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Monte Carlo methods for yrast spectroscopy

G. Puddu[a]

Dipartimento di Fisica dell'Università di Milano, I-20133 Milano, Italy and INFN sezione di Milano, Milano, Italy

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Abstract. We discuss the details of the recently proposed Monte Carlo method to evaluate the exact energies of yrast levels. Energy levels are evaluated up to $J = 18$ with small statistical errors using the Metropolis method for the case of ^{166}Er using the pairing plus quadrupole model within one major shell. We also discuss the evaluation of the probabilities of the Hartree-Fock-Bogoliubov wave functions in the corresponding yrast eigenstates and they are found to be large. The model displays a too strong backbending behaviour not seen experimentally.

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1 Introduction

The shell model method has been a valuable tool for a detailed description of nuclear eigenstates. Its application has been limited by the large size of the Hamiltonian matrix to be diagonalized. Although it has been used extensively for light nuclei, heavy and medium-heavy nuclei have been up to date outside of the reach of the shell model approach. In the past decades, the application of the Hubbard-Stratonovich (HS) transformation, ref. [1], to the nuclear many-body problem has been extensively explored (see, for example, ref. [2]). The essential physical content of this transformation is the evaluation of the exponential of the many-body Hamiltonian $\mathrm{e}^{-\beta\hat{H}}$ in terms of a sum of an infinite number of exponentials of one-body Hamiltonians. The above operator, for sufficiently large-β projects the exact ground state of the many-body Hamiltonian out of a trial wave function. Observables can in principle be computed using such a projected wave function.

Recently we have introduced a method that allowed the Monte Carlo evaluation, of the energies of angular momentum and parity projected eigenstates of the form $\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle$, where $\hat{P}_{JJ}$ is the projector to good angular momentum J and z-projection $J_z = J$ and $|\psi\rangle$ is a particle number projected HFB wave function (ref. [3]). With this method yrast energies have been evaluated with a small statistical error using the Metropolis sampling method (ref. [4]), including the full many-body basis, without any remnant of the shell model diagonalization method.

In ref. [5] it has been proposed that the same HS transformation, applied to $\mathrm{e}^{-\beta\hat{H}}$ acting on trial Hartree-Fock wave functions, could be used to construct an optimized many-body basis in which the shell model Hamiltonian can be diagonalized. Although in this last approach there is no guarantee that the many-body basis is sufficiently large and no method was given to estimate the statistical error, it was shown that properties of yrast levels, and of excited states, could be evaluated. The most advanced form of this approach uses angular-momentum projected Hartree-Fock-Bogoliubov (HFB) wave functions, rather than Hartree-Fock wave functions, as trial states.

In ref. [6], Monte Carlo calculations in the rare-earth region have been discussed in order to extract thermal properties of nuclei. In the approach we propose, individual excited states can be studied explicitly rather than as a statistical average.

The purpose of this article is to describe the details of the method used in ref. [3] and to complete the calculation of the yrast band up to $J = 18$. The functional integral formulation which was used, is the same used in the Monte Carlo calculations of refs. [7]. This functional integral formulation, because of the small number of auxiliary fields, allows a reasonably fast sampling of the functional integral compared to other formulations.

Since HFB wave functions are considered accurate approximations to the exact wave functions, they were selected so that small values of β are necessary to converge to the yrast levels. This has the advantage that sampling the integration volume with the Metropolis method is reasonably fast. Since we evaluate only angular-momentum projected energies, only high-lying excited states of the

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

same angular momentum have to be filtered out by the operator $\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}$ and this itself implies the need of small values of the parameter β.

Moreover, since sign oscillations usually appear at large values of β, the use of these wave functions could potentially mitigate the sign problem.

The outline of this paper is as follows. In sect. 2 we discuss the method for the evaluation of the yrast energies. In sect. 3 we give explicit expressions for the matrix elements for one particle species which enter the calculation. In sect. 4 we discuss the problem of the overlaps of HFB wave functions with yrast eigenstates, and in sect. 5 we summarize and discuss the numerical results obtained so far.

