Eur. Phys. J. A **9**, 171–181 (2000)

**THE EUROPEAN PHYSICAL JOURNAL A**

© Società Italiana di Fisica
Springer-Verlag 2000

# Monte Carlo calculations of angular momentum projected many-body matrix elements in the Pairing Plus Quadrupole Model

G. Puddu[a]

Dipartimento di Fisica dell'Universitá di Milano, I-20133 Milano, Italy

Received: 28 April 2000 / Revised version: 6 July 2000
Communicated by P. Schuck

**Abstract.** We extend the recently presented formalism for Monte Carlo calculations of the partition function, for both even and odd particle number systems (Phys. Rev. C **59**, 2500 (1999)), to the calculation of many-body matrix elements of the type $\langle\psi|e^{-\beta\hat{H}}|\psi\rangle$ where $|\psi\rangle$ is a many-body state with a definite angular momentum, parity, neutron and proton numbers. For large $\beta$ such matrix elements are dominated by the lowest eigenstate of the many-body Hamiltonian $\hat{H}$, corresponding with a given angular momentum parity and particle number. Emphasis is placed on odd-mass nuclei. Negligible sign fluctuations in the Monte Carlo calculation are found provided the neutron and proton chemical potentials are properly adjusted. The formalism is applied to the $J^\pi = 0^+$ state in $^{166}$Er and to the $J^\pi = 9/2^-,\ \ 13/2^+,\ \ 5/2^-$ states in $^{165}$Er using the pairing-plus-quadrupole model.

**PACS.** 05.30.-d Quantum statistical mechanics – 02.70.Lq Monte Carlo and statistical methods – 21.60.Ka Monte Carlo models

## 1 Introduction

A fundamental problem in nuclear physics is the calculation of observables associated with exact eigenstates of interacting many-particle systems using Monte Carlo methods.

Recently a formalism to compute the fermionic partition function using Monte Carlo methods for Hamiltonians containing pairing terms has been introduced (ref. [1]) which is equally applicable to even and odd numbers of particles. The formalism is based on a functional integral expression of the partition function containing pairing fields. The physical content of the partition function is intrinsically statistical. The only eigenstate of the Hamiltonian reachable via the partition function is the ground-state (as the temperature tends to 0). However, because of the very small level spacing in heavy nuclei, extremely large values of $\beta = 1/T$ are required. The situation considerably improves if the partition function with a definite value of the angular momentum and parity is considered. Here, we discuss a method of computing matrix elements of the type

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

where $|\psi\rangle$ is a trial many-particle state having a given angular momentum, parity and particle numbers $J, M, \pi, N, Z$. Computation of the above matrix elements allows the calculation of the lowest-energy levels of a given angular momentum and parity. We present this method not as an alternative to the method of angular momentum projected partition function but simply as an additional possibility. For large $\beta$, $\mathcal{B}$ is determined solely by the lowest state of a given angular momentum and parity. It should be mentioned that the large-scale shell-model method using a quantum Monte Carlo diagonalization technique (ref. [2]) is capable of giving information on the low-lying part on the energy spectrum in many-particle systems.

With the availability of ever faster computers, the study of quantal systems with stochastic Monte Carlo integration techniques is becoming increasingly powerful (see for example ref. [3]).

The ideas implemented in this work differ from the methods used in ref. [4], where angular-momentum projection (without parity projection) is implemented only approximately with the cranking method. Here we use a functional integral method which is exactly angular momentum and parity projected from the start. The angular momentum and parity projection is not, as usually done, carried out with the familiar angular-momentum projectors, but rather with the choice of the the trial wave functions which have good angular momentum and parity. To the author's knowledge, this idea was never used before for Monte Carlo calculations.

[a] e-mail: giovanni.puddu@mi.infn.it

If the pairing interaction has a large effect, the methods of ref. [4], used to determine the canonical partition function, give strong sign fluctuations in the case of an odd number of particles and small sign fluctuations for an even number of particles ( although these sign fluctuations are absent in the grand canonical partition function and in the ground state). The reason for this effect is the sign of the real parts of the eigenvalues of the evolution operator appearing in the functional integral in the density decomposition. In order to make this obvious consider the functional integral expression for the canonical partition function in the density decomposition, which schematically we write as

$$Z = \int \mathrm{d}\sigma G(\sigma) \mathrm{Tr}\, \hat{U} \quad ,$$

where we called $\sigma$ the integration variables, $G$ is the Gaussian weight and $\hat{U}$ is the evolution operator which depends on the integration variables. Consider any contribution to this integral and let $x_1, x_2, ...$, the largest eigenvalues of the first quantized evolution operator associated with $\hat{U}$ . To a very good approximation, especially at low temperature, the trace of the second quantized evolution operator (*i.e.* the one for $N$ particles) is given by $x_1 x_2 ... x_N$. Since the eigenvalues come in complex conjugate pairs, this quantity is positive for an even number of particles. For an odd number of particles the sign of the trace is the sign of the real part of the unpaired eigenvalue $x_N$. If the pairing force is strong, this sign can be negative with large probability (see ref. [5] for a detailled discussion). Thus we would like to construct a formalism which can be applied both to an even and odd particle number and is angular momentum and parity projected. This is precisely the goal of the method we propose in this work. An accurate evaluation of the matrix elements of eq. (1) gives information about the spectrum of the many-body Hamiltonian.

It should be stressed that another ingredient of the method we propose is the use of a trial Gaussian density distribution for the computation of the functional integral itself. This is different from the Metropolis method usually employed in Monte Carlo calculations. The main reason for using this method, which is discussed later in this work, is that the approximations commonly used in nuclear physics (mean-field and RPA) can be derived by approximating the integrand in the functional integral, with a Gaussian around the mean field (the highest value of the integrand). Therefore it is reasonable to use such approximations as a trial probability density to compute the full functional integral. As discussed later, much of the computational effort goes in the construction of such a trial probability density . Although intrinsically less accurate than the Metropolis methods, the Monte Carlo integration performed with these trial probabilbity densities can be a few orders of magnitude faster since this method does not require the computationally expensive number of decorrelation steps necessary in the Metropolis method to guarantee the statistical independence of the the sample.

Methods for the computation of matrix elements, as in eq. (1), can be particularly useful for odd-even and odd-odd nuclei. Of course much relies on the expression for the trial state $|\psi\rangle$ one adopts. A good choice allows small values of $\beta$, but a poor choice of the trial state would require large values of $\beta$. Matrix elements are amenable to Monte Carlo calculations with small sign fluctuations; this seems to be the case in the examples discussed below for odd-even nuclei using the pairing+quadrupole force. Although calculations were not performed, this is very encouraging also for odd-odd nuclei, since sign fluctuations in the formalism of ref. [1] do not depend on whether the particle number is even or odd. The outline of this paper is the following. In section 2 we present the formalism for the computation of the matrix elements. In subsections 2.1 and 2.2 specific cases are discussed in detail. In subsection 2.3 the phase ambiguity associated with the generalized quasi-particle formalism is discussed. In section 3 we discuss some examples with Monte Carlo calculations; the limitations of the present implemetation are also discussed. In section 4, we present some conclusions.

