values of the chemical potential until the minimum value of the effective action, as a function of the chemical potential, is found.

Time-dependent mean-field equations of this type, although in a different context have, also been discussed in Ref. [10]. Here, they appear because the static mean-field equations do not represent the maximum of the effective action.

III. MONTE CARLO CALCULATIONS

Let us now discuss the numerical results. The model Hamiltonian is the pairing plus quadrupole Hamiltonian with a restricted single-particle basis. The neutron states comprising the basis are $0h9/2$, $1f7/2$, $1f5/2$, $2p3/2$, $2p1/2$, and $0i13/2$, and the proton states $0g7/2$, $1d5/2$, $1d3/2$, $2s1/2$, and $1h11/2$. The strength of the forces, the single-particle energies, and the matrix elements of the quadrupole operator are taken from Ref. [7], except for the size of the basis, which is restricted here to one major shell. The quantities that are evaluated are the energies, given by

$$\langle \hat{H} \rangle = - \partial_\beta \ln \langle \psi, J, M, \pi, N, Z | e^{-\beta \hat{H}} | \psi, J, M, \pi, N, Z \rangle. \qquad (39)$$

We rewrite the functional integral expression for the matrix elements in Eq. (39) schematically as

$$\langle \psi, J, M, \pi, N, Z | e^{-\beta \hat{H}} | \psi, J, M, \pi, N, Z \rangle = \int dx \, e^{S_{\text{eff}}(\beta, x)} s, \qquad (40)$$

where $se^{S_{\text{eff}}(\beta, x)}$ is the real part of the integrand of the functional integral, x denotes the set of integration variables, and s is the sign; then we have

$$\langle \hat{H} \rangle = \frac{\int dx \, e^{S_{\text{eff}}(\beta, x)} s[- \partial_\beta S_{\text{eff}}(\beta, x)]}{\int dx \, e^{S_{\text{eff}}(\beta, x)} s}. \qquad (41)$$

This expression is rewritten as the ratio of expectation values

$$\langle \hat{H} \rangle = \frac{\langle s[- \partial_\beta S_{\text{eff}}(\beta, x)] \rangle}{\langle s \rangle}, \qquad (42)$$

where the expectation values in the right-hand side are evaluated with the probability density $e^{S_{\text{eff}}}$, for example,

$$\langle s[- \partial_\beta S_{\text{eff}}(\beta, x)] \rangle = \frac{\int dx \, e^{S_{\text{eff}}(\beta, x)} s[- \partial_\beta S_{\text{eff}}(\beta, x)]}{\int dx \, e^{S_{\text{eff}}(\beta, x)}}.$$

Each expectation value in the right-hand side of Eq. (42) is evaluated using the method of Metropolis *et al.* [4]. The statistical error of the ratio in Eq. (42) is evaluated using the following expression for the variance of two random variables r_1 and r_2 with variances ϵ_1 and ϵ_2:

$$\sigma(r_1/r_2)$$

$$= \left| \frac{\langle r_1 \rangle}{\langle r_2 \rangle} \right| \sqrt{\left(\frac{\epsilon_1}{\langle r_1 \rangle} \right)^2 + \left(\frac{\epsilon_2}{\langle r_2 \rangle} \right)^2 - 2 \frac{\langle r_1 r_2 \rangle - \langle r_1 \rangle \langle r_2 \rangle}{\langle r_1 \rangle \langle r_2 \rangle}}. \qquad (43)$$

In this expression, the variances ϵ_1 and ϵ_2 and the correlation $\langle r_1 r_2 \rangle - \langle r_1 \rangle \langle r_2 \rangle$ refer to the Monte Carlo averages and not to the corresponding quantities of set of the samples generated during the Monte Carlo calculation. The variances and correlation of the averages are related to the corresponding quantities computed using the samples by the familiar factor $1/\sqrt{n_{\text{sample}}}$, where n_{sample} is the number of uncorrelated samples.

The calculation is performed as follows. First the chemical potentials, for both neutrons and protons, are determined as discussed in Sec. II C; then sample points of the integration domain are generated by updating all variables. A full update is performed by first updating all variables at a fixed time interval (for this model we have only five deformation variables, and four pairing variables in every time interval) while keeping all other variables fixed, then by repeating the procedure at every time interval in sequence. The starting configuration is usually the solution of the mean-field equations (since it is determined anyway); sometimes, however, we start the calculation from the typical values of the integration variables in neighboring systems. We took the as transition probability from one integration point x to $y \neq x$,

$$T(x \rightarrow y) = N(x-y) \min[1, \exp(S_{\text{eff}}(y) - S_{\text{eff}}(x))],$$

where $N(x-y)$ is a Gaussian distribution of $x-y$.