2 The method for the evaluation of the yrast energies

If $\hat{H}$ is the many-body shell model Hamiltonian and $\hat{P}_{JM}$ is the projector to good angular momentum J and z-component of the angular momentum M, the basic quantity we want to evaluate is

$$E(\beta,N,Z,J)=\frac{\langle\psi NZ|\hat{P}^{(J)}_{JJ}\hat{H}\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}{\langle\psi NZ|\hat{P}^{(J)}_{JJ}\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}, \quad (1)$$

where $\hat{J}_z$ is the z-component of the angular-momentum operator, ω is a cranking frequency, $\hat{N}_{n(p)}$ is the neutron (proton) particle number operator and $\mu_{n(p)}$ is neutron (proton) chemical potential. The trial wave function $|\psi NZ\rangle$ is a particle number projected HFB wave function for N valence neutrons and Z valence protons and, in terms of the neutron (proton) particle number projector $\hat{P}_{N(Z)}$, is given by

$$|\psi NZ\rangle=\hat{P}_N|\psi_n\rangle\hat{P}_Z|\psi_p\rangle,$$

where $|\psi_\tau\rangle$ $(\tau=n,p)$ is a wave function of the type

$$|\psi\rangle=\exp\left(\frac{1}{2}\sum_{i,j}a^\dagger_i X_{ij}a^\dagger_j\right)|0\rangle \quad (2)$$

$a^\dagger_i$ being the creation operator of the single-particle (neutron or proton) state i, X a variationally determined antisymmetric matrix and $|0\rangle$ is the particle vacuum. In eq. (1), the cranking frequency has been introduced so that the unprojected lowest-energy state has $J_z=J$ and the chemical potential so that the lowest-energy state has neutron (proton) particle number $N\,(Z)$. This is done in view of the fact the functional integral expression for the exponential of the Hamiltonian in eq. (1) breaks the rotational symmetry and therefore the propagator in the functional integral (see below) propagates all angular-momentum components of the HFB wave function, and not just the desired one, giving stronger weight to the angular-momentum component having the lowest energy. Since the Monte Carlo evaluation of eq. (1) hinges on the method of importance sampling, the lack of the cranking term would lead to the sampling of states which would have to be cancelled out by the angular-momentum projection. In principle one could use the angular-momentum projector both at the left and at the right of the propagator in eq. (1), but such a double angular-momentum projection, besides being prohibitively expensive, would not prevent the propagation of angular-momentum components different from the desired J value. Analogous considerations can be made to justify the presence of the chemical potentials.

The energy evaluated using eq. (1) is a monotonically decreasing function of the parameter β and for $\beta=0$ eq. (1) gives the expectation value of the Hamiltonian with angular-momentum projected HFB wave functions

$$E_{\mathrm{HFB}}(N,Z)=\frac{\langle\psi NZ|\hat{P}^{(J)}_{JJ}\hat{H}|\psi NZ\rangle}{\langle\psi NZ|\hat{P}^{(J)}_{JJ}|\psi NZ\rangle}. \quad (3)$$

Therefore it is quite reasonable to expect that the best variational wave functions will lead to the yrast energies even at small values of β. In this context, these wave functions should be selected so that they minimize the right-hand side of eq. (3). In practice, since the variational determination of $|\psi NZ\rangle$ is by itself computationally time consuming, we selected only wave functions which minimize the J_z projected energy functional of eq. (3). In the case of the ground state no angular-momentum projector is necessary in the determination of the trial wave function, although the full projector was used in the evaluation of eq. (1) as discussed below.

The calculations which will be discussed later, are relative to the pairing plus quadrupole model limited to one major shell for neutrons and one major shell for protons. For this model the functional integral for the exponential of the Hamiltonian, which we use for the evaluation of eq. (1), has a simple and appealing form. It leads to the smallest number of integration variables. The model Hamiltonians is

$$\hat{H}=\hat{H}_{0n}+\hat{H}_{0p}+\hat{V}_Q-G_n\hat{P}^\dagger_n\hat{P}_n-G_p\hat{P}^\dagger_p\hat{P}_p, \quad (4)$$

with $\hat{H}_{0n}$ $(\hat{H}_{0p})$ being the spherical independent single-particle Hamiltonian for the neutrons (protons), $\hat{V}_Q$ is the quadrupole interaction

$$\hat{V}_Q=-\frac{1}{2}\chi\sum_{a=-2}^{a=2}(c^2_n\hat{Q}_{na}+c^2_p\hat{Q}_{pa})(c^2_n\hat{Q}_{na}+c^2_p\hat{Q}_{pa}) \quad (4')$$

with the allowance of different n-n, p-p and n-p quadrupole coupling constants[1]. The operators appearing in eq. (4′) are the Cartesian components of the spherical tensor operators. In eq. (4), $\hat{P}^\dagger$ is the monopole pair creation operator. Using the Hubbard-Stratonovich transformation