## 2 The functional integral expression for matrix elements $\mathcal{B}$

The Hamiltonian we consider in the next section, as a numerical example, is the Pairing+Quadrupole Hamiltonian. Since the formalism does not depend on the details of the Hamiltonian, we consider such a model. In order to simplify the formulae we shall consider one particle type although the numerical calculations have been performed including both neutron and proton degrees of freedom. The Hamiltonian used is (ref. [6])

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

where $\hat{H}_0 = \sum_{i=-\Omega}^{\Omega} E_i a_i^\dagger a_i$ is the single-particle Hamiltonian, $\hat{Q}^{(2)}_a = \sum_{i,j} (q^{(2)}_a)_{ij} a_i^\dagger a_j$ (for $a = -2, .., 2$) are the spherical components of the quadrupole operator and $\hat{P} = \sum_{i>0} a_{\bar{i}} a_i$ is the monopole pairing operator. The label $i > 0$ denotes a single-particle orbit $njm$, and $\bar{i}$ refers to its time reversed orbit, defined as $|\overline{njm}\rangle = (-)^{j+1/2} |nj-m\rangle$. The total number of single-particle states is $N_\mathrm{s} = 2\Omega$. The pairing operator is of the form

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

where $\mathcal{P}$ is an antisymmetric matrix in the single-particle indices. As in ref. [1], the details of the pairing matrix $\mathcal{P}$ as well as of the quadrupole force are irrelevant for the purpose of introducing the formalism. In what follows $\hat{Q}_a$ ($a = -2, -1, 0, 1, 2$) are the Cartesian components (*i.e.* the real and imaginary parts) of the quadrupole operator in (2). In the following we consider rather than $e^{-\beta \hat{H}}$, the operator $e^{-\beta \hat{H} + \alpha \hat{N}}$ Let $\beta = \epsilon N_t$, then the Hubbard-Stratonovich transformation (ref. [7]) gives the following

expression for the evolution operator $e^{-\beta\hat{H}+\alpha\hat{N}}$ (cfr. ref. [1]):

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

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

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

$$\hat{U}_n = e^{-\epsilon[\hat{H}_0'-k\sum_a\sigma_{an}\hat{Q}_a-G(\phi_n\hat{P}+\phi_n^\star\hat{P}^\dagger)]} \quad , \quad (6)$$

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

$$\mathcal{N} = (\frac{\epsilon k}{2\pi})^{\frac{5N_t}{2}}(\frac{\epsilon G}{\pi})^{N_t} \quad .$$

Equation (4) becomes exact in the limit $\epsilon \to 0$. We preferred this functional integral since its mean-field (*i.e.* the time-independent values of the integration variables, which give the highest integrand in eq. (4)) describes the familiar Hartree-Bogoliubov mean field. This functional integral was also used in ref. [8] and is a particular case of the more general class of functional integrals described in ref. [9].

Second quantized operators are denoted with capitals with a carret and their corresponding first quantized operators with small letters, for example $\hat{Q}_a = \sum_{rs}(q_a)_{rs}a_r^\dagger a_s$. As discussed in ref. [1], the chemical potential $\mu$ is adjusted so that sign fluctuations are supressed.

Inserting eq. (4), in eq. (1) one derives, for $A$ particles,

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

In order to compute eq. (7) one needs matrix elements of the type

$$\langle\psi, J, M, \pi, A|\hat{U}|\psi, J, M, \pi, A\rangle \quad ,$$

with $\hat{U}$ given by eq. (5) and (6). As in ref. [1] , we make use of the general quasi-particle formalism of ref. [10].

The operator $\hat{U}$ in eq. (7) conserves neither particle number nor angular momentum, while the original many-body matrix element in eq. (1) does . The restoration of conserved quantum numbers is therefore achieved after the functional integration is performed. This implies that spurious particle number and angular momentum violating components in $\hat{U}$ have to be cancelled statistically. If we decompose $\hat{U}$ in its spherical tensor components, only its scalar part is physically meaningful (this is obvious from eq. (4) since the result of the integral is a scalar). Higher angular momentum tensor components in $\hat{U}$ must give 0 after the integration is performed. Therefore, it is desirable to cancel all spurious particle number and angular momentum components in (7) *before* the integration. Non-zero angular momentum components in $\hat{U}$ are cancelled simply by considering the following matrix elements:

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

instead of the matrix elements eq. (7). The expression for $\mathcal{B}$ then becomes

$$\mathcal{B} = e^{-\beta G\Omega/2}\mathcal{N}\int\prod_{n=1}^{N_t}(\mathrm{d}\phi_{xn}\mathrm{d}\phi_{yn}\prod_{a=-2}^{2}\mathrm{d}\sigma_{an}) \times e^{-\frac{\epsilon}{2}k\sum_{an}\sigma_{an}^2-\epsilon G\sum_n(\phi_{xn}^2+\phi_{yn}^2)}e^{-\alpha A}\ B\ . \quad (9)$$

Exact particle number is preserved if the trial states have good particle number (see below). If this is not the case, one has to insert particle number projectors $\wp_A$ ($|JM\pi A\rangle = \wp_A|JM\pi\rangle$) in eq. (8), thus

$$B = \sum_M \frac{1}{2J+1}\langle J, M, \pi|\wp_A\hat{U}\wp_A|J, M, \pi\rangle \quad . \quad (10)$$

This is the expression (modified to account for two particle types) that has been computed in the Monte Carlo calculation discussed in section 3.

Usually one constructs trial states with good angular momentum by projecting the desidered angular-momentum component from a state which breaks rotational invariance (see for ex. ref. [11]). Here we take a different approach, by only using angular-momentum eigenstates. Consider the following state with an even particle number:

$$|\psi\rangle = \hat{C}|0\rangle = e^{\frac{1}{2}a^\dagger Xa^\dagger}|0\rangle \quad , \quad (11)$$

in which $|0\rangle$ is the particle vacuum and $X$ is an antisymmetric matrix in the space of single-particle indices ($a^\dagger Xa^\dagger = a_i^\dagger X_{ij}a_j^\dagger$). Let us take the simple case of $X$ given by a combination of Clebsh-Gordan coefficients which couple the particle operators to zero angular-momentum [1], *i.e.*

$$a^\dagger Xa^\dagger = \sum_i f_i[a_{j_i}^\dagger \times a_{\overline{j_i}}^\dagger]^{(0)}, \quad (12)$$

which is a linear combination of zero angular-momentum coupled pairs constructed in each subshell. The state in

[1] Actually these Clebsh-Gordan coefficients are modified by the following phase factor in the definition of the time-reversed partner of $|jm\rangle$, since $a_{\overline{jm}}^\dagger = (-1)^{j+1/2}a_{j-m}^\dagger$

eq. (11) then carries angular momentum zero and positive parity. Higher angular momenta and/or different parity can be constructed by considering states like

$$|\psi\rangle = g_{kh}[a_k^\dagger \times a_h^\dagger]_M^{(J)} e^{\frac{1}{2}a^\dagger X a^\dagger}|0\rangle + g_{khk'h'}[[a_k^\dagger \times a_h^\dagger]^{(J')} \times [a_{k'}^\dagger \times a_{h'}^\dagger]^{(J'')}]^{(J)} \times e^{\frac{1}{2}a^\dagger X' a^\dagger}|0\rangle + \ldots \ .$$

For an odd particle number one can take combinations of $|\text{odd}\rangle = a_k^\dagger|\text{even}\rangle$ with the appropriate C-G coefficients to ensure good rotational invariance. Ideally one should choose the coefficients appearing in the trial states variationally so as to maximize the overlap with the exact eigenstates of the starting two-body Hamiltonian. In the example discussed in the next section we simply take

$$|0^+\rangle = e^{1/2\sum_{jm} a_{jm}^\dagger a_{\overline{jm}}^\dagger}|0\rangle \quad ,$$

for $0^+$ state of even-even systems and $a_{jm}^\dagger|0^+\rangle$ for the trial state with an odd particle number. No attempt is made here to fix the coefficients $f_k$ in eq. (12) optimally . These coefficients can be determined using variational methods.

