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General canonical ensemble functional integral formalism with Hamiltonians containing pairing interactions and Monte Carlo calculations for even-even, even-odd, and odd-odd nuclei

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We present a functional integral formulation in the canonical ensemble for Hamiltonians containing pairing interactions, equally applicable for even-even, even-odd, and odd-odd nuclei. A general stabilization technique, necessary for Monte Carlo calculations is discussed and applied, within the Gaussian path Monte Carlo method, to nuclei in the rare-earth region. Approximations, such as the Hartree-Bogoliubov mean-field, and the static path approximations, defined directly in the canonical ensemble, are discussed.
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I. INTRODUCTION

The problem of the proper inclusion of pairing effects in the low-energy nuclear structure is an old and important one (see, for example, Ref. [1], and references therein). In this work we present the details of a new formalism which incorporates the pairing terms in the Hamiltonian in the calculation of the nuclear partition function, applicable for both even and odd particle numbers. So far, no Monte Carlo calculations for both an even and odd number of particles have been performed, because of strong sign fluctuations for an odd number of particles. The method presented in this work seems to solve such a problem, at least in the cases studied so far. The principal motivation behind this work is, first of all, that the Hamiltonian relevant for nuclear physics can be studied in an exact fashion and also we can understand quantitatively the validity of approximation schemes for realistic models. Usually approximation schemes are tested in solvable models rather than realistic models and their validity in the solvable models is extrapolated to the realistic cases. In particular, the formalism, well suited for both even and odd particle systems, allows a systematic study of the validity of approximations (such as the Hartree-Bogoliubov approximation) in a fashion that strictly conserves the particle number as well as computation of the partition function via the Monte Carlo integration technique. The details of the Monte Carlo technique used to carry out the actual integration are discussed somewhere else (Refs. [2–4]), and will not be reviewed here. We entirely avoid the use of particle number projection techniques (Ref. [1]), rather we offer a new way of computing traces in the canonical ensemble (i.e., with a given number of particles) of evolution operators which do not conserve the particle number. The method we shall discuss gives, as a bonus, also a simple way to perform calculations in the grand-canonical ensemble. An intrinsic ambiguity in all approximation schemes in the canonical ensemble is also brought into light by the new formalism.

Pairing effects are parametrized, in the nuclear Hamiltonian, with nonlocal interaction terms $a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$ where $i,\bar{i}$ are single-particle time-reversal orbits (monopole pairing). Sometimes higher angular momentum pairing terms are considered, such as quadrupole pairing. The formalism and techniques, such as computation of traces in the canonical ensemble, discussed in this work apply to general pairing interactions; only for sake of argument (the numerical calculations have been performed using the pairing+quadrupole model), we shall work with monopole pairing interaction. In order to make the formalism applicable to nuclei in the low-temperature region, we shall also present numerical stabilization techniques, which are necessary for the Monte Carlo calculations. The simplest instance of these techniques has been used in a preliminary report of this work (Ref. [5]).

The idea of parametrizing the short-range part of the residual interaction with pairing terms is the traditional one, and the standard theory of collective motion in nuclei is based on it. However, one can speculate, since the pairing term comes from a short-range part of the residual interaction, whether the same physics can be recast in terms of local (e.g., δ forces) rather than nonlocal forces.

The residual two-body interaction can be written either as a sum of squares of one-body operators containing terms like $a_i^\dagger a_j$, or a sum of pairing operators, containing terms like $a_i^\dagger a_j^\dagger$ times their Hermitian conjugates, or a combination of both. The separation of the residual interaction into a sum of squares of the particle-number preserving part and into a pairing part is here model given. In principle however, one has the freedom of casting the full Hamiltonian or just parts of it, in terms of the pairing field. The separation is, to some extent, arbitrary. Ideally one would like to make such a separation so that, once the Hubbard-Stratonovich transformation is applied, sign fluctuations in the functional integral expression of the partition function, as well as other sources of statistical errors, are suppressed in the Monte Carlo integration. This, however, can be decided *a posteriori*, rather than *a priori*. As one *a-priori* criterion we take a decomposition so that the resulting integrand inside the functional integral (FI) has the same symmetry properties of the original two-body Hamiltonian (in our case rotational invariance).

An additional motivation for this work is that we would like to make the bridge between the exact FI and standard approaches (such as the Hartree-Bogoliubov approximation in the Grand-Canonical ensemble) conceptually simple and natural. If the monopole pairing interaction would be written in a particle number preserving form the rotational invariance of the integrand would be destroyed and there is no simple way of connecting the Hartree-Bogoliubov approximation to the FI.

This ambiguity expresses only one of the freedoms of writing the FI for a given Hamiltonian. Another important one, pointed out in Ref. [2], is the following. In the grand-canonical ensemble the chemical potential is fixed so that the average particle number has a desired value. In a canonical ensemble FI, a term like $-\mu\hat{N}$ in the Hamiltonian (where μ is the chemical potential and $\hat{N}$ is the particle number operator) does not change the exact partition function; however, it leads to a different functional integral, and therefore to different canonical ensemble mean fields (defined as the maximum of the functional integrand), one for each value of the chemical potential. This freedom (or ambiguity) was used in order to suppress sign fluctuations in Ref. [2]. Since this point is important, it will be emphasized in the discussion below.

From a broader theoretical point of view one would like to have a formalism which systematically allows one to correct known approximation schemes in the grand-canonical and in the canonical ensemble, starting from the underlying two-body Hamiltonian. Our main concern is, however, the application of this formalism to exact calculations relevant to nuclear problems for both even and odd neutron and proton numbers, but the formalism, because of its generality, could also be useful in other context such as pairing phenomena in condensed-matter physics.

The theoretical starting point is provided by the Hubbard-Stratonovich transformation (Ref. [6]) and by a new general method of computing fermionic traces in the canonical ensemble in the presence of pairing operators. In order to elucidate the features of the canonical ensemble partition function, brought into light by the new formalism, we shall also discuss widely used schematic pairing model (i.e., without the quadrupole force) the degenerate version of which is widely used in testing approximation schemes.

The outline of this paper is as follows: in Sec. II we shall recall the derivation of the FI starting from the two-body Hamiltonian. In Sec. III we shall go into the details of a general method of computing traces in the canonical and grand-canonical ensembles when pairing terms are present. In Sec. IV we discuss the mean-field, and the static path approximations (Ref. [7]) as an application of the formalism and apply it to the schematic pairing model. In Sec. V we discuss Monte Carlo calculation in the canonical ensemble. Some of the elements of the formalism discussed here in detail were introduced in Ref. [5].