[1] In the numerical calculations described later these coupling constants were chosen as in ref. [8], with $c_n=(2N/A)^{1/3}$ and $c_p=(2Z/A)^{1/3}$.

(ref. [1]) one obtains

$$\mathrm{e}^{-\beta(\hat{H}-\mu_n\hat{N}_n-\mu_p\hat{N}_p-\omega\hat{J}_z)} = \mathrm{e}^{-\beta G_n\Omega_n/2-\beta G_p\Omega_p/2}\mathcal{N} \times\int\prod_{m=1}^{N_t}\prod_{\tau=n,p}(\mathrm{d}\phi_{xm}^{(\tau)}\mathrm{d}\phi_{ym}^{(\tau)}) \times\prod_{a=-2}^{2}\mathrm{d}\sigma_{am}\mathrm{e}^{-\frac{1}{2}\sum_{am}\sigma_{am}^2-\frac{1}{2}\sum_{m\tau}(\phi_{xm}^{(\tau)2}+\phi_{ym}^{(\tau)2})}\hat{U}. \quad (5)$$

In this equation $\mathcal{N}$ is an irrelevant normalization constant and

$$\hat{U} = \hat{U}^{(n)}\hat{U}^{(p)}\,,$$
$$\hat{U}^{(\tau)} = \hat{U}_{N_t}^{(\tau)}\hat{U}_{N_t-1}^{(\tau)}\ldots\hat{U}_1^{(\tau)}\,, \qquad (\tau=n,p)\,, \quad (6)$$
$$\hat{U}_m^{(\tau)} = \exp\Big[-\epsilon\hat{H}^{(\tau)\prime}_0-\sqrt{\epsilon\chi}\sum_a\sigma_{am}c_\tau^2\hat{Q}_a^{(\tau)} -\sqrt{\epsilon G_\tau/2}(\phi_m^{(\tau)}\hat{P}^{(\tau)}+\phi_m^{(\tau)\star}\hat{P}^{(\tau)\dagger})\Big]\,, \quad (7)$$

for $m=1,\ldots,N_t$ and $\phi_m^{(\tau)}=\phi_{xm}^{(\tau)}+i\phi_{ym}^{(\tau)}$.
In eq. (7), $\hat{H}^{(\tau)\prime}_0=\hat{H}_0^{(\tau)}-\omega\hat{J}_z^{(\tau)}-\mu^{(\tau)\prime}\hat{N}^{(\tau)}$ and $\mu'_\tau=\mu_\tau+G_\tau/2$ and Ω_τ is one half of the number of single particle states. The label $\tau=n,p$ refers to the neutrons or to the protons. N_t is the number of time intervals and $\epsilon=\beta/N_t$.

The propagator $\hat{U}$ for both neutrons and protons is Hermitian in the static limit (*i.e.* $N_t=1$). In order not to overburden the equation, since the propagator $\hat{U}$ is a product of a neutron propagator and a proton propagator, we shall simply write for each particle species at any time interval

$$\hat{U}_m = \exp\Big[\hat{K}_m+\frac{1}{2}(\hat{\Pi}_m+\hat{\Pi}_m^\dagger)\Big]\,, \quad (8)$$

with $\hat{K}_m$ being a Hermitian operator of the type, in a matrix notation, $a^\dagger K_m a$ and $\hat{\Pi}_m$ a pairing operator of the type $a\Pi_m a$. For later convenience we rewrite eq. (8) as

$$\hat{U}_m = \exp\Big[\frac{1}{2}(a^\dagger a)\begin{pmatrix}K_m & -\Pi_m^\star\\ \Pi_m & -\tilde{K}_m\end{pmatrix}\begin{pmatrix}a\\ a^\dagger\end{pmatrix}\Big]\exp\Big[\frac{1}{2}\mathrm{tr}K_m\Big] \equiv \hat{W}_m\exp\Big[\frac{1}{2}\mathrm{tr}K_m\Big] \quad (9)$$