To ensure a proper particle number, these states are particle number projected as explained below. Since the operator $\hat{U}$ in eq. (8) does not conserve particle number, the projection in eq. (8) must be done both at the left and at the right of $\hat{U}$. Thus, in this scheme, both particle number and angular momentum projections are taken care of with a double particle number projection.

To appreciate how crucial these projections are in order to suppress sign fluctuations in Monte Carlo calculations, let us mention that for the quadrupole-quadrupole Hamiltonian ($\hat{U}$ in this case does not change particle number) a single-particle number projection is sufficient to fix both angular momentum and particle number, in this scheme, and the resulting functional integral behaves very well from the point of view of the Monte Carlo integration; however a single particle number projection, if pairing is included, gives rise to very strong sign oscillations of the integrand in the functional integral. This is not surprising since spurious particle number components in the matrix element $B$ have to be cancelled out by the integration.

The operator $\wp_A$ which projects the component having $A$ particles is

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

Hence the matrix elements to be studied are ($z_{p,q} = e^{\alpha_{p,q}}$)

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

and eq. (8) becomes

$$B = (2\pi i)^{-2} \int_0^{2\pi i} \mathrm{d}\alpha_p \mathrm{d}\alpha_q B'(z_p, z_q) e^{-(\alpha_p+\alpha_q)A} \quad . \tag{14}$$

In the case of a single-particle number projector (say $\alpha_q = 0$) it is possible to decompose eq. (13) into a polynomial of $e^{\alpha_p}$ using recursion relations, as done in ref. [1], for the calculation of the partition function. In the case of double-particle number projection, for an even particle number, one of the integrals over $\alpha$ in eq. (14) can be carried out in a similar way using recursion relations in a numerically stable way. For an odd particle number, we prefer a direct numerical integration over $\alpha_p$ and $\alpha_q$ in order to compute the $A$-particle matrix elements in eq. (10) from eq. (13) and (14) (this is actually computationally expensive, but rather stable from a numerical point of view).

In the present paper we consider matrix elements $B'(\alpha_p, \alpha_q)$ for the following forms of trial states:

Case 1) $|\psi\rangle = e^{\frac{1}{2}a^\dagger X a^\dagger}|0\rangle$,

Case 2) $|\psi\rangle = a_k^\dagger e^{\frac{1}{2}a^\dagger X a^\dagger}|0\rangle$.

More complicated cases like $[a^\dagger \times a^\dagger]^{(0)}|\text{Case1}\rangle$ will not be considered, although the technique which will be used in case 1) and case 2) can be implemented also in this case.

The technique employed makes use of the formalism described in ref. [1] and ref. [10]. In what follows $\gamma_\mathrm{c} = \mathrm{col}(a, a^\dagger)$ is a column vector consisting of all annihilation and all creation oparators, $\gamma_\mathrm{r}$ is the corresponding row vector and $\overline{\gamma}_\mathrm{r} = (a^\dagger, a)$ and $\overline{\gamma}_\mathrm{c} = \mathrm{col}(a^\dagger, a)$. Every operator of the form

$$\hat{K} = e^{a^\dagger R_{11} a + \frac{1}{2}[a R_{21} a + a^\dagger R_{12} a^\dagger]} \quad , \tag{15}$$

can be rewritten as

$$\hat{K} = e^{\frac{1}{2}\overline{\gamma}_\mathrm{r}\mathcal{R}\gamma_\mathrm{c} - 1/2 \mathrm{tr} R_{22}} \quad , \tag{15'}$$

where $\mathcal{R}$ is a $2N_s \times 2N_s$ matrix which can be obtained, by inspection, from eq. (15) and $R_{22} = -\tilde{R}_{11}$. In particular, every evolution operator at a given time interval $n$, $\hat{U}_n$ (see eq. (6)) can be rewritten as

$$\hat{U}_n = \mathcal{C}_n \hat{W}_n \quad , \tag{16}$$

with

$$\hat{W}_n = e^{\frac{1}{2}\overline{\gamma}_\mathrm{r}\mathcal{R}_n\gamma_\mathrm{c}} \quad . \tag{17}$$

The matrix $\mathcal{R}_n$ and the complex number $\mathcal{C}_n$ can be obtained, by inspection of eq. (6). The matrix elements we wish to calculate are of the type

$$B'(z_p, z_q) = \frac{\mathcal{C}}{2J+1} \sum_M (z_p z_q)^{N_s/2} \times \langle \psi J M \pi | e^{1/2\alpha_p \overline{\gamma}_r N \gamma_\mathrm{c}} \hat{W} e^{1/2\alpha_q \overline{\gamma}_r N \gamma_\mathrm{c}} | \psi J M \pi \rangle \ , \tag{18}$$

$$= \frac{\mathcal{C}}{2J+1} \sum_M B''(z_p, z_q) \quad ,$$

with

$$\mathcal{C} = \prod_n \mathcal{C}_n \quad , \tag{19}$$

$$\hat{W} = \hat{W}_{N_t}\hat{W}_{N_t-1}...\hat{W}_2\hat{W}_1 \quad . \tag{20}$$

$N$ in eq. (18) is the matrix

$$N = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad . \tag{21}$$

Thus we need to give prescriptions for the calculation of the following matrix elements:

$$\text{(Case1)} \quad B''(z_p z_q) = (z_p z_q)^{N_s/2} \times \langle 0|\hat{C}^\dagger e^{1/2\alpha_p \overline{\gamma}_r N\gamma_c}\hat{W}e^{1/2\alpha_q\overline{\gamma}_r N\gamma_c}\hat{C}|0\rangle, \tag{22}$$

$$\text{(Case2)} \quad B''(z_p z_q) = (z_p z_q)^{N_s/2} \times \langle 0|a_k\hat{C}^\dagger e^{1/2\alpha_p \overline{\gamma}_r N\gamma_c}\hat{W}e^{1/2\alpha_q\overline{\gamma}_r N\gamma_c}\hat{C}a_k^\dagger|0\rangle, \tag{23}$$

with $\hat{C}$ given by eq. (11). We now make use of the group properties satisfied by the exponentials of quadratic forms in the creation and anihilation operators (ref. [10]). These properties state that, if

$$\hat{W}_1 = e^{1/2\overline{\gamma}_r \mathcal{R}_1\gamma_c} \quad , \tag{24a}$$

$$\hat{W}_2 = e^{1/2\overline{\gamma}_r \mathcal{R}_2\gamma_c} \quad , \tag{24b}$$

then

$$\hat{W} = \hat{W}_2\hat{W}_1 = e^{1/2\overline{\gamma}_r \mathcal{R}\gamma_c} \quad , \tag{24c}$$

with the matrix $\mathcal{R}$ given by

$$e^{\mathcal{R}} = e^{\mathcal{R}_2}e^{\mathcal{R}_1} \quad . \tag{24d}$$

That is, to the operators $\hat{W}_n$, as in (17), there are associated matrices $W_n = e^{\mathcal{R}_n}$ which have the same group multiplication law. In order to compute products of evolution operators one has to compute the product of their associated matrices and then evaluate its logarithm. The matrix associated with $\hat{C}$, defined in eq. (11), is

$$C = \begin{pmatrix} 1 & X \\ 0 & 1 \end{pmatrix} \quad , \tag{25}$$

and to $\hat{C}^\dagger$ (we choose $X$ real)

$$D = \begin{pmatrix} 1 & 0 \\ -X & 1 \end{pmatrix} \quad . \tag{26}$$

In the next three subsections we shall treat separately case 1) and case 2) and the problem of the determination of the sign of the matrix elements $B''$ defined by (22) and (23).