II. THE FI FOR THE PARTITION FUNCTION

We shall consider for sake of argument the pairing plus quadrupole Hamiltonian of Baranger and Kumar (Ref. [8])

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

where $\hat{H}_0=\Sigma_{i=-\Omega}^{\Omega}E_i a_i^\dagger a_i$ is the single-particle Hamiltonian, $\hat{Q}^{(2)}_a=\Sigma_{i,j}(q^{(2)}_a)_{ij}a_i^\dagger a_j$ (for $a=-2,\dots,2$) are the spherical components of the quadrupole operator and $\hat{P}=\Sigma_{i>0}a_{-i}a_i$ is the monopole pairing Hamiltonian. The labels $i>0$, $-i$ $(=\overline{i})$ refer to time-reversal orbits. $N_s=2\Omega$ is the total number of available single-particle states.

$$\hat{P}=\frac{1}{2}a^\dagger\mathcal{P}a^\dagger, \tag{2}$$

where $\mathcal{P}$ is an antisymmetric matrix in the single-particle indices. In the discussion that follows the details of the pairing matrix $\mathcal{P}$ as well as of the quadrupole force are irrelevant, as the considerations below apply regardless of the specific form of these matrices. To shorten the formulas we shall consider one particle species. By defining the real and imaginary parts of the quadrupole operators as

$$\hat{Q}_2=(\hat{Q}^{(2)}_2+\hat{Q}^{(2)}_{-2})/\sqrt{2},\quad \hat{Q}_{-2}=(\hat{Q}^{(2)}_2-\hat{Q}^{(2)}_{-2})/i\sqrt{2},$$

$$\hat{Q}_1=(\hat{Q}^{(2)}_1-\hat{Q}^{(2)}_{-1})/i\sqrt{2},\quad \hat{Q}_{-1}=(\hat{Q}^{(2)}_2+\hat{Q}^{(2)}_{-2})/\sqrt{2},$$

$$\hat{Q}_0=\hat{Q}^{(2)}_0 \tag{3}$$

the quadrupole part of Eq. (1) can be rewritten as

$$\sum_{a=-2}^{2}\hat{Q}_a^2,$$

and by defining the real and imaginary parts of the pairing operators as

$$R=(\hat{P}^\dagger+\hat{P})/2,\quad I=(\hat{P}^\dagger-\hat{P})/2i, \tag{4}$$

the pairing part can be rewritten as

$$\hat{P}^\dagger\hat{P}=R^2+I^2+\frac{1}{2}[\hat{P}\hat{P}^\dagger], \tag{5}$$

where the commutator $[\hat{P}\hat{P}^\dagger]$ gives rise to an additional one-body term in the Hamiltonian and to a constant. In the case of the monopole pairing R,I, $[\hat{P},\hat{P}^\dagger]$ give the familiar quasispin operators. In the following we shall set

$$\hat{H}'_0=\hat{H}_0-\left(\mu+\frac{G}{2}\right)\hat{N}. \tag{6}$$

We shall apply the Hubbard-Stratonovich transformation to the partition function for A particles defined as

$$Z=e^{-\alpha A}\,\mathrm{Tr}[e^{-\beta\hat{H}+\alpha\hat{N}}], \tag{7}$$

where $\alpha=\beta\mu$ with μ being the chemical potential, and $\hat{N}$ is the particle number operator. In the grand-canonical ensemble, the trace is taken over the full Hilbert space and μ (or better α) is fixed by the condition that

$$\frac{\partial\ln Z}{\partial\alpha}=0, \tag{8}$$

which is equivalent to $\langle\hat{N}\rangle=A$. The value of α obtained by solving Eq. (8) is a minimum for $\ln Z$ if the trace is taken in the grand-canonical ensemble. In the canonical ensemble the trace in Eq. (7) is taken in the subspace of the full Hilbert space spanned by A particles only. In this case, since the full two-body Hamiltonian commutes with the particle number operator, the chemical potential is, in principle, arbitrary. However, as pointed out in Ref. [2], the value of the chemical potential affects the computability of the functional integral in the canonical ensemble (i.e., the statistical error depends on the chemical potential while the value of the integral does not). Therefore, the chemical potential is selected so that the statistical error in the Monte Carlo evaluation of the canonical ensemble functional integral is the smallest.

In order to apply the Hubbard-Stratonovich transformation the interval $[0,\beta]$ is divided in M intervals of length ϵ $(\beta=\epsilon M)$ so that one can approximate with sufficient accuracy $e^{-\epsilon(\hat{H}_0+\hat{V})}=e^{-\epsilon\hat{H}_0}e^{-\epsilon\hat{V}}$. The Hubbard-Stratonovich transformation

$$e^{(\epsilon/2)\hat{O}^2}=\sqrt{\frac{\epsilon}{2\pi}}\int d\sigma\, e^{(-\epsilon/2)\sigma^2}e^{\epsilon\sigma\hat{O}} \tag{9}$$

is then applied to each interaction term in the Hamiltonian at each time interval ϵ. In our case this leads to, in the limit of $\epsilon\rightarrow 0$,

$$\begin{aligned}Z=e^{-\beta G\Omega/2}\mathcal{N}\int\prod_{n=1}^{M}\left(d\phi_{xn}d\phi_{yn}\prod_{a=-2}^{2}d\sigma_{an}\right)\\ \times e^{-(\epsilon/2)k\Sigma_{an}\sigma_{an}^2-\epsilon G\Sigma_n(\phi_{xn}^2+\phi_{yn}^2)}e^{-\alpha A}\,\mathrm{Tr}(\hat{U}),\end{aligned} \tag{10}$$

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

$$\hat{U}=\hat{U}_M\hat{U}_{M-1}\cdots\hat{U}_1, \tag{11}$$

$$\hat{U}_n=e^{-\epsilon[\hat{H}_0'-k\Sigma_a\sigma_{an}\hat{Q}_a-G(\phi_n\hat{P}+\phi_n^\star\hat{P}^\dagger)]} \tag{12}$$

with $\phi_n=(\phi_{xn}+i\phi_{yn})$, and $\mathcal{N}$ is the normalization constant

$$\mathcal{N}=\left(\frac{\epsilon k}{2\pi}\right)^{5M/2}\left(\frac{\epsilon G}{\pi}\right)^{M}.$$

Equation (10) applies for both the grand-canonical ensemble partition function (with the trace in Eq. (10) taken over the full Fock space) and the canonical ensemble partition function [in this case the trace in Eq. (10) is restricted to the subspace spanned by A particles].

The difficulty with these FI's lies in the fact that the evolution operator does not conserve particle number (although the original two-particle Hamiltonian does), while we are primarily interested in traces having a fixed particle number. For small systems such as nuclei this could pose a problem. Contrary to the usual way of proceeding we will prove that canonical ensemble calculations are possible without using particle number projectors as usually done.

III. COMPUTATION OF THE TRACE

In order to compute the trace in Eq. (10) (whether in the grand-canonical or in the canonical ensemble) we make use of the generalized nonsingular (and in general nonunitary) quasiparticle transformation introduced in Ref. [9]. First let us rewrite any operator, quadratic in the creation and annihilation operators, of the type

$$\hat{K}=a^\dagger K_{21}a+\frac{1}{2}[aK_{11}a+a^\dagger K_{22}a^\dagger] \tag{13}$$

as

$$\hat{K}=\frac{1}{2}(a\quad a^\dagger)\begin{pmatrix}K_{11} & K_{12}\\ K_{21} & K_{22}\end{pmatrix}\begin{pmatrix}a\\ a^\dagger\end{pmatrix}-\frac{1}{2}\sum_i (K_{12})_{ii} \tag{14}$$

(here and in the following $a^\dagger K_{21}a$ is short hand for $\Sigma_{ij}a_i^\dagger K_{21ij}a_j$, etc.). In Eq. (14) $K_{21}=-\tilde{K}_{12}$. Since $a^\dagger$ and a are treated on an equal footing, let us consider the row vector $\gamma_r=(aa^\dagger)$ [the corresponding column vector will be denoted as $\gamma_c=\mathrm{col}(a,a^\dagger)$ so that we can use matrix notations]. Matrices in Eq. (14) have dimensions $N_s\times N_s$. In short

$$\hat{K}=\frac{1}{2}\gamma_r\mathcal{R}\gamma_c-\frac{1}{2}\mathrm{tr}\,K_{12}, \tag{15}$$