with the matrix K_m given by

$$(K_m)_{ij} = -\epsilon(\varepsilon_i-\mu'-\omega m_i)\delta_{ij}-\sqrt{\epsilon\chi}c^2\sum_a\sigma_{am}(q_a)_{ij} \quad (10)$$

with ε_i being the single-particle energies, m_i the single-particle eigenvalues of j_z and q_a the single-particle quadrupole moment. The skew-symmetric matrix Π_m in eq. (9) for the monopole pairing interaction has non-zero matrix elements $(\Pi_m)_{ij}=\sqrt{2\epsilon G}\phi_m\delta_{-ij}$, where $-i$ denotes the time-reversal partner of the single-particle state i. The operator $\hat{W}_m$ is defined by eq. (9). Schematically, if we denote by $\mathrm{d}x$ the integration volume, by $G(x)$ the Gaussian weight and the numerical factors appearing in eq. (5), the functional integral can be written in a compact form as

$$\mathrm{e}^{-\beta(\hat{H}-\mu_n\hat{N}_n-\mu_p\hat{N}_p-\omega\hat{J}_z)} = \int\mathrm{d}xG(x)\hat{W}^{(n)}\hat{W}^{(p)} \quad (11)$$

and the neutron (proton) propagator is the time-ordered product of the N_t operators $\hat{W}_m$. The angular-momentum projector in eq. (1) is given by

$$\hat{P}_{JJ}^{(J)} = \frac{2J+1}{8\pi^2}\int\mathrm{d}\Omega_E D_{JJ}^{(J)*}(\Omega_E)\hat{R}(\Omega_E), \quad (12)$$

where $\Omega_E=(\theta_1\theta_2\theta_3)$ is the collection of the three Euler angles, $\mathrm{d}\Omega_E=\mathrm{d}\theta_1\sin\theta_2\mathrm{d}\theta_2\mathrm{d}\theta_3$, $D_{JJ}^{(J)}$ is the Wigner function and

$$\hat{R}(\Omega_E) = \mathrm{e}^{i\theta_3\hat{J}_z}\mathrm{e}^{i\theta_2\hat{J}_y}\mathrm{e}^{i\theta_1\hat{J}_z}, \quad (13)$$

is the rotation operator. The evaluation of eq. (1) is then reduced to the evaluation of the following functional integrals (separately or their ratio):

$$\langle\hat{O}\rangle = \int\mathrm{d}xG(x)\int\mathrm{d}\Omega_E D_{JJ}^{(J)\star} \times\langle\psi NZ|\hat{R}(\Omega_E)\hat{O}\hat{W}^{(n)}\hat{W}^{(p)}|\psi NZ\rangle \quad (14)$$

for $\hat{O}=1$ and $\hat{O}=\hat{H}$. Since sampling the integration space with the the angular-momentum projection is very time consuming we rewite eq. (14) as

$$\langle\hat{O}\rangle = \mathrm{Re}\int\mathrm{d}xG(x)\langle\psi NZ|W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle \times\frac{\int\mathrm{d}\Omega_E D_{JJ}^{(J)\star}\langle\psi NZ|\hat{R}(\Omega_E)\hat{O}\hat{W}^{(n)}\hat{W}^{(p)}|\psi NZ\rangle}{\langle\psi NZ|W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle}, \quad (15)$$

where Re denotes the real part. If we set $G(x)\langle\psi NZ|W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle=\mathrm{e}^{A+iB}$, call $\mathcal{E}$ the ratio in eq. (15), $s(x)$ the sign of $\cos B$ and define the probability distribution in the importance sampling as $p(x)=\mathrm{e}^{A+\ln|\cos B|}$, then

$$\langle\hat{O}\rangle = \int\mathrm{d}x\ \ p(x)s(x)[\mathrm{Re}(\mathcal{E})-\tan B\ \ \mathrm{Im}(\mathcal{E})]. \quad (16)$$

This quantity is evaluated, up to the normalization of $p(x)$, which cancels out in the ratio of eq. (1), with the Metropolis method (ref. [4]). In other words we evaluate $\langle\hat{H}\rangle$ and $\langle 1\rangle$ by sampling the functional integrals in eq. (16) with an unprojected probability distribution.