### 2.1 Case 1)

In ref. [10] it is proven that for any operator of the form (15′) the vacuum expectation value of any operator $\hat{K}$ of the class of eq. (24) is given by

$$\langle 0|\hat{K}|0\rangle = s[\det(K_{22})]^{1/2} \quad . \tag{27}$$

This expression is defined up to a sign $s = \pm 1$ which will be discussed in detail in section 2.3. $K_{22}$ in eq. (27) is the $(2,2)$ submatrix of the matrix $K$ associated with $\hat{K}$. For compactness let

$$\hat{P}_{p,q} = e^{1/2\alpha_{p,q}\overline{\gamma}_r N\gamma_c} \quad . \tag{28}$$

We now have to compute the vacuum expectation value of the operator (see eq. (22))

$$\hat{W}' = \hat{C}^\dagger\hat{P}_p\hat{W}\hat{P}_q\hat{C} \quad . \tag{29}$$

Let $W'$ be the matrix associated with $\hat{W}'$. The multiplication law of eq. (24) gives

$$W' = D\begin{pmatrix} z_p & 0 \\ 0 & 1/z_p \end{pmatrix} W \begin{pmatrix} z_q & 0 \\ 0 & 1/z_q \end{pmatrix} C \quad , \tag{30}$$

and $W$ is the matrix associated with $\hat{W}$ of eq. (20) and $C$ and $D$ are given in eqs. (25) and (26). Thus, using eq. (27) and extracting the $(2,2)$ submatrix, we obtain

$$B''(z_p, z_q) = (z_p z_q)^{N_s/2}\langle 0|\hat{W}'|0\rangle = s(z_p z_q)^{N_s/2}[\det W'_{22}]^{1/2} = s[\det(-z_p^2 z_q^2 X W_{11} X - z_p^2 X W_{12} + z_q^2 W_{21} X + W_{22})]^{1/2} \quad . \tag{31}$$

It is obvious that $s$ does not depend on $z_p, z_q$. In fact $B''$ must be a polynomial in $z_p^2$ and $z_q^2$ (the trial state contains only an even particle number), therefore $B''$ and also $s$ must be continous functions of $z_p, z_q$; since $s = \pm 1$, $s$ cannot depend on the values of $z_{p,q}$. In particular $s$ can be determined from

$$B''(z_p = 0, z_q = 0) = s[\det W_{22}]^{1/2} = \langle 0|\hat{W}|0\rangle \quad . \tag{32}$$

The matrix element $\langle 0^+A|\hat{W}|0^+A\rangle$ (for $A$ particles), is the coefficient of $(z_p z_q)^A$ in the polynomial expansion of eq. (31). The simplest way to extract $\langle 0^+A|\hat{W}|0^+A\rangle$ is to evaluate

$$\langle 0^+A|\hat{W}|0^+A\rangle = (2\pi i)^{-2}\int_0^{2\pi i} \mathrm{d}\alpha_p \mathrm{d}\alpha_q B''(z_p, z_q)/(z_p z_q)^A \quad . \tag{33}$$

This is not the least expensive way (it requires the computation of a large number of determinants). A faster method can be obtained using the following reasoning. Let us rewrite the determinant in eq. (31) as

$$(B'')^2 = \det(z_p^2 U(z_q) + V(z_q)) = \det V(z_q)\det[1 + z_p^2 U(z_q)V(z_q)^{-1}] = \det V(z_q)\det[1 + z_p^2 Y(z_q)] \quad . \tag{34}$$

The matrices $U$ and $V$ can be read from eq. (31), and $Y$ is defined by the above. The coefficients in the polynomial expansion of $\det[1 + z_p^2 Y(z_q)]$ in powers of $z_p^2$ can be obtained with recursion relations as in ref. [1] (cfr. eq. (41)-(44) of ref. [1] ). Since also the square root of the

determinant has to be a polynomial in $z_p^2$ and $z_q^2$, it follows that the eigenvalue spectrum of $Y$ in (34) consists of degenerate doublets for all values of $z_q$. These degeneracy properties are essential if we are to compute the square root of these determinants. Similarly, since the matrix $V(z_q)$ is of the type $z_q^2 A + B$ (with $A$ and $B$ being matrices), it can be rewritten in the form $B(z_q^2 B^{-1}A+1)$. For $z_p = 0$ the right-hand side of (34) has to be a polynomial in $z_q^2$, therefore all eigenvalues of $B^{-1}A$ have to be degenerate. The criterion for numerical stability, adopted in this work, is that these degeneracy properties be preserved to a reasonable accuracy. Let $\xi_n(z_q^2)$ be the coefficient of $z_p^{2n}$ in $\det(1+z_p^2 Y)^{1/2}$ (which can be computed with the afore-mentioned recursion relations), then

$$B''s = [\det V(z_q)]^{1/2} \sum_n z_p^{2n} \xi_n(z_q^2) \quad . \tag{35}$$

Then it follows that we need only to perform the integral over $\alpha_q$ in order to complete the projection of $B''$ in eq. (33).

In this discussion we have assumed that all matrices can be computed accurately. This is actually not so: as $\beta$ becomes larger and larger, some eigenvalues of the evolution operator in the functional grow exponentially. The problem can be cured using the root method, introduced in ref. [1] , with some modifications to allow for the double particle number projection. The method consists in working with a decomposition $\hat{W} = \hat{W}_b \hat{W}_a ...$ so that each factor of the evolution operator is not exponentially large. Consider the case $\hat{W} = \hat{W}_b \hat{W}_a$. In ref. [1] it is shown that the vacuum expectation value of an evolution operator, which in our case is $\hat{W}'$ (eq. (29)), is equal to

$$\langle 0|\hat{W}'|0\rangle = s \det \begin{pmatrix} A_{11}^{(a)'} & A_{12}^{(a)'} \\ W_{21}^{(b)'} & W_{22}^{(b)'} \end{pmatrix}^{1/2} \quad , \tag{36}$$

where $A_{i,j}^{(a)'}$ are the submatrices of $(W^{(a)'})^{-1}$ and $W^{(a)'}$ $W^{(b)'}$ are the matrices associated with the operators $\hat{W}'_a$ and $\hat{W}'_b$ with $\hat{W}' = \hat{W}'_b \hat{W}'_a$ and

$$\hat{W}'_b = \hat{C}^\dagger \hat{P}_p \hat{W}_b \ , \quad \hat{W}'_a = \hat{W}_a \hat{P}_q \hat{C} \quad .$$

It is not difficult, although tedious, to apply the same reasoning, as done in eqs. (34)-(36). One can easily determine the matrices $A_{i,j}^{(a)'}$ of eq. (36) because the inverse of the matrix $W'$ is given by (ref. [10])

$$W'^{(-1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tilde{W}' \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad . \tag{37}$$

It then becomes easy to determine the matrix coefficients of $z_p^2$ and $z_q^2$ in the argument of determinant of eq. (36). Once these matrices are known one can repeat the considerations leading from eq. (31) to eq. (34).