$\mathcal{R}$ being antisymmetric. Every evolution operator at a given time interval n can be written as in Eq. (15). Consider the set of operators

$$\hat{W}=e^{(1/2)\gamma_r\mathcal{R}\gamma_c}. \tag{16}$$

To every evolution operator $\hat{U}_n$ one can associate an operator $\hat{W}_n$, a matrix $\mathcal{R}_n$ and a complex number C_n as follows:

$$\begin{aligned}\hat{U}_n&=C_n\hat{W}_n,\\ C_n&=e^{-\mathrm{tr}\,K_{12}(n)/2}=e^{\mathrm{tr}\,K_{21}(n)/2},\\ \hat{W}_n&=e^{(1/2)\gamma_r\mathcal{R}(n)\gamma_c}.\end{aligned} \tag{17}$$

The set of the operators $\hat{W}$ transforms the creation and annihilation operators γ_r and γ_c in the following way (cf. Ref. [9]):

$$\begin{aligned}\hat{W}^{-1}\gamma_r\hat{W}&=\gamma_r\tilde{W},\\ \hat{W}^{-1}\gamma_c\hat{W}&=W\gamma_c,\end{aligned} \tag{18}$$

where the matrix W (not to be confused with the second quantized operator $\hat{W}$) is given by

$$W=e^{\hat{\sigma}\mathcal{R}},\quad \hat{\sigma}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{19}$$

$\tilde{W}$ in Eq. (18) is the transpose of W. Transformation (18) preserves the anticommutation rules of the creation and destruction operators. It is easy to see that

$$\hat{\sigma}W\hat{\sigma}=\tilde{W}^{-1}. \tag{20}$$

This property follows from the antisymmetry of $\mathcal{R}$. It is convenient to define also the vectors

$$\overline{\gamma_r}=\gamma_r\hat{\sigma},\quad \overline{\gamma_c}=\hat{\sigma}\gamma_c. \tag{21}$$

Trivially $\overline{\gamma_r}=(a^\dagger,a)$. Then, using Eq. (20), one has

$$\hat{W}^{-1}\overline{\gamma_r}\hat{W}=\overline{\gamma_r}W^{-1}. \tag{22}$$

Equation (20) implies that $\mathcal{R}$ in Eq. (19) is antisymmetric. The product of two such matrices W_2 and W_1 also satisfies Eq. (20), and such matrices form a group which is a representation of the group of the nonsingular, nonunitary (in general) transformations $\hat{W}$ defined in Eq. (18).

From the Baker-Campbell-Hausdorff theorem (see, for instance, Ref. [10]) the product of two operators of type (16) is also of type (16), since the quadratic forms in the creation and annihilation operators form a Lie algebra. That is if $\hat{W}_2,\hat{W}_1$ are two operators of type (16) and

$$\hat{W}=\hat{W}_2\hat{W}_1, \tag{23a}$$

then

$$\hat{W}=e^{(1/2)\gamma_r\mathcal{R}\gamma_c} \tag{23b}$$

with

$$W=e^{\hat{\sigma}\mathcal{R}},\quad W=W_2W_1. \tag{23c}$$

One practical use of this group properties is that one can immediately calculate the product of the transformations $\hat{W}_M\hat{W}_{M-1}\dots\hat{W}_1$ by computing

$$W=W_MW_{M-1}\cdots W_1, \tag{24}$$

and from this $\mathcal{R}=\hat{\sigma}\ln W$. Another important implication is the following. Let us consider the grand-canonical trace of an operator $\hat{W}$ (which is the product of the operators at each time interval), and a transformation (undefined for the moment) $\hat{\zeta}$, then

$$\mathrm{Tr}\,\hat{W}=\mathrm{Tr}[\hat{\zeta}^{-1}\hat{W}\hat{\zeta}]=\mathrm{Tr}[e^{(1/2)\hat{\zeta}^{-1}\gamma_r\mathcal{R}\gamma_c\hat{\zeta}}]. \tag{25}$$

If T is the matrix associated with $\hat{\zeta}$ according to the association law (18), then applying Eqs. (18) and (22) to $\hat{\zeta}$,

$$\hat{\zeta}^{-1}\overline{\gamma_r}\hat{\sigma}\mathcal{R}\gamma_c\hat{\zeta}=\overline{\gamma_r}T^{-1}\hat{\sigma}\mathcal{R}T\gamma_c. \tag{26}$$

Among the possible T matrices there are those which bring $\hat{\sigma}\mathcal{R}$ in diagonal form. In order to see this consider the eigenvalue problem for the matrix $W=\exp(\hat{\sigma}\mathcal{R})$ written as

$$WX=X\begin{pmatrix} e^{\lambda} & 0\\ 0 & e^{\lambda'}\end{pmatrix}$$

with λ,λ' being diagonal. Then by multiplying to the left and to the right by $\hat{\sigma}$ one has

$$\hat{\sigma}W\hat{\sigma}(\hat{\sigma}X\hat{\sigma})=\hat{\sigma}X\hat{\sigma}\begin{pmatrix} e^{\lambda'} & 0\\ 0 & e^{\lambda}\end{pmatrix},$$

and using Eq. (20)

$$\widetilde{W}^{-1}(\hat{\sigma}X\hat{\sigma})=\hat{\sigma}X\hat{\sigma}\begin{pmatrix} e^{\lambda'} & 0\\ 0 & e^{\lambda}\end{pmatrix},$$

which implies that $\lambda'=-\lambda$. Therefore, by taking the transpose

$$(\hat{\sigma}\widetilde{X}\hat{\sigma})W^{-1}=\begin{pmatrix} e^{\lambda'} & 0\\ 0 & e^{\lambda}\end{pmatrix}(\hat{\sigma}\widetilde{X}).$$

Since the matrix of the left eigenvectors of W (or of W^{-1}) is the inverse of the matrix formed with the right eigenvectors we have $X^{-1}=\hat{\sigma}\widetilde{X}\hat{\sigma}$, which proves the assertion that the matrix of eigenvalues of W (or equivalently $\hat{\sigma}\hat{R}$) has the property of Eq. (20). Therefore, going back to Eq. (26), taking T as the matrix which diagonalizes $\hat{\sigma}\hat{R}$, we have

$$T^{-1}\hat{\sigma}\mathcal{R}T=\begin{pmatrix} \lambda & 0\\ 0 & \lambda'\end{pmatrix} \tag{27}$$

with $\lambda'=-\lambda$, or

$$\mathcal{R}=T\begin{pmatrix} 0 & \lambda\\ -\lambda & 0\end{pmatrix}T^{-1}, \tag{28}$$

$$W=T\begin{pmatrix} e^{\lambda} & 0\\ 0 & e^{-\lambda}\end{pmatrix}T^{-1}, \tag{29}$$

which gives the eigenvalue structure of an arbitrary W. In the grand-canonical ensemble, therefore,

$$\mathrm{Tr}\,\hat{W}=\mathrm{Tr}[e^{(1/2)\gamma_r\left(\begin{smallmatrix} 0 & \lambda\\ -\lambda & 0\end{smallmatrix}\right)\gamma_c}], \tag{30}$$

and an elementary calculation gives

$$\mathrm{Tr}\,\hat{W}=e^{\Sigma_i\lambda_i/2}\prod_i\,(1+e^{-\lambda_i}), \tag{31}$$

which is the final result for the grand-canonical trace of $\hat{W}$.