After all variables have been updated, the value of $[-\partial_\beta S_{\text{eff}}(\beta, x)]s$ and of the sign s are calculated. Strictly speaking, all values generated in this way should be statistically independent and distributed according to the probability density $e^{S_{\text{eff}}(\beta, x)}$. Since the initial integration point usually has a small probability of being generated during the Monte Carlo calculation, a number of values generated initially have to be discarded (this is the so-called "thermalization step").

The values of $\partial_\beta S_{\text{eff}}(\beta, x)$ are generated sequentially, and therefore they are strongly correlated. Therefore we consider, as is usually done for the statistical analysis, only one value for every n_{dec} value (this is the so-called decorrelation step). As a consequence, most of the data set is discarded and we are left with a small fraction of the initial data set.

The mean-field effective action, although being the largest effective action, is not the most probable one. This implies that the region close to the mean field (e.g., mean field with small-amplitude perturbations) are not generated during the Monte Carlo simulation. In order to determine the most probable value of the effective action, let us assume that it can be expanded with a quadratic form in the vicinity of the mean-field x_0, i.e.,

$$e^{S_{\text{eff}}(\beta, x)} = \approx e^{S_{\text{eff}}(\beta, x_0) - (x_i - x_{0i}) M_{ij}(x_j - x_{0j})/2},$$

where M is the matrix of the second derivative of the effective action as a function of the integration variable x_i. Almost all the eigenvalues m_k of the matrix M are between 0 and 1 (only the eigenvalue corresponding to the deformation variable γ is much larger than 1). Using the eigenvectors v of this matrix, $M_{ij} = v_{ik} m_k v_{jk}$, we can perform a change in the integration variables to new variables u_k, defined as x_j

$-x_{0j} = \Sigma_k \sqrt{m_k} v_{jk} u_k$. The variables u_k have a Gaussian distribution $\exp(-\frac{1}{2}\Sigma_k u_k^2)$. The region $u_k \approx 0$ has a negligibly small probability of being generated in the Monte Carlo simulation. The most probable effective action has $\Sigma_k u_k^2$ approximately equal to the dimensionality of the integral, as can be seen using polar coordinates.

Differently stated, the probability of having a particular value S for the effective action is given by $e^S V(S) dS$, where $V(S) dS = \int dx \, \delta(S - S_{\text{eff}})$ is the volume of the integration domain in which the action equals S. It is not the absolute value of S that matters, but rather, the product $e^S V(S)$. This is readily verified in the Monte Carlo calculation, where the effective actions, generated by the Metropolis algorithm, show very large deviations from their mean-field value.

If we start the calculation near the mean field, all integration points generated with the Metropolis method quickly depart from this initial point and never approach it again. Typically we have to discard the first few thousand integration points to avoid sensitivity to the initial start.

In the Metropolis algorithm, each integration point is updated in the neighborhood of the previous one. Since we have only nine variables at each time interval, we can perform updates with a large step and still have a large acceptance ratio (typically, at any time interval, acceptance ratios are as high as 50% and 70% with a step size of about 0.25–0.5. Even with such large steps, considerable correlation remains between one integration point and the next. Typically we keep one point about every 10 or 20 steps. The sizes of these decorrelation steps are decided by keeping the energy autocorrelation function ≈ 0.4 or smaller. The numerical results are summarized in Table I. Together with the nuclei, the J^π values, the energies, and the inverse temperatures that have been used, we also show the average sign $\langle s \rangle$, the number of decorrelation steps n_{dec} (we took 2000 thermalization steps), and the residual number of samples n_{sample} used in the statistical analysis after thermalization and decorrelation. We consider a single long Markov chain.

Despite the large number of decorrelation steps, the residual autocorrelations in the samples remains high, which probably leads to underestimated statistical errors.

It is worth mentioning that the energies evaluated near the time-dependent mean field, during the calculation, are several MeV (typically 5–7 MeV) higher than the expectation values. All calculations have been performed with the weights, defined by Eqs. (10) and (11), $f_i = 1$ and with $\beta/N_t = 0.0625$.