### 2.2 Case 2)

In ref. [10] it is proven that every operator $\hat{K}$ of the class (24) can be written as a product of the form

$$\hat{K} = \hat{\zeta}_c \hat{\zeta}_0 \hat{\zeta}_d \ , \tag{38}$$

where

$$\begin{aligned} &\hat{\zeta}_c = e^{1/2 a^\dagger C a^\dagger} \ , \\ &\hat{\zeta}_0 = e^{1/2 \overline{\gamma}_r \mathcal{R}_0 \gamma_c} \quad \left( \mathcal{R}_0 = \begin{pmatrix} (R_0)_{11} & 0 \\ 0 & -(\tilde{R}_0)_{11} \end{pmatrix} \right), \\ &\hat{\zeta}_d = e^{1/2 a D a} \quad . \end{aligned} \tag{39}$$

The matrices associated with $\hat{\zeta}_c, \hat{\zeta}_0, \hat{\zeta}_d$ are, respectively,

$$\begin{aligned} &Z_c = \begin{pmatrix} 1 & C \\ 0 & 1 \end{pmatrix} \ , \\ &Z_0 = \begin{pmatrix} (z_0)_{11} & 0 \\ 0 & (z_0)_{22} \end{pmatrix} \quad (z_0)_{ii} = e^{(R_0)_{ii}} \ \ (i=1,2), \\ &Z_d = \begin{pmatrix} 1 & 0 \\ D & 1 \end{pmatrix} \quad . \end{aligned} \tag{40}$$

The matrices $C, Z_0, D$ can easily be obtained if the matrices associated with $\hat{K}$, $K$, are known. Using the multiplication law $K = Z_c Z_0 Z_d$, the result is (ref. [10])

$$(Z_0)_{22} = K_{22} \quad D = K_{22}^{-1} K_{21} \quad C = K_{12} K_{22}^{-1} \quad . \tag{41}$$

Using this theorem, it is easy to compute matrix elements of the type $\langle 0|a_k \hat{K} a_h^\dagger|0\rangle$, $\langle 0|a_i a_j \hat{K} a_h^\dagger a_k^\dagger|0\rangle$ etc. The results are

$$\langle 0|a_k \hat{K} a_h^\dagger|0\rangle = (Z_{022})^{-1}_{hk} \langle 0|\hat{K}|0\rangle \ , \tag{42}$$

$$\begin{aligned} &\langle 0|a_i a_j \hat{K} a_h^\dagger a_k^\dagger|0\rangle = \\ &[-C_{ji} D_{hk} + (Z_{011})_{jh} (Z_{011})_{ik} - (Z_{011})_{jk} (Z_{011})_{ih}] \langle 0|\hat{K}|0\rangle \ . \end{aligned} \tag{43}$$

The last matrix elements are the ones we need to consider states like $0^-, 2^\pm, ..,$ etc. We consider eq. (42) for $k = h$. We need

$$B''(z_p, z_q) = (z_p z_q)^{N_s/2} \langle 0|a_k \hat{W}' a_k^\dagger|0\rangle \quad , \tag{44}$$

with $\hat{W}'$ given by eq. (29). Using the relation (42), together with the expression for the matrix $W'$ (eq. (30)) associated with $\hat{W}'$, we obtain

$$\begin{aligned} &B''(z_p, z_q) = s z_p z_q (-z_p^2 z_q^2 X W_{11} X \\ &- z_p^2 X W_{12} + z_q^2 W_{21} X + W_{22})^{-1}_{kk} \\ &\times [\det(-z_p^2 z_q^2 X W_{11} X - z_p^2 X W_{12} + z_q^2 W_{21} X + W_{22})]^{1/2} . \end{aligned} \tag{45}$$

The matrix elements $B$ of eq. (14) are then given by

$$\begin{aligned} B = &\frac{\mathcal{C}}{2J_k + 1} \\ &\times \sum_{M_k} (2\pi i)^{-2} \int_0^{2\pi i} \mathrm{d}\alpha_p \mathrm{d}\alpha_q B''(z_p, z_q)/(z_p z_q)^A \ , \end{aligned} \tag{46}$$

with $M_k$ being the value of the $z$-component of the angular momentum for the single-particle state $k$. Straightforward evaluation of the right-hand side of this equation requires a large number of inversions and determinants. In the case of an odd number of particles, we use a direct evaluation of eqs. (45) and (46). Again, for large $\beta$, all $W$ matrices involved in the evaluation of (45) grow exponentially and a prescription must be given to deal with this problem. The solution implemented in this work, makes use of the factorization theorem, recalled at the begining of this subsection, applied to the operator $\hat{W} = \hat{W}^{(b)}\hat{W}^{(a)}$. In practice $\hat{W}^{(a)}$ is the evolution operator from 0 to $\beta/2$ and $\hat{W}^{(b)}$ is the evolution operator from $\beta/2$ to $\beta$, to optimize the decomposition. Then (see eq. (29))

$$\hat{W}' = \hat{C}^\dagger \hat{P}_p \hat{W}^{(b)} \hat{W}^{(a)} \hat{P}_q \hat{C} = \hat{W}^{(b)'} \hat{W}^{(a)'} \quad . \tag{47}$$

The matrix elements $B''$ are computed in terms of the associated matrices of $\hat{W}^{(b,a)'}$ rewritten using the factorization theorem. The result for the matrix elements in terms of the associated matrices of $\hat{W}^{(b)}$ and $\hat{W}^{(a)}$ is written in the following form:

$$\begin{aligned} B''(z_p, z_q) &= z_p z_q |1 - z_p^2 W_{22}^{(b)-1} X W_{12}^{(b)}|^{1/2} \\ &\times |1 + z_q^2 W_{21}^{(a)} X W_{22}^{(a)-1}|^{1/2} \\ &\times |1 + D^{(b)} C^{(a)}|^{1/2} |W_{22}^{(b)}|^{1/2} |W_{22}^{(a)}|^{1/2} \\ &\times \big[ W_{22}^{(a)-1} (1 + z_q^2 W_{21}^{(a)} X W_{22}^{(a)-1})^{-1} (1 + D^{(b)} C^{(a)})^{-1} \\ &\times (1 - z_p^2 W_{22}^{(b)-1} X W_{12}^{(b)})^{-1} W_{22}^{(b)-1} \big]_{kk}, \end{aligned} \tag{48}$$

with $D$ and $C$ given by

$$D^{(b)} = (-z_p^2 X W_{12}^{(b)} + W_{22}^{(b)})^{-1} (-z_p^2 X W_{11}^{(b)} + W_{21}^{(b)}) \, , \tag{49}$$

$$C^{(a)} = (z_q^2 W_{11}^{(a)} X + W_{12}^{(a)})(z_q^2 W_{21}^{(a)} X + W_{22}^{(a)})^{-1} \, . \tag{50}$$

The reason for rewriting $B''$ in this complex form is that it is numerically rather stable. Each factor behaves much better than the corresponding product, and moreover, it is not difficult to take the square root of the determinants without having to recompute the sign for every $z_p$ and $z_q$ (as the numerical computation of the determinant, as it is stands, would require). The method we have used in this case is the following ( note first that eq. (48) holds for any $W^{(a)}$ and $W^{(b)}$). If we set $W^{(a)} = 1$ in eq. (48) and $z_q = 0$ in eq. (31), we immediately obtain that the eigenvalues of $W_{22}^{(b)-1} X W_{12}^{(b)}$ are two-fold degenerate (see also the discussion following eq. (34)). So in taking the square root of $|1 - z_p^2 W_{22}^{(b)-1} X W_{12}^{(b)}|$, in eq. (48), we take one eigenvalue for every degenerate pair. Similarly, one can apply the same argument to $|1 + z_q^2 W_{21}^{(a)} X W_{22}^{(a)-1}|$ (cfr. eq. (31) for $z_p = 0$). To take the square root of $|1 + D^{(b)}(z_p^2) C^{(a)}(z_q^2)|$ let us prove first that the eigenvalues of $DC$ are degenerate. Consider the matrix elements

$$v = \langle 0 | \hat{\zeta}_d \hat{P} \hat{\zeta}_c | 0 \rangle \quad \hat{P} = z^{\hat{N}} \quad ,$$

where the operators $\hat{\zeta}_{d,c}$ are built from the matrices $D^{(b)}$ and $C^{(a)}$ using eq. (40) ($v$ is a polynomial in the fugacity $z$). Using eq. (27) for the vacuum expectation values, we have

$$v = z^{N_s/2} |Z_d \begin{pmatrix} z & 0 \\ 0 & 1/z \end{pmatrix} Z_c|_{2,2}^{1/2} = |1 + z^2 D^{(b)} C^{(a)}|^{1/2} \, .$$