Let us now focus on the canonical trace $\mathrm{Tr}\,\hat{W}$. Equation (25) no longer holds, since the operator $\hat{\zeta}$ which brings $\hat{W}$ in a diagonal form changes the particle number [the familiar identity $\mathrm{Tr}(A)=\mathrm{Tr}(B^{-1}AB)$ holds only if the trace is taken over the full space over which A and B are defined]. The difficulty is avoided with the formal device of introducing an arbitrary complex variable $z=e^{\alpha'}$ and considering the grand-canonical trace

$$\mathrm{Tr}(e^{\alpha'\hat{N}}\hat{W})=\sum_{A=0}^{N_s}z^A\,\mathrm{Tr}_A(\hat{W}), \tag{32}$$

here N_s is the highest possible value for the particle number ($N_s=2\Omega$) and the Tr_A denotes the trace in the subspace with exactly A particles. First we will compute the left-hand side of Eq. (32) and then we will perform the polynomial expansion in powers of $z=e^{\alpha'}$ in order to extract algebraically $\mathrm{Tr}_A(\hat{W})$ which is the quantity of interest. We stress that $\alpha'\neq\alpha$; we perform exact particle number projection by polynomial expansion of the generating function Eq. (32), while we keep the original chemical potential $\mu=\alpha/\beta$ fixed. Stated differently we use two chemical potentials: with one (α'/β) we extract exact expressions for the traces in the canonical ensemble and the other (unrelated to the first) is fixed so that the canonical ensemble trace is mostly positive. The canonical ensemble traces in Eq. (32) are traces of operators which do not conserve the particle number and they do not depend on α' [Eq. (32) is simply an exact expansion] but they do depend on α since the evolution operators does. If we would use only one chemical potential (α') we would be selecting $\mu=0$) and lose the freedom of modifying the evolution operator. Before proceeding we point out that the final formulas, should be applicable to numerical cases of physical interest. In these cases all matrices under consideration tend to become numerically pathologically large as the temperature is decreased. This can be seen very simply by looking at the grand-canonical expressions themselves. Consider for example the matrix W which has to be diagonalized in order to find the eigenvalues λ_i which appear in the grand-canonical trace (31). This matrix has eigenvalues of the type $e^{\lambda_i}, e^{-\lambda_i}$; in the mean-field case the λ_i are the quasiparticles energies multiplied by $-\beta$, and, depending on the single-particle space can be low and negative in energy (they are generated by the high-lying single-particle states). Thus because of the structure of the matrix W the eigenvalues are very large and loss of numerical accuracy easily follows. To deal with the problem we introduce the following method. Instead of the eigenvalue problem for W we consider the eigenvalue problem for the supermatrix

$$W^{[2]}=\begin{pmatrix} 0 & W_a \\ W_b & 0 \end{pmatrix}, \tag{33}$$

where $W_a=W_{M/2}\cdots W_2 W_1$ and $W_b=W_M W_{M-1}\cdots W_{M/2+1}$, in other words W_a is the result of the evolution for the first $M/2$ time intervals, and W_b is the result of the evolution for the last $M/2$ intervals. Both matrices are better behaved than their product. It is easy to see that the eigenvalues of $W^{[2]}$ are the square roots of the eigenvalues of the original matrix W. So the eigenvalues of $W^{[2]}$ are better defined numerically and from these the λ_i can be directly extracted. Even better behaved are the eigenvalues of the supermatrix

$$W^{[3]}=\begin{pmatrix} 0 & 0 & W_a \\ W_b & 0 & 0 \\ 0 & W_c & 0 \end{pmatrix}, \tag{34}$$

where W_a, W_b, W_c are the result of the evolution from 0 to $\beta/3$ from $\beta/3$ to $2\beta/3$ and from $2\beta/3$ to β. It is easy to see that the eigenvalues of $W^{[3]}$ are the cubic roots of the eigenvalues of W, and therefore can be used to extract directly the λ_i. It is straightforward to generalize this ''root'' method to fourth roots and so on. This method can of course be used (and it has been implemented in Ref. [3]) in the case where the pairing interaction is absent, in such a case canonical ensemble Monte Carlo calculations are straightforward. The implementation of this idea in the Canonical ensemble in the case pairing is present and nontrivial. We shall keep the name ''root'' method, although strictly speaking we do not take the root of the evolution operator in this case. To be clear, ''square root'' applies to the decomposition of W in two factors and nth root to the decomposition of W in n factors.

We shall discuss the method up to fourth roots (again it can be generalized to higher roots). We stress that the method is essential in order to do Monte Carlo calculations in the canonical ensemble. We shall start with the case where no root is taken (i.e., W is not factorized). From the point of view of Monte Carlo calculations in the canonical ensemble this is purely academic, since the numerical pathology is so strong that it can be implemented only at high temperatures (at least in the erbium region) where pairing is no longer effective. At least squares, cubic, and quartic roots of W are necessary.

Let us go back to Eq. (33) and rewrite the operator inside the trace in the form (16)

$$\hat{W}(z)=e^{\alpha'\hat{N}}\hat{W}=e^{\alpha N_s/2}e^{(1/2)\gamma_r\left(\begin{smallmatrix}0 & -1\\ 1 & 0\end{smallmatrix}\right)\gamma_c}\hat{W}. \tag{35}$$

The operator product can easily be taken into account using Eqs. (21)–(23). Thus the matrix associated with $\hat{W}(z)$ [call it $W(z)$] is given by

$$W(z)=e^{\alpha\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)}W=\begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix}W. \tag{36}$$

Then one has, by taking the square in Eq. (31) for $\hat{W}(z)$

$$\begin{aligned}[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2&=z^{N_s}\det[1+W(z)]\\ &=\det\left[\begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix}+\begin{pmatrix} z & 0 \\ 0 & 1 \end{pmatrix}W\right],\end{aligned} \tag{37}$$

where the fact that

$$z^{N_s}=\det\begin{pmatrix} 1 & 0 \\ 0 & z \end{pmatrix} \tag{38}$$

has been used. One can rewrite Eq. (38) as

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det(S_v+zS_p), \tag{39}$$

where the matrices S_v and S_p do not depend on z and can be expressed in terms of the block forming W as

$$S_v=\begin{pmatrix} 1 & 0 \\ W_{21} & W_{22} \end{pmatrix}, \quad S_p=\begin{pmatrix} W_{11} & W_{12} \\ 0 & 1 \end{pmatrix}. \tag{40}$$

The matrix S_v is the contribution from the vacuum (of particles) since it is obtained for $z=0$. From Eq. (39) one has

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det(S_v)\det(1+zS_v^{-1}S_p). \tag{41}$$

Let μ_j (not to be confused with the chemical potential) be the eigenvalues of the matrix $S_v^{-1}S_p$. Since the left-hand side of Eq. (41) is the square of a polynomial in z all eigenvalues μ_i must come in degenerate pairs. Therefore, to reconstruct the left-hand side we can simply write

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]=s\sqrt{\det(S_v)}\prod_i^{N_s}{}'(1+z\mu_i), \tag{42}$$

where the product is only over the distinct eigenvalues and $s=\pm 1$ is an overall sign necessary in taking the square root of Eq. (41). s can be determined by considering Eq. (42) for $z=1$ (i.e., $\alpha'=0$). In order to extract the canonical traces from Eq. (42), i.e., the coefficient of z^A in Eq. (42), one can use the recursion relation of Ref. [4]. Let us set

$$\prod_{i}^{N_s}{}'(1+z\mu_i)=1+z\xi(1,N_s)+z^2\xi(2,N_s)+z^3\xi(3,N_s)+\cdots . \tag{43}$$

Then the quantities $\xi(n,N_s)$ satisfy the recursion relation

$$\xi(n,s)=\mu_s\xi(n-1,s-1)+\xi(n,s-1), \tag{44}$$

where $\xi(n,s)$ is constructed from the first s eigenvalues μ_i only. The canonical trace for A particles is finally given by

$$\mathrm{Tr}_A\,\hat{W}=s\sqrt{\det(S_v)}\,\xi(A,N_s). \tag{45}$$

As mentioned before, Eq. (46) is not numerically applicable in Monte Carlo calculations at low temperature because very large numbers are involved in both the computation of S_v and of the μ_i. Rather we use the method of roots, previously discussed.