The first task in a Monte Carlo calculation is to obtain a set of statistically independent integration points $\{x\}$ according to the distribution $p(x)$, without actually evaluating the observables; only after a set of statistically independent integration points has been obtained the angular-momemtum projected matrix elements are evaluated. The criterion that we use in fixing $p(x)$ is that it must approximate as much as possible the angular-momentum projected matrix elements $G(x)\langle\psi NZ|\hat{P}_{JJ}W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle$

for the most relevant integration points. That is the integral $\int \mathrm{d}x\, G(x)\langle\psi NZ|W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle$ should be the best approximation to $\langle\psi NZ|\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}|\psi NZ\rangle$. In turn this implies that the cranking frequency in principle should be fixed by a Monte Carlo calculation (see also sect. 5). This completes the discussion of the basic idea behind the method used in the evaluation of the yrast energies.

The remaining task is to give explicit expressions, for matrix elements for one particle species, of the type

$$\mathcal{O}_1(\hat{M}) = \langle\psi N|\hat{R}(\Omega_E)\hat{M}\hat{W}|\psi N\rangle \tag{17}$$

which appear in the evaluation of the integrand in eq. (15), where $\hat{M}$ can be a one-body operator, a two-body operator for a single particle species, or 1.

3 Expressions for the one particle species matrix elements

The evaluation of eq. (17) implies a double particle number projection for every set of the Euler angles. As usually done, we first evaluate

$$\mathcal{O}_1(\hat{M},\alpha_p,\alpha_q) = \langle\psi|\mathrm{e}^{\alpha_p\hat{N}}\hat{R}(\Omega_E)\hat{M}\hat{W}\mathrm{e}^{\alpha_q\hat{N}}|\psi\rangle \tag{18}$$

and then isolate the N-th power of both $z_p = \mathrm{e}^{\alpha_p}$ and $z_q = \mathrm{e}^{\alpha_q}$. The calculation is summarized in the appendix. The results are as follows. First the single-particle matrix W_{ij} defined as the time-ordered product

$$W = \prod_{m=1}^{N_t} \exp\begin{pmatrix} K_m & -\Pi_m^\star \\ \Pi_m & -\tilde{K}_m \end{pmatrix}, \tag{19}$$

is constructed. From the square submatrices W_{11}, W_{12}, W_{21} and W_{22} of W, the matrices $C = W_{12}W_{22}^{-1}$ and $D = W_{22}^{-1}W_{21}$ are then evaluated. The single-particle representation (first quantized), r, of the rotation operator is constructed. Then

$$\mathcal{O}_1(M=1,z_p,z_q) = |W_{22}|^{1/2}|1+z_q^2DX|^{1/2}|1-z_p^2\tilde{r}X^\star r\overline{X}_q|^{1/2} \tag{20}$$

with

$$\overline{X}_q = C + z_q^2\tilde{W}_{22}^{-1}X(1+z_q^2DX)^{-1}W_{22}^{-1} \tag{21}$$

and, if $\hat{T} = a^\dagger Ta$ in a matrix notation is a one-body operator,

$$\mathcal{O}_1(\hat{M}=\hat{T},z_p,z_q) = \mathcal{O}_1(M=1,z_p,z_q)\mathrm{tr}(\rho T) \tag{22}$$

and, if $\hat{V}_2$ is a two-body operator, then

$$\mathcal{O}_1(\hat{M}=\hat{V}_2,z_p,z_q) = \mathcal{O}_1(\hat{M}=\hat{Q},z_p,z_q) \times\left[-\frac{1}{4}z_p^2\overline{K}_{ji}\overline{V}_{ijsr}K_{sr} + \frac{1}{2}\rho_{si}\overline{V}_{ijsr}\rho_{rj}\right] \tag{23}$$

with $\overline{V}$ being the antisymmetrized two-body potential, and

$$\rho = 1-\tilde{F}, \qquad F = (1-z_p^2\tilde{r}X^\star r\overline{X}_q)^{-1}, \tag{24}$$