The eigenvalues of $DC$ must therefore be degenerate. Again to take square root of $|1 + DC|$ we take only one eigenvalue per doublet. This recipe takes care of the intrinsic ambiguity of the square root of the 1st, 2nd and 3rd determinant in eq. (48). However we still have to evaluate two more square roots of a determinant in eq. (48). In order to remove this remaining ambiguity we argued as follows. In eq. (48), let us set $z_p = z_q = 0$ in the determinants only. We obtain the product

$$|1 + D^{(b)}(z_p{=}0) C^{(a)}(z_q{=}0)|^{1/2} |W_{22}^{(b)}|^{1/2} |W_{22}^{(a)}|^{1/2} = |W_{22}|^{1/2}.$$

Since we can take care (by eliminating one eigenvalue in each pair of degenerate eigenvalues) of the ambiguity in the first determinant we rewrite the 4th and the 5th square root of determinants in (48) as

$$|W_{22}|^{1/2} |1 + D^{(b)}(z_p = 0) C^{(a)}(z_q = 0)|^{-1/2} \quad .$$

We are still left with the ambiguity in $|W_{22}|^{1/2}$ but this is equal to $\langle 0 | \hat{W} | 0 \rangle$. Thus we only have to fix an overall sign for this last matrix element. This vacuum expectation value has also been studied in ref. [1] where a recipe was given for the determination of its overall phase. In the following subsection we shall re-examine this issue and clarify a missing point in the sign recipe given in ref. [1].

### 2.3 The sign of the vacuum contribution

A basic shortcoming of the generalized quasi-particle formalism is that the sign of the vacuum expectation value $\langle 0 | \hat{W} | 0 \rangle$ is left undetermined. This is of course not a problem if $\hat{W}$ is the exponential of a Hermitian Hamiltonian. However, in a functional integral $\hat{W}$ is not Hermitian and the phase of the vacuum expectation values must be fixed. In ref. [1] the sign of the vacuum expectation value was fixed by noting that it is the zero particle number contribution in the grand canonical partition function, which can be rewritten as

$$\mathrm{tr}_{\mathrm{gc}}[e^{\alpha \hat{N}} \hat{W}] = \langle 0 | \hat{W} | 0 \rangle f(z) \quad . \tag{51}$$

The function $f$ is a polynomial in $z = e^\alpha$ (ref. [1] eqs. (41)-(45)) that can be determined without any sign ambiguity. The recipe given in ref. [1] is simply to compute the sign of the vacuum term from eq. (51) as a ratio for a particular value of the fugacity after its modulus is calculated from its determinant [2]. In ref. [1] was shown that

[2] It should be mentioned that one of the criteria for numerical stability is precisely $|s| = 1$ to some accuracy, as determined by eq. (51)

the eigenvalues of $W$ come in pairs the type $e^{\pm\lambda}$ and that the grand-canonical trace is given by (let us take $z = 1$)

$$\mathrm{tr}_{\mathrm{gc}}\hat{W} = \prod_r (e^{\lambda_r/2} + e^{-\lambda_r/2}) \quad , \tag{52}$$

(the product is over different pairs). The above expression has a phase ambiguity (the matrix $W$ is $2N_s \times 2N_s$), for the knoweledge of $W$ gives $e^{\lambda}$ and $e^{-\lambda}$ but not $e^{\pm\lambda/2}$, which is defined up to a sign. In the calculation discussed in ref. [1] this sign ambiguity is removed using the fact that the $\pm\lambda$ values have small imaginary parts. The fact that these imaginary parts are small can qualitatively be understood with the following argument. In the functional integral $W = W_N ... W_1$; if we consider static values of the integration variables, $W$ becomes the exponential of a Hermitian matrix and therefore its eigenvalues are real and positive and one can choose real $\lambda$ values. Moreover, the $\lambda$ values are also degenerate (these degeneracy is due to the time-reversal invariance of the quadrupole force, as in the familar Nilsson model). We therefore must assign the same arbitrary multiple of $2\pi$ to the imaginary part of the degenerate $\lambda$ values, since the trace given by eq. (52) is positive. In the Monte Carlo calculation, the matrices $W_n$ vary with the index $n$ and the degeneracy of the $\lambda$ values is removed and they are no longer real. However, the time-reversed $\lambda$ values are still recognizable since the imaginary parts are small and the real parts are close to form degenerate pairs. We therefore give the same arbitrary number of $2\pi$ to the imaginary parts of the (almost) degenerate $\lambda$. In practice, since they are small, we use the prescription to define all phases of $\lambda$ values between $-\pi$ and $\pi$. In the code used in this work, a warning message is printed if the largest imaginary part of $\lambda_r$'s exceeds 1. No such cases were obtained for values of $\beta$ discussed in this work.

In principle a rigorous way to determine the proper imaginary part of $\lambda_r/2$ could be done in the following way: consider the $\beta$ dependence of each $\lambda_r$ (in practice since the imaginary part is small only few values of $\beta$ should be necessary); every time (as a function of $\beta$ ) an imaginary part increases and approaches $\pi$ linearly ( or $-\pi$) its imaginary part should be kept and not readjusted so that it is in the interval $-\pi, +\pi$.

Another way could be to compute the grand-canonical partition function considering only the first $n$ evolution operators for $n = 2, .., N_t$, in order to check whether the phase rule given above for the eigenvalues $\lambda$ agrees with the behavior of the grand-canonical partition function as a function of $n$. In case a disagreement is found, the phase of one the $\lambda$'s should be changed by $2\pi$. Perhaps the most practical way to check the phase rule given above is to apply the method, given in section 2.2, about the decomposition of the evolution operator $W = W^{(b)}W^{(a)}$. The factors are the evolution operators in the time interval $\beta/2, \beta$ and $0, \beta/2$, respectively. We have shown that $W_{22} = W_{22}^{(b)}(1 + D^{(b)}(z = 0)C^{(a)}(z = 0))W_{22}^{(a)}$. From this expression we can obtain the square root of $\det(W_{22})$ in terms of the the square roots of $\det(W_{22}^{(b)})$ and $\det(W_{22}^{(a)})$ (as discussed in the previous subsection there is no sign ambiguity in the evaluation of the square root of $\det(1 + D^{(b)}(z = 0)C^{(a)}(z = 0))$ ). The sign of the square roots relative to the $a$ and $b$ vacuum expectation values is statistically better defined, since $\beta$ is one-half of the original value, using the phase rule given before. In principle, this recipe can be iterated until the value of $\beta$ is small enough such that the above phase rule is mathematically exact. We actually performed a test of this method by evaluating the sign of the square root of $|W_{22}|$ using eq. (51) (for $z = 1$) and by evaluating the sign using the decomposition formula just described. We took about three thousand evolution operators for the pairing-plus-quadrupole model, applied to $^{166}$Er. First the sign was determined by simple application of eq. (51) with the left-hand side evaluated with the phases of the $\lambda$'s between $-\pi$ and $\pi$. Then the sign was determined using the factorization of $W_{22}$ just given above. The sign of the individual vacua was again determined using eq. (51) with the same phase prescription for the eigenvalues of $W^{(b)}$ and $W^{(a)}$. No discrepancy was found between the two methods. If a single discrepancy was obtained we would have repeated the decomposition into smaller and smaller values of $\beta$ untill the phase rule would have been satisfied. This was done at $\beta = 2$ in order to check whether the simple phase rule is statistically satisfied in the other cases discussed in the next section.