Consider first the square-root method. Let us write $W=W_bW_a$ with W_a being the result form the evolution from 0 to $\beta/2$ and W_b the result form the evolution from $\beta/2$ to β. Then Eq. (37) becomes

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det\left[\begin{pmatrix}1 & 0\\ 0 & z\end{pmatrix}+\begin{pmatrix}z & 0\\ 0 & 1\end{pmatrix}W_bW_a\right]. \tag{46}$$

Let us note first that $\det W_a=1$ (the matrices W are such that they have eigenvalues where one is the inverse of the other). Let $A_a=W_a^{-1}$. Then

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det\left[\begin{pmatrix}1 & 0\\ 0 & z\end{pmatrix}A_a+\begin{pmatrix}z & 0\\ 0 & 1\end{pmatrix}W_b\right]. \tag{47}$$

Let

$$A_a=\begin{pmatrix}(A_a)_{11} & (A_a)_{12}\\ (A_a)_{21} & (A_a)_{22}\end{pmatrix},$$

$$W_b=\begin{pmatrix}(W_b)_{11} & (W_b)_{12}\\ (W_b)_{21} & (W_b)_{22}\end{pmatrix},$$

then Eq. (47) can be rewritten as

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det\left[\begin{pmatrix}(A_a)_{11} & (A_a)_{12}\\ (W_a)_{21} & (W_a)_{22}\end{pmatrix}+z\begin{pmatrix}(W_a)_{11} & (W_a)_{12}\\ (A_a)_{21} & (A_a)_{22}\end{pmatrix}\right]. \tag{48}$$

Equation (41) still holds with new matrices S_v and S_p which can be read off from Eq. (48)

$$S_v=\begin{pmatrix}(A_a)_{11} & (A_a)_{12}\\ (W_a)_{21} & (W_a)_{22}\end{pmatrix}, \tag{49a}$$

$$S_p=\begin{pmatrix}(W_a)_{11} & (W_a)_{12}\\ (A_a)_{21} & (A_a)_{22}\end{pmatrix}. \tag{49b}$$

These matrices are better behaved numerically than the matrices defined by Eq. (40) since A_a and W_b contain only half of the time intervals. The same considerations made in Eqs. (41)–(45) still apply including the argument about the degeneracy of the eigenvalues of $S_v^{-1}S_p$. More powerful decompositions are the cubic and fourth roots where $W=W_cW_bW_a$ and $W=W_dW_cW_bW_a$. For the cubic let us set

$$h=\begin{pmatrix}1 & 0\\ 0 & z\end{pmatrix},\quad k=\begin{pmatrix}z & 0\\ 0 & 1\end{pmatrix}, \tag{50}$$

then

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det[hA_a+hkW_cW_b], \tag{51}$$

and using the matrix identity

$$\det\begin{pmatrix}P_{11} & P_{12}\\ P_{21} & P_{22}\end{pmatrix}=\det P_{22}\det[P_{11}-P_{12}P_{22}^{-1}P_{21}], \tag{52}$$

one can rewrite Eq. (50) as

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det\begin{pmatrix}hA_a & hk\\ -W_b & A_c\end{pmatrix} \tag{53}$$

($A_c=W_c^{-1}$). It is important to realize that we had to double the size of the matrix from which we are taking the determinant in Eq. (52). The right-hand side of Eq. (54) can be written now explicitly as

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det\left[\begin{pmatrix}(A_a)_{11} & (A_a)_{12} & 0 & 0\\ 0 & 0 & 0 & 1\\ -(W_b)_{11} & -(W_b)_{12} & (A_c)_{11} & (A_c)_{12}\\ -(W_b)_{21} & -(W_b)_{22} & (A_c)_{21} & (A_c)_{22}\end{pmatrix}+z\begin{pmatrix}0 & 0 & 1 & 0\\ (A_a)_{21} & (A_a)_{22} & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}\right]. \tag{54}$$

Again in this expression the structure of the determinant is

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det[S_v+zS_p] \tag{55}$$

with S_v and S_p that can be found by inspection of Eq. (54). Therefore,

$$[\mathrm{Tr}_{gc}\,\hat{W}(z)]^2=\det S_v\det[1+zS_v^{-1}S_p]. \tag{56}$$

There is a difference between this case and the previous ones. Every submatrix S_v and S_p have twice the dimension (i.e., $4N_s$) of the matrices appearing in the case of the square-root decomposition. The polynomial in Eq. (56), on the other hand, has to be the square of a polynomial of degree N_s. Therefore, half of the eigenvalues of $S_v^{-1}S_p$ are zero and the remaining half consists of degenerate doublets of which we keep only eigenvalue per doublet in taking the square root Eq. (56). From the ‘‘purged’’ set of eigenvalues of $S_v^{-1}S_p$ one can compute the canonical partition function using Eqs. (43) and (44). In the case of the fourth-root decomposition $W=W_dW_cW_bW_a$, one can proceed in a similar way and obtain the following results for S_v and S_p:

$$S_v=\begin{pmatrix} (A_a)_{11} & (A_a)_{12} & 0 & 0 \\ 0 & 0 & (W_d)_{21} & (W_d)_{22} \\ -(W_b)_{11} & -(W_b)_{12} & (A_c)_{11} & (A_c)_{12} \\ -(W_b)_{21} & -(W_b)_{22} & (A_c)_{21} & (A_c)_{22} \end{pmatrix}, \tag{57a}$$

$$S_p=\begin{pmatrix} 0 & 0 & (W_d)_{11} & (W_d)_{12} \\ (A_a)_{21} & (A_a)_{22} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{57b}$$

Again the size of these matrices are $4N_s$; therefore, since $\det(1+zS_v^{-1}S_p)$ has to be the square of a polynomial of degree N_s, half of the eigenvalues of $S_v^{-1}S_p$ have to be zero and the remaining $2N_s$ have to come in degenerate doublets of which we keep only one per doublet in Eqs. (43) and (44). In principle (although it has not be done in practice), one can go forward and construct matrices S_v and S_p for higher-order decompositions $W=W_pW_{p-1}\cdots W_2W_1$; however, they were not deemed necessary for the numerical cases discussed in this paper. They would, however, be necessary if one would consider more complicated models than the one considered in this paper, like pairing+quadrupole+octupole.

As a concluding remark we note that the matrices S_v and $S_v^{-1}S_p$ for the no root, square, cubic, and quartic root cases [given by Eqs. (40), (49), (54), and (57), respectively], although differing in each case, have the following properties: $\det S_v$ is the same regardless of the root and $S_v^{-1}S_p$ have the same eigenvalues for all roots except when the matrix has larger dimensions, in which case the additional eigenvalues are zero.

IV. APPLICATIONS OF THE FORMALISM: THE PURE PAIRING MODEL AND APPROXIMATION SCHEMES

Before discussing Monte Carlo calculations, which are the main purpose of this work, we apply the formalism constructed in the previous section to a simplified model and to the mean-field approximation. This is not meant to imply that such an approximation is uniquely defined or a good approximation. The goodness of the approximation ultimately relies in how well the approximation reproduces the exact Monte Carlo results. However, even in cases where the approximation is not accurate, the mean field plays a central role in the construction of the Gaussian path Monte Carlo method and moreover it offers at least a qualitative understanding of the exact results.