There are several features that emerge from the results. Together with the erbium isotopes we also show some calculations for ^{153}Dy and ^{157}Dy. Typically, the statistical errors are rather small; they range from about 100 keV in the case of large neutron number to few hundred keV for small neutron number. This is true for both even and odd nuclei, and despite the small number of samples remaining after the thermalization and decorrelation steps (about 400 for the heavy systems and 900 for the light dysprosium isotopes). The number of decorrelation steps depends on the number of neutrons: is relatively small for light systems but large for the heavy ones. The average sign is nearly 1 for heavy systems,

TABLE I. Monte Carlo results for the energies E. n_{dec} is the number of decorrelation steps. $\langle s \rangle$ is the average sign.

Nucleus	J^{π}	β	n_{dec}	n_{sample}	Autocorrelation	$\langle s \rangle$	$E \pm \delta E$ (MeV)
^{171}Er	$\frac{13}{2}+$	4.0	23	348	0.5	0.99	-125.587 ± 0.105
^{169}Er	$\frac{9}{2}-$	4.0	20	401	0.3	0.99	-120.67 ± 0.097
^{168}Er	0^+	2.0	30	600	0.5	1.0	-118.961 ± 0.116
^{167}Er	$\frac{9}{2}-$	4.0	20	378	0.4	0.92	-114.436 ± 0.175
		3.0	20	401	0.5	0.95	-114.517 ± 0.136
		2.0	20	401	0.4	0.99	-114.747 ± 0.147
^{166}Er	0^+	4.0	20	344	0.5	0.91	-112.802 ± 0.131
		3.0	20	378	0.5	0.98	-112.951 ± 0.151
		2.0	20	318	0.5	1.0	-112.772 ± 0.182
^{165}Er	$\frac{9}{2}-$	4.0	20	408	0.4	0.82	-108.475 ± 0.116
		3.0	20	428	0.5	0.91	-108.365 ± 0.131
		2.0	20	417	0.4	0.99	-107.836 ± 0.130
^{165}Er	$\frac{13}{2}+$	4.0	20	424	0.4	0.92	-108.656 ± 0.103
		3.0	20	396	0.4	0.90	-108.068 ± 0.132
		2.0	20	401	0.5	1.0	-107.829 ± 0.138
^{165}Er	$\frac{7}{2}-$	4.0	15	490	0.4	0.94	-108.200 ± 0.95
		3.0	20	436	0.5	0.97	-108.467 ± 0.105
		2.0	20	445	0.4	0.99	-107.443 ± 0.125
^{164}Er	0^+	2.0	20	402	0.5	0.98	-106.352 ± 0.141
^{162}Er	0^+	2.0	20	401	0.4	0.95	-98.309 ± 0.140
^{160}Er	0^+	2.0	12	667	0.4	0.72	-90.434 ± 0.138
^{158}Er	0^+	2.0	12	667	0.4	0.75	-81.780 ± 0.136
^{156}Er	0^+	2.0	12	1010	0.3	0.60	-72.994 ± 0.127
^{154}Er	0^+	2.0	12	784	0.4	0.43	-63.726 ± 0.217
^{157}Dy	$\frac{7}{2}-$	4.0	10	1257	0.3	0.23	-82.393 ± 0.313
^{153}Dy	$\frac{7}{2}-$	4.0	10	901	0.3	0.29	-64.877 ± 0.330
		3.0	10	801	0.3	0.31	-64.636 ± 0.250

but sign statistics tend to worsen as the neutron number is decreased. Despite this, errors are reasonable. Numerically the three terms appearing inside the square-root expression of Eq. (43) nearly cancel each other out.