## 3 A Monte Carlo calculation

As an example of the formalism described in the previous section we considered the pairing +quadrupole model for the $J^\pi = 0^+$ state of $^{166}$Er and the $J^\pi = 9/2^-, \ 13/2^+$ states of $^{165}$Er. The single-particle basis, energy levels, quadrupole and paring forces are taken from ref. [6]. The matrix elements $\mathcal{B}$ of eq. (9), to be computed in the case of two particle types are

$$\begin{aligned}\mathcal{B} &= \langle\psi, J, M, \pi, N, Z|e^{-\beta\hat{H}+\alpha_n\hat{N}_n+\alpha_p\hat{N}_p}|\psi, J, M, \pi, N, Z\rangle \\ &\times e^{-\alpha_n N-\alpha_p Z} = \frac{1}{2J+1} \\ &\times\sum_M \langle\psi, J, M, \pi, N, Z|e^{-\beta\hat{H}+\alpha_n\hat{N}_n+\alpha_p\hat{N}_p}|\psi, J, M, \pi, N, Z\rangle \\ &\qquad \times e^{-\alpha_n N-\alpha_p Z} \ . \end{aligned} \tag{53}$$

The Hubbard-Stratonovich transformation applied to the pairing+quadrupole Hamiltonian with both neutrons and protons gives

$$\begin{aligned}\mathcal{B} &= \mathcal{N}_n\mathcal{N}_p \int \prod_{n=1}^{N_t} \Big( \prod_{\tau=n,p} \mathrm{d}\phi_{xn}^{(\tau)}\mathrm{d}\phi_{yn}^{(\tau)} \\ &\times \prod_{a=-2}^{2} \mathrm{d}\sigma_{an}\Big)\, e^{-\frac{\epsilon}{2}k\sum_{an}\sigma_{an}^2 - \epsilon\sum_\tau G_\tau \sum_n (\phi_{xn}^{(\tau)2}+\phi_{yn}^{(\tau)2})} \\ &\times e^{-\sum_{\tau=n,p}(\beta G_\tau \Omega_\tau/2+\alpha_\tau N_\tau)} \times \frac{1}{2J+1} \\ &\times\sum_M \langle\psi, J, M, \pi, N, Z|\hat{U}^{(n)}\hat{U}^{(p)}|\psi, J, M, \pi, N, Z\rangle, \end{aligned} \tag{54}$$

where $N_n = N$ and $N_p = Z$; the label $\tau$ identifies either neutrons or protons. The evolution operator in the above equation is the product of the evolution operator for the neutrons and the one for the protons. As before we perform the sum over the $\hat{J}_z$ quantum number, $M$, in order to eliminate spurious angular momentum components in the integrand of (54).

We have tested the computer program by first considering a pure pairing model without the quadrupole interaction and with all single-particle energies equal to each other. The total number of single-particle states was fixed to 40 for both neutrons and protons. The strength of the interaction was set to $G = 0.1$MeV for both particle types. For 20 neutrons and 20 protons we reproduced the energy of the ground state within the statistical error ($\beta = 2.5$). Similarly for 19 neutrons and 20 protons the program was succesfully tested.

Going back to the full pairing+quadrupole model, the trial states are states with both neutrons and protons degrees of freedom. For an even-even nucleus, $(0^+)$ one can take

$$|0^+\rangle = |n, 0^+\rangle|p, 0^+\rangle + \sum_J b_J[|n, J^+\rangle \times |p, J^+\rangle]^{(0)} + ... \ ,$$

with the trial state formed by coupling neutrons and protons to angular momentum (parity) $J^\pi = 0^+$. In our sample calculation for $^{166}$Er only the first term was considered. For the odd-neutron, even-proton case we took for the trial state

$$|J, M, \pi\rangle = a^\dagger_{JM}{}^{(n)}|n, 0^+\rangle|p, 0^+\rangle \quad .$$

The $|\tau, 0+\rangle$ is of type (11) with all $f_i = 1$ in eq. (12) for all subshells.

The calculation of the functional integral in eq. (54) was performed using the Gaussian Path Method (ref. [12]). Actually, in order to reach reasonable statistical errors, a much more refined version of the method which we discuss below, is implemented. The idea behind the Gaussian Path method is the following. Let us rewrite schematically the functional integral as

$$\mathcal{B} = \int \mathrm{d}v \ e^{S(v)} \quad ,$$

where $v$ are the integration variables, and $e^{S(v)}$ is the integrand. $S(v)$ is called the effective action. $S(v)$ is expanded up to quadratic terms around the maximum (the mean-field) $\bar{v}$ and gives the approximate effective action $S(v)_a$

$$S(v)_a = S(\bar{v}) + 1/2\tilde{(}v - \bar{v})M(v - \bar{v}) \quad . \tag{55}$$

We use the matrix notation and $M$ is the matrix of the second derivatives of the effective action with respect to the integration variables, calculated at the mean-field values $\bar{v}$. Then we rewrite

$$\mathcal{B} = \int \mathrm{d}v \ e^{S_a(v)} e^{S(v)-S(v)_a} \quad , \tag{56}$$

and we compute the ratio of integrals

$$\left[\int \mathrm{d}v \, e^{S_a(v)}\right]^{-1} \mathcal{B} = \left[\int \mathrm{d}v \, e^{S_a(v)}\right]^{-1} \int \mathrm{d}v \, e^{S_a(v)} e^{S(v)-S(v)_a} \quad , \tag{57}$$

which is the expectation value of $e^{S(v)-S(v)_a}$.

Since the integrand in the functional integral is invariant with respect to rotations, we prefer to work with the Fourier components of the integration variables, since symmetry requirements need to be taken into account when using such variables. We work in the intrinsic system by selecting the 0-mode Fourier components of the deformation variables in the intrinsic frame. The intrinsic frame is defined as that frame for which the time average of the Cartesian (not spherical) variables $\sigma_a$ is zero at $a = -2, -1, 1$. The same is done to take into account the gauge symmetry of the pairing fields.