The mean-field approximation (at finite temperature) is defined as the maximum of the integrated in the FI representation of the partition function. Since the integrand changes depending on the value of α so does its maximum, i.e., the mean field. This is true even if the trace inside the FI is taken in the subspace having a good particle number.

Thus by changing the value of α we obtain a family of FI. This peculiarity was used in Ref. [2], where α was selected so that sign fluctuations are suppressed in the Monte Carlo sampling. In order to choose a value of α we make the following qualitative reasoning. Reasonable values of α are close to the one that minimizes the canonical ensemble mean-field partition function (this may not be the optimal value of α for Monte Carlo calculations but is close to it). In fact if, for a given value of α, the contributions to the exact partition function in the vicinity of the mean field are too large, there has necessarily to be a cancellation from some other contributions. If the mean-field contribution is the smallest possible (for the appropriate value of α), then the contributions from the other regions in the integration domain should act coherently, i.e., with the same sign. This argument is of course qualitative. In practice we start from the chemical potentials from approximate grand canonical calculations [the actual values are the ones used in Ref. [11] in the framework of the static path approximation (SPA)] modify them if the sign fluctuations are too large. This feature, i.e., that the feasibility of Monte Carlo canonical ensemble calculation depends on the grand-canonical ensemble should not be regarded as obvious. In fact in the case the evolution operator conserves particle number, it is possible to perform directly in the canonical ensemble, calculations either exact (Monte Carlo) or approximate [Mean field, SPA, random-phase approximation (RPA) at finite temperature, RPA-SPA) without any reference to the grand-canonical ensemble (without the aid of particle number projectors). In the case of pairing forces part of this desirable feature is lost. An input value from the grand-canonical ensemble is essential or somehow the chemical potentials should be predetermined before any Monte Carlo calculation.

In order to elucidate some peculiar features of the canonical ensemble and also in order to see how the formalism constructed in the previous section works in a simple case, the remaining of this section is devoted to the static path approximation (SPA) and the mean field for both the pure pairing model and for the pairing+quadrupole model. The static path approximation is defined by setting $M=1$, $\epsilon=\beta$ in the functional integral. Let us consider first the pure pairing model.

This model has been studied numerically in Ref. [2] using the Gaussian path method. In order to simplify formulas the index r will be reserved for either $i>0$ or $\bar{i}$. Equation (10), in the SPA, simplifies to

$$Z=e^{-\alpha A-\beta\Omega G/2}\mathcal{N}\int (d\phi_x\, d\phi_y)e^{-\beta G(\phi_x^2+\phi_y^2)}\mathrm{Tr}(\hat{U}), \tag{58}$$

the evolution operator $\hat{U}$, is now

$$\hat{U}=e^{-\beta[\hat{H}_0'-G(\phi\hat{P}+\phi^\star\hat{P}^\dagger)]} \tag{59}$$

with $\phi=\phi_x+i\phi_y$ and

$$\mathcal{H}_0'=\sum_{r=1}^{2\Omega}(E_r\hat{n}_r) \quad (E_r=\epsilon_r-q), \tag{60}$$

and $q=\mu+G/2$. Let us write the evolution operator $\hat{U}$ in the form (17). Then

$$\mathrm{Tr}\,\hat{U}=\mathcal{C}\,\mathrm{Tr}\,\hat{W},$$

$$\mathcal{C}=e^{-\beta\Sigma_{i>0}E_i}, \tag{61}$$

$$\sigma\mathcal{R}=\begin{pmatrix} -\beta E & -\beta G\phi^{\star}\mathcal{P} \\ \beta G\phi\mathcal{P} & \beta E \end{pmatrix}. \tag{62}$$

Here E is the diagonal matrix with elements $E_i, E_{\bar{i}}=E_i$. The matrix $\mathcal{P}$ is in block form

$$\mathcal{P}=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{63}$$

with 1 being the unit matrix of dimensions $\Omega\times\Omega$. More explicitly

$$\sigma\mathcal{R}=\begin{pmatrix} -\beta E_i & 0 & 0 & -\beta G\phi^{\star} \\ 0 & -\beta E_i & \beta G\phi^{\star} & 0 \\ 0 & \beta G\phi & \beta E_i & 0 \\ -\beta G\dot{\phi} & 0 & 0 & \beta E_i \end{pmatrix}. \tag{64}$$

Clearly only $i,\bar{i}$ levels are coupled. Let $\Delta=G\phi$, $\omega_r=\sqrt{E_r^2+\Delta^2}$, and let $C_r=\cosh(\beta\omega_r)$, $S_r=\sinh(\beta\omega_r)$ for short, then

$$W=\begin{pmatrix} C_i-\dfrac{E_i}{\omega_i}S_i & 0 & 0 & -\dfrac{G\phi^{\star}}{\omega_i}S_i \\ 0 & C_i-\dfrac{E_i}{\omega_i}S_i & \dfrac{G\phi^{\star}}{\omega_i}S_i & 0 \\ 0 & C_i-\dfrac{E_i}{\omega_i}S_i & \dfrac{G\phi^{\star}}{\omega_i}S_i & 0 \\ 0 & \dfrac{G\phi}{\omega_i}S_i & C_i+\dfrac{E_i}{\omega_i}S_i & 0 \\ -\dfrac{G\phi}{\omega_i}S_i & 0 & 0 & C_i+\dfrac{E_i}{\omega_i}S_i \end{pmatrix} \tag{65}$$

or in short

$$W=\begin{pmatrix} C_{-,i} & 0 & 0 & -a^{\star} \\ 0 & C_{-,i} & a^{\star} & 0 \\ 0 & a & C_{+,i} & 0 \\ -a & 0 & 0 & C_{+,i} \end{pmatrix}. \tag{65$'$}$$

The meaning of the symbols in Eq. (65′) can be obtained by inspection from Eq. (65). It is simple to construct the matrix $S_v^{-1}S_p$ and to diagonalize it. The root method described in the previous section is not needed in this case since we carry out the calculations analytically. The result is

$$\det S_v^{1/2}=\prod_{i>0} C_{+,i}, \tag{66}$$

$$S_v^{-1}S_p=\begin{pmatrix} C_{-,i} & 0 & 0 & -a^{\star} \\ 0 & C_{-,i} & a^{\star} & 0 \\ 0 & -a\,\dfrac{C_{-,i}}{C_{+,i}} & \dfrac{1-|a|^2}{C_{+,i}} & 0 \\ a\,\dfrac{C_{-,i}}{C_{+,i}} & 0 & 0 & \dfrac{1-|a|^2}{C_{+,i}} \end{pmatrix}. \tag{67}$$

The eigenvalues of this matrix, as mentioned earlier, are degenerate, and are complex. The fact that the eigenvalues are complex is crucial to understand how a purely single-particle picture, as the mean-field canonical ensemble is, contains correlations caused by pairing. The eigenvalues μ_r (one per doublet) of $S_v^{-1}S_p$ come in complex conjugate pairs. In the very low-temperature limit for even particle number $A=2N$ the quantity ξ of Eq. (46) is dominated by

$$|\mu_1|^2|\mu_2|^2\cdots|\mu_N|^2.$$

If the last particle is removed (the factor of 2 is brought by the trace)

$$|\mu_1|^2|\mu_2|^2\cdots 2\,\mathrm{Re}(\mu_N).$$

Thus the correlations caused by pairing are contained also in the imaginary part of the μ_i; in fact a large imaginary part on the last occupied eigenvalue implies a large canonical trace in the case of even number of particles, that is more binding for the last pair. Weak pairing effects are obtained if the eigenvalues are almost real (in such a case no extra contribution to the trace is obtained in the case of even particle number). Rather than being a mathematical unphysical artifact of the mean-field approximation, the fact that the eigenvalues are complex is a necessity to obtain an even-odd effect. The explicit expression for the eigenvalues μ_i is

$$\mu_k=2\,\frac{e^{-\beta\omega_k}\pm i[G|\phi|(1-e^{-2\beta\omega_k})/2\omega_k]}{1+e^{-2\beta\omega_k}+(E_k/\omega_k)(1-e^{-2\beta\omega_k})}. \tag{68}$$