In order to understand qualitatively the reason why the statistical errors are so small in the case of strong sign oscillations (we obtained average signs as small as 0.2), let us note that, apart from the sign, the quantity $a \equiv -\partial_{\beta} S_{eff}(\beta, x)$ is nearly constant, especially at low temperature. Let us consider for the sake of argument the sign as an integer random variable approximately uncorrelated to a. Then one has (here σ denotes the variance)

$$\langle \hat{H} \rangle = \langle a \rangle, \quad \sigma(\langle \hat{H} \rangle) = \sigma(a)/\langle s \rangle. \tag{44}$$

Therefore, if the derivative of the effective action is nearly constant in the important region of the integration domain, the error of the ratio is small and the sign does not affect the expectation values of $\hat{H}$. This is true if the sign and the derivative of the effective action are decorrelated. Since some correlations are present, some deviations from the approximate expressions presented above should be expected. The deviations of $\langle \hat{H} \rangle$ from the approximate expression of Eq. (44) induced by the correlation between a and s are

typically few to several hundreds of keV for the light systems and only in the case of ^{154}Er is the deviation 1 MeV. The approximate error formula is rather accurate. Apart from these small deviations occurring for light systems, the energy expectation values are not strongly affected by the sign. The statistical error instead is inversely proportional to the average sign, but the fluctuations of a are small and this results in a tolerable statistical error of the energy.

The energy $-\partial_{\beta} S_{eff}(\beta, x)$ decreases as we depart from the mean-field region, and since we never sample this region with appreciable probability, we sample a region in the integration volume in which the above-noted quantity assumes values substantially lower than the mean-field value by several MeV. Also, the difference between the effective action evaluated at the mean field and the typical effective action of the samples is rather large, as previously explained; for $\beta = 2$, for example, this difference fluctuates around 100–140. Although the relative probability of the integration points versus the mean-field probability is rather small, they have a much larger volume.

To summarize the findings of this work, we have shown that sign fluctuations decrease as we increase the particle number. Moreover, despite sign fluctuations in light systems, the samples generated by the Monte Carlo method give small

statistical errors, since apart from the sign $\langle s \rangle$ the energy is nearly a constant. In this respect, it is conceivable that also other functional integrals having sign fluctuations could be evaluated using Monte Carlo techniques. Finally, we have discussed an improved method for the evaluation of the functional integral in the case of odd systems.

APPENDIX

Here we prove Eq. (30), which we found numerically stabler than Eq. (29). The matrices W satisfy the identity (cf. Ref. [8])

$$W^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \widetilde{W} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{A1}$$

If we set

$$C = W_{12} W_{22}^{-1}, \quad D = W_{22}^{-1} W_{21}, \tag{A2}$$

expanding Eq. (A1), we obtain

$$\widetilde{C} = -C, \quad \widetilde{D} = -D, \tag{A3}$$

and

$$W_{11} = \widetilde{W}_{22}^{-1} + W_{12} D. \tag{A4}$$

If we set

$$M_q = -X(z_q^2 W_{11} X + W_{12}),$$

$$N_q = z_q^2 W_{21} X + W_{22}, \tag{A5}$$

we have, from Eq. (29),

$$W_{22}' = (z_p z_q)^{-1} [1 + z_p^2 M_q N_q^{-1}] N_q. \tag{A6}$$

The matrix N_q can be written as

$$N_q = W_{22}'(1 + z_q^2 D X). \tag{A7}$$

Combining Eqs. (A5) and (A4), we have

$$M_q = -X[z_q^2 \widetilde{W}_{22}^{-1} X + W_{12}(1 + z_q^2 D X)], \tag{A8}$$

and using Eq. (A7)

$$M_q N_q^{-1} = -X[C + z_q^2 \widetilde{W}_{22}^{-1} X(1 + z_q^2 D X)^{-1} W_{22}^{-1}], \tag{A9}$$

from which Eq. (30) follows directly.

[1] J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959); R. D. Stratonovich, Dokl. Akad. Nauk SSSR **115**, 1907 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)].

[2] G. Puddu, Eur. Phys. J. A **9**, 171 (2000).

[3] G. Puddu, J. Phys. G **26**, 1635 (2000).

[4] N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[5] J. A. White, S. Koonin, and D. J. Dean, Phys. Rev. C **61**, 034303 (2000), and references therein.

[6] G. Puddu, J. Phys. G **27**, L1 (2001).

[7] K. Kumar and M. Baranger, Nucl. Phys. **A110**, 529 (1968).

[8] R. Balian and E. Brezin, Nuovo Cimento Soc. Ital. Fis., B **64**, 37 (1969).

[9] G. Puddu, Phys. Rev. C **59**, 2500 (1999).

[10] S. Levit, J. W. Negele, and Z. Paltiel, Phys. Rev. C **21**, 1603 (1980); A. K. Kerman and S. Levit, *ibid.* **24**, 1029 (1981).