If the approximation $S(v)_a$ is a good approximation to the exact effective action we expect the Monte Carlo integration to converge reasonably rapidly, if not, a large number of samples are needed. For the method to be meaningful, the maximum of $S(v)$ should be unconstrained, *i.e.* the expansion should be carried out around the highest value of $S$ throughout the integration volume. The variables $v$ are the time-dependent fields $\sigma$ and $\phi_x, \phi_y$ considered in the previous sections. We therefore expect, on very general grounds, that the mean-field is time-dependent and not static. We found that a static mean-field for our problem does not exist. This is very surprising since the Hartree-Bogoliubov mean-field is static [3]. The Hartree-Bogoliubov mean-field can be obtained only if time independence is enforced (strictly it is not a maximum for the effective action). Using time-dependent mean-fields one can proceed to compute the matrix $M$. We have done so with the following considerations, since the calculation of the full matrix is expensive. We assumed that only the lowest Fourier frequencies of the time dependent variables $\sigma(t_n), \phi_x(t_n), \phi_y(t_n)$ affect that integrand. Therefore, instead of computing the second derivatives against the time dependent variables, we compute the second derivatives against their Fourier transforms. Typically we take up to 8 or 9 modes for all fields. We found that there is a very strong interplay between shape and pairing degrees of freedom. In previous works the GPM has been implemented only by constructing approximations to the matrix $M$ (strictly $M$ needs not to be the matrix of the derivatives). In all cases a crude approximation to $M$ was used, we still could compute the functional integral with a statistical error of about 10%, but not in the case of the pairing plus quadrupole model. A rather accurate matrix $M$ is

[3] The Hartree-Bogoliubov mean-field can be obtained in correspondance of the maximum of the Grand-Canonical partition function. In this work we deal with matrix elements, rather than partition functions, and therefore the identification of the mean-field with the Hartree-Bogoliubov mean-field is only qualitative.

needed. Fortunately the computation of $M$ lends itself to be distributed over any number of computers (up to the total number of matrix elements to be calculated), so the calculation can be performed despite the large number of matrix elements.

Qualitatively we distinguish 3 regions in the integration domain. The near mean-field region where the Gaussian approximation of eq. (55) is accurate; the far away region where the whole functional integral is dominated by the Gaussian weight of the Hubbard-Stratonovich transformation and the intermediate region of the integration variables. The far away region does not contribute to the functional integral since it is very unlikely to occur in the calculation and we are left with the near mean-field and intermediate region. Also the mean-field region is unlikely to occur (in a large dimensional space it has a very small volume). Since we compute expectation values of $e^{S(v)-S(v)_a}$, using $e^{S_a}$ as a probability density, the intermediate region gives the largest contribution to the variance, since there, the approximation of eq. (55) is less accurate (anharmonicities can play a large role). To smooth out these fluctuations, in some test cases not discussed here, instead of the matrix $M$, we use a rescaled matrix $rM$ with $r$ smaller but close to 1. Thus the sampled values of $e^{S(v)-S(v)_a}$ are smaller in the intermediate region but hardly affect the ratio in the near mean-field region. The majority of the sampled values fall in the intermediate region. One can raise the following objection: both $e^{S(v)}$ and $e_a^{S(v)}$ are exponentially small in the intermediate region but their ratio can be very large or very small giving a very large contribution to the variance. The answer to this objection is precisely the rescaling we mentionned, which gives smaller ratios.

There are some distinct advantages in using this integration method. It is rather easy to sample $e^{S_a}$ and the integration points generated in this way are statistically fully independent. Moreover the computation of the ratio in eq. (57) can be rigorously divided equally over several computers thus effectively increasing the speed of the calculation.

The method described gives the value of the full functional integral $\mathcal{B}$. The energy levels of the pairing+quadrupole Hamiltonian are then obtained using the expression

$$-\partial_\beta \ln \mathcal{B} = -[\ln \mathcal{B}(\beta + \delta\beta) - \ln \mathcal{B}(\beta)]/\delta\beta \quad . \tag{58}$$

Strictly, $\delta\beta$ should be small, but it can be taken large since at low temperatures $\mathcal{B}$ is essentially the exponential of $-\beta E_{J\pi}$.

The calculation with the full basis, used in ref. [6], is computationally heavy (few computers were used), but it can be done. With the full basis we evaluated the energy by calculating $\mathcal{B}$ at $\beta = 1.0$ and $\beta = 2.0$. In the calculation we took $\epsilon = 0.03$. We obtained the following values for the energies. For $Er^{166}$ , 0+ state, $E = -308.77 \pm 0.10$ MeV For $Er^{165}$, $E(9/2^-) = -303.38 \pm 0.11$ MeV, $E(13/2^+) = -303.34 \pm 0.13$ MeV and $E(5/2^-) = -302.73 \pm 0.12$ MeV. Of course, it is not the absolute values of the energies which matter, but rather the separation between the levels. At this stage we do not express any judgement about the validity of the pairing + quadrupole model in reproducing spectra for the following reasons. First of all, we do not know how accurate our ansatz for the trial wave functions is: at these temperatures mixture with excited states of the same angular momentum and parity can occur. Presumably a more complicated ansatz is necessary if we choose to use only relatively large temperatures. If we choose to keep these ansatzs the calculations have to be performed at reasonably large $\beta$ values. At the moment we are limited by the CPU time necessary. The above numbers have been obtained with Monte Carlo runs ranging from about 6000 to 14000 data points. The percentage of negative contributions in the integration is kept to a few percent by proprerly selecting both neutron and proton chemical potentials as discussed in ref. [13].

## 4 Conclusions

The formalism and the calculations described in this work prove that spectral properties of nuclear models can be studied in an exact way using Monte Carlo methods. These techniques might be very useful in testing the validity of model Hamiltonians using their lowest energy levels of given angular momentum and parity. An obvious improvement will be to consider a better ansatz for the trial states with good angular momentum and parity (we took the simplest ansatz from a computational point of view) and/or implement the method at very low temperatures so that the ground state energy with a given $J\pi$ can be unambigously calculated. A better ansatz for the trial states would allow the computation of the ground-state energy for a given angular momentum and parity, without having to consider very low temperatures.

We found no difference in behaviour between cases with an even and an odd number of particles, as far as the sign problem is concerned. Also, to the author's knoweledge, no Monte Carlo calculation with the full single-particle basis of ref. [6], at these temperatures, has been carried out before. We were able to perform such a calculation thanks to the computational speed, compared with the Metropolis method, of the Gaussian Path method as described in this work.

## References

1. G. Puddu, Phys. Rev. C **59**, 2500 (1999).
2. T. Mizusaki, T. Otsuka, Y. Utsuno, M. Honma and T. Sebe, Phys. Rev. C **59**, R1846 (1999) and references in there.
3. R. Blankenbecler, D.J. Scalapino and R.L. Sugar, Phys. Rev. D **24**, 2278 (1981). S.R. White, D.J. Scalapino, R.L. Sugar, E.Y. Loh, J.E. Gubernatis and R.T. Scarlettar, Phys. Rev. B **40**, 506 (1989). G.H. Lang, C.W. Johnson, S.E. Koonin and W.E. Ormand Phys. Rev. C **48**, 1518 (1993). N.J. Cerf, Phys. Rev. Lett. **76**, 2420 (1996). S.M.A. Rombouts, K. Heydem and N. Jachowicz, Phys. Rev. Lett. **82**, 4155 (1999).

4. J.A. White, S. Koonin and D.J. Dean Phys. Rev. C **61**, 034303 (2000).
5. G. Puddu, Nuovo Cimento B **113**, 543 (1998).
6. K. Kumar and M. Baranger, Nucl. Phys. A **110**, 529 (1968).
7. J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959). R.D. Stratonovich. Dokl. Akad. Nauk. SSSR **115**, 1907 (1957). [English translation Soviet Phys. Dokl. **2**, 416 (1958)].
8. G. Puddu, Phys. Rev. C **47**, 1067 (1993).
9. A.K. Kerman and T. Troudet, Ann. Phys. (N.Y.) **154**, 456 (1984). See especially sec. 2.3.
10. R. Balian and E. Brezin, Nuovo Cimento B **64**, 37 (1969).
11. J.M. Eisenberg, W. Greiner, *Nuclear Theory*, Vol. **3** (North Holland Publ. New York, 1972).
12. G. Puddu, Nuovo Cimento A **111**, 317 (1998).
13. G. Puddu, Nuovo Cimento A **111**, 311 (1998).