As $\beta\rightarrow\infty$ this gives

$$\mu_k=\frac{\pm i(G|\phi|/\omega_k)}{1+E_k/\omega_k}. \tag{68$'$}$$

These are the eigenvalues of the evolution operator to be filled to construct the canonical trace at very low temperature. As these eigenvalues do not have the usual exponential dependence on β considerable excitation might take place. Putting the various terms together, Eq. (60) becomes

$$Z=e^{-\alpha A-\beta\Omega G/2}\frac{\beta G}{\pi}\int(d\phi_x\,d\phi_y)$$

$$\times e^{-xbG(\phi_x^2+\phi_y^2)}e^{-\beta\Sigma_{i>0}E_i}\prod_{i>0} C_{+,i}\,\xi(A,N_s), \tag{69}$$

where $\xi(A,N_s)$ is the canonical ensemble trace formed with the A particles distributed in the set of eigenvalues μ_k given by Eq. (70). Usually the integral is reexpressed using as the integration variable the gap Δ, since the integrand is invariant under rotations of the variables ϕ_x, ϕ_y; integration of the rotation angle gives

$$Z = e^{-\alpha A - \beta \Omega G/2} \frac{2\beta}{G} \int_0^\infty \Delta d\,\Delta e^{-\beta \Delta^2/G} e^{-\beta \Sigma_{i>0} E_i} \times \prod_{i>0} C_{+,i} \xi(A, N_s). \tag{69$'$}$$

On the other hand, the particle number dependence in the integrand is contained in $\xi(A,N_s)$. In order to get further insight, let us specialize to the particular case of the degenerate pure pairing model, where all single-particle unperturbed levels are zero, i.e., $E_r = -q$. In this case all ω_k have a common value

$$\omega = \sqrt{q^2 + \Delta^2},$$

letting also $\mathcal{E}$ be the common value of all μ_k. Equation (69) can be approximated using the saddle-point method and the leading contribution is the mean field. The mean-field partition function is therefore

$$Z_{\rm mf} = e^{-\alpha A - \beta \Omega G/2} e^{-\beta \Delta^2/G} e^{\beta q \Omega} C_+^{\Omega} \xi(A, 2\Omega)$$

with Δ being the value that gives the maximum of the integrand. To obtain the energy, in the low-temperature limit, one has to compute $-\partial_\beta \ln Z$. The quantity $-\partial_\beta \ln \xi$ tends to 0, leaving the only dependence of the energy from the particle number in the external input chemical potential μ. While in the grand-canonical ensemble the chemical potentials are implicitly determined by the number of particles in the canonical ensemble, instead, the chemical potential is (at least in principle) a free parameter. This is the structure of the fully particle-number-projected mean-field partition function, for the degenerate pairing model as well as of the static path approximation for the same model.

Let us now consider the pairing+quadrupole model of heavy nuclei, in the SPA. The SPA expression for the partition function is

$$Z = e^{-\beta G \Omega/2} \mathcal{N} \int \left(d\phi_x \, d\phi_y \prod_{a=-2}^{2} d\sigma_a \right) \times e^{-(\beta/2) k \Sigma_a \sigma_a^2 - \beta G (\phi_x^2 + \phi_y^2)} e^{-\alpha A} \, \mathrm{Tr}(\hat{U}), \tag{70}$$

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

$$\hat{U} = e^{-\beta [\hat{H}_0' - k \Sigma_a \sigma_a \hat{Q}_a - G(\phi \hat{P} + \phi^\star \hat{P}^\dagger)]} \tag{71}$$

with $\phi = (\phi_x + i\phi_y)$ and $\mathcal{N}$ is the normalization constant

$$\mathcal{N} = \left(\frac{\beta k}{2\pi} \right)^{5/2} \left(\frac{\beta G}{\pi} \right). \tag{72}$$

It is more convenient to work in the intrinsic frame. This is accomplished by performing a transformation from the variables σ_a $(a = -2, \ldots, 2)$ to the new variables $\sigma_2', \sigma_0', \theta_1, \theta_2, \theta_3$, with the constraint $\sigma_{-1}' = \sigma_1' = 0$ and $\sigma_{-2}' = \sigma_2'$ (these are not the spherical but the cartesian components of a rank-2 tensor). The variables $\theta_1, \theta_3, \theta_3$ are the Euler angles, and the standard deformation variable which we call here δ, γ instead of β, γ (in order to avoid confusion with the inverse of the temperature) are related to σ_2', σ_0' by

$$\sigma_2' = c\,\delta \sin\gamma, \quad \sigma_0' = c\,\delta \cos\gamma, \tag{73}$$

where $c = \hbar\omega_0/k$ and ω_0 is the harmonic oscillator frequency. The final expression for the partition function in the SPA is obtained after performing the integration over the Euler angles and in using δ, γ, Δ as integration variables is given by

$$Z = e^{-\beta G \Omega/2} \mathcal{N}' \int \Delta d\,\Delta\,\delta^4 \sin(3\gamma) d\delta\, d\gamma \times e^{-(\beta\hbar\omega_0/2k)\delta^2 - \beta/G \Delta^2} e^{-\alpha A} \, \mathrm{Tr}(\hat{U}) \tag{74}$$

with $\mathcal{N}'$ being

$$\mathcal{N}' = \mathcal{N} 16\pi^2 (\hbar\omega_0/k)^5/G.$$

The evolution operator in Eq. (74) is

$$\hat{U} = e^{-\beta[\hat{H}'' - \Delta(\hat{P} + \hat{P}^\dagger)]} \tag{75a}$$

with

$$\hat{H}'' = \hat{H}_0' - \hbar\omega_0 \delta (\cos\gamma \hat{Q}_2 + \sin\gamma \hat{Q}_0). \tag{75b}$$

The trace in Eq. (76), whether in the canonical or in the grand-canonical ensemble, can be conveniently computed in the representation that diagonalizes $\hat{H}''$. Since time-reversal orbits are not mixed by the quadrupole potential in Eq. (75b) the eigenvalues of $\hat{H}''$ are degenerate and the transformation that diagonalizes $\hat{H}''$ in one set of levels is the same as the one that diagonalizes $\hat{H}''$ in the time-reversal levels. As a consequence the pairing operators in the bases that diagonalizes $\hat{H}''$ retains the same form. Therefore, we can work in this single-particle basis and the problem becomes the previous one (the pure pairing case), except that we also have an integration over the deformation variables. Although in principle both the mean-field partition function and the SPA partition function in the canonical ensemble depend on the chemical potential, because of the pairing terms, they have different sensitivity to it; not surprisingly the mean field is much more sensitive to variation of the chemical potential than the SPA: the more accurate the approximation the less the partition function is sensitive to the chemical potentials, until any dependence disappears altogether in the exact partition function.

V. MONTE CARLO CALCULATION WITH THE PAIRING PLUS QUADRUPOLE MODEL

In this section we shall discuss Monte Carlo calculations using the pairing plus quadrupole model of Baranger and Kumar (Ref. [8]). The method of performing the functional integral stochastically is the Gaussian path method, as discussed in Refs. [2–4], etc. Essentially it consists of the following steps.

TABLE I. Canonical ensemble free energies for several nuclei obtained from the Gaussian path Monte Carlo method. The rightmost column shows the free energies obtained in the static path approximation in the grand-canonical ensemble.

$1/T$	Nucleus	F (exact)	F (SPA)
3.0	Dy162	−301.72 (−0.06, +0.07)	−293.1317
2.5	Dy162	−302.61 (−0.14, +0.21)	−294.3684
2.0	Dy162	−303.30 (−0.10, +0.13)	−296.4250
3.0	Dy163	−305.02 (−0.10, +0.15)	−296.7328
2.5	Dy163	−306.26 (−0.17, +0.30)	−297.9815
2.0	Dy163	−306.52 (−0.13, +0.17)	−300.0526
3.0	Dy164	−308.84 (−0.11, +0.16)	−300.1281
2.5	Dy164	−309.06 (−0.16, +0.28)	−301.3883
2.0	Dy164	−310.02 (−0.16, +0.24)	−303.4726
3.0	Ho163	−301.73 (−0.10, +0.15)	−293.6146
2.5	Ho163	−302.39 (−0.15, +0.25)	−294.8953
2.0	Ho163	−303.45 (−0.16, +0.25)	−297.0243
3.0	Ho164	−304.88 (−0.12, +0.19)	−297.1913
2.5	Ho164	−305.16 (−0.09, +0.11)	−298.4802
2.0	Ho164	−306.70 (−0.14, +0.20)	−300.6196
3.0	Ho165	−308.62 (−0.12, +0.18)	−300.5570
2.5	Ho165	−308.83 (−0.15, +0.24)	−301.8551
2.0	Ho165	−310.10 (−0.20, +0.34)	−304.0057
3.0	Er167	−311.90 (−0.13, +0.21)	−303.6765
2.5	Er167	−312.00 (−0.09, +0.12)	−304.9702
2.0	Er167	−313.45 (−0.13, +0.17)	−307.1237
3.0	Tm168	−311.24 (−0.10, +0.15)	−303.4195
2.5	Tm168	−311.66 (−0.14, +0.22)	−304.7026
2.0	Tm168	−311.89 (−0.12, +0.16)	−306.8530

TABLE II. Sensitivity of the canonical ensemble mean field as a function of the neutron chemical potential. Shown are the free energies, the gaps (n and p), and the deformation variable.

Dy164 ($1/T=3.0$)					
μn	μp	F	Gap n	Gap p	Deform.
−5.30	−1.6	−295.3	1.0798	1.5680	0
−5.10	−1.6	−293.0	1.1207	1.5680	0
−4.90	−1.6	−290.6	1.1681	1.5680	0
−4.70	−1.6	−288.5	1.2217	1.5680	0
−4.50	−1.6	−286.5	1.2800	1.5680	0
−4.45	−1.6	−294.2	0.4872	0.7373	0.368
−4.40	−1.6	−294.2	0.4387	0.7359	0.368
−4.35	−1.6	−294.13	0.0000	0.7326	0.370
−4.30	−1.6	−294.13	0.0000	0.7326	0.370
−4.25	−1.6	−294.13	0.0000	0.7326	0.370
−4.20	−1.6	−294.13	0.0000	0.7326	0.370
−4.15	−1.6	−294.13	0.0001	0.7326	0.370
−4.10	−1.6	−294.13	0.0779	0.7323	0.370
−4.05	−1.6	−294.14	0.3819	0.7273	0.373
−4.00	−1.6	−294.16	0.4719	0.7227	0.375
−3.95	−1.6	−294.18	0.5845	0.6669	0.419
−3.90	−1.6	−294.25	0.6135	0.6652	0.428
−3.70	−1.6	−294.7	0.6752	0.6678	0.439
−3.50	−1.6	−295.3	0.7192	0.6708	0.445
−3.30	−1.6	−296.0	0.7627	0.6743	0.450

(1) First a preliminary calculation as done in Ref. [11] is performed in order to have approximate values of the chemical potentials, in the grand-canonical ensemble.

(2) A canonical ensemble mean-field calculation is performed. It gives the maximum of the integrand in the functional integral. The action we maximize includes also the volume elements of the gap and deformation variables. This helps smooth out phase changes as a function of the chemical potentials.

(3) The integration variables in the functional integral are decomposed in two groups. One group generates the symmetries in the integrand (Euler angles and gauge angles for the pairing fields). The other generates the remaining integration variables, as done in Refs. [2,3]. The symmetry variables are approximated with their time average (this is to avoid a constraint on the remaining variables), i.e., they are the zero Fourier components of the integration variables. The remaining variables (nonzero Fourier components) are generated with an approximate Gaussian probability distribution (hence the name of the method) about their mean-field values [see (2)]. The integration variables in the original exact functional integral are then reconstructed.

(4) Since the FI is rewritten as an expectation value with a Gaussian probability density, the exact integral is computed with the distribution function generated in (3).

(5) Typically, with a good choice of the chemical potentials, only a few percent of the contributions are negative. In cases where the percentage is higher the chemical potentials are adjusted and the calculation is repeated from point (2). This percentage of negative contributions does not depend on whether the particle number is even or odd. There are integration variables (as the gaps, the deformation variables δ,γ) which are constrained to be positive (or, in the case of γ between 0 and $\pi/3$); step (3) generates them around the mean-field with a Gaussian distribution, thus a θ function is included in the integrand. Some integration points fall outside the allowed range. Acceptance ratio is kept at about 0.4.

(6) The result of the calculation is the partition function itself (although the method can be extended to compute matrix elements). In the simplest version of the Gaussian path method (i.e., all Gaussians have width set to 1) statistical errors on the partition function are large. But since we deal with very large numbers the corresponding errors on the free energies are quite small.

Although free energies are not immediately related to quantities of experimental interest, comparison of the exact free energies with the ones determined with an approximation scheme, helps determine the degree of validity of the approximation schemes themselves in realistic models. All calculations discussed below are performed with a few up to several thousands Monte Carlo sweeps. The value of β/M was kept almost constant and equal to about 0.025 MeV^{-1}. The results are shown in Table I. The rightmost column shows the grand-canonical SPA results. The discrepancy between the canonical and grand-canonical SPA free energies was found to be small (so only the grand-canonical SPA results are shown) and both are about 7 MeV higher than the exact Monte Carlo free energies. The source of this large discrepancy is the number of time slices ($M=1$ for the SPA and 60 to about 100 in the exact case). This discrepancy, of course, disappears as M is decreased, so the source of the discrepancy is identified unambiguously.

In Table II we study the sensitivity of the canonical ensemble mean-field result (the one obtained by varying the effective action without the inclusion of volume elements) as a function of the neutron chemical potential. Also shown are the gap variable (for both neutrons and protons) and the standard deformation variable. The canonical ensemble SPA calculation for the free energy (not shown in Table II) is about 300 MeV and varies by about 2 MeV in the same interval of chemical potentials.

As a concluding remark, the scheme proposed in this work suggests a functional integral formulation which is free of pathological sign fluctuations in the case of an odd number of particles when the Hamiltonian contains pairing terms. At least for the cases studied so far, this method does not seem to have the limitations of the one used in Ref. [12], which is ill-behaved for even-odd and odd-odd nuclei.

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