$$\overline{K} = F\tilde{r}X^\star r, \qquad K = \overline{X}_qF. \tag{25}$$

The remaining point is the determination of the sign of the square root of the determinants in eq. (20). Here we recall the results of ref. [7]. The square root of $|1+z_q^2DX|$ is evaluated by considering one eigenvalue of DX for every degenerate pair (since the product of two skew-symmetric matrices as D and X has a degenerate spectrum). No additional sign is present. Similarly one argues for $|1-z_p^2\tilde{r}X^\star r\overline{X}_q|$. For the square root of $|W_{22}|$ we make use of the following formula for the trace of $\mathrm{e}^{\alpha\hat{N}}\hat{W}$ in the grand canonical ensemble (ref. [7]):

$$\mathrm{tr}_{\mathrm{g.c.}}[\mathrm{e}^{\alpha\hat{N}}\hat{W}] = |W_{22}|^{1/2}|1+z\mathcal{M}|^{1/2}, \tag{26}$$

where $\mathcal{M}$ can be proven to be given by

$$\mathcal{M} = \begin{pmatrix} \tilde{W}_{22}^{-1} & C \\ -D & W_{22}^{-1} \end{pmatrix}. \tag{27}$$

Since the eigenvalues of $\mathcal{M}$ must be degenerate (since the left-hand side is a polynomial in $z = \mathrm{e}^\alpha$), $|1+z\mathcal{M}|^{1/2}$ can be evaluated by taking one eigenvalue of $\mathcal{M}$ for every degenerate pair, without extra sign[2] since z can be taken close to zero. Hence the evaluation of the left-hand side of eq. (26) gives the proper sign of $|W_{22}|^{1/2}$, say for $z = 1$. At high temperature the sign of $\mathrm{tr}_{\mathrm{g.c.}}\hat{W}$ is free of ambiguities since the eigenvalues of W are nearly real. If the temperature is not too high, as in ref. [7] one divides the interval $[0,\beta]$ into two intervals say 1 and 2. Then $W_{22} = W_{22}^{(2)}(1+D^{(2)}C^{(1)})W_{22}^{(1)}$ and one can proceed by evaluating the square root of W_{22} at smaller values of β. This last method has been implemented in the computer programs by iterating twice.

4 The evaluation of the overlaps

Although not essential for the method described in the previous section, we describe here a method for the evaluation of the probabilities of Monte Carlo yrast wave functions in the HFB wave functions. To motivate this problem let us assume that any yrast HFB wave function $|\psi\rangle$, inclusive of the projectors, can be expanded in terms of the exact eigenstates of the Hamiltonian with small coefficients for excited states, *i.e.* $|\psi\rangle = \sum_i c_i|i\rangle$ with $c_0 \approx 1$ and $c_k \approx 0$ for $k = 1,2,\ldots$ and let us estimate qualitatively the Monte Carlo error for the energies. Schematically the Hubbard-Stratonovich transformation can be rewritten as

[2] Such an extra sign is independent of z since the left-hand side is a polynomial in z, $|W_{22}|^{1/2}$ is a c-number and $|1+z\mathcal{M}|^{1/2}$ is also a polynomial of z and both polynomials are continous functions of z. Hence such an extra sign which could take the values ±1 must be a constant.

$\mathrm{e}^{-\beta\hat{H}} = \sum_x \hat{W}(x)$, where x is the multidimensional integration point and $\hat{W}(x)$ denotes the propagators (here inclusive of all coefficients) in the functional integral. Then, up to first order,

$$\langle\psi|\hat{H}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle = \sum_x \{E_0[\langle 0|\hat{W}(x)|0\rangle + \sum_{i>0}(\langle 0|\hat{W}(x)|i\rangle c_i + \langle i|\hat{W}(x)|0\rangle c_i^\star)] + \sum_{i>0} c_i^\star (E_i - E_0)\langle i|\hat{W}(x)|0\rangle\} \quad (28)$$

and

$$\langle\psi|\mathrm{e}^{-\beta\hat{H}}|\psi\rangle = \sum_x [\langle 0|\hat{W}(x)|0\rangle + \sum_{i>0}(\langle 0|\hat{W}(x)|i\rangle c_i + \langle i|\hat{W}(x)|0\rangle c_i^\star)]. \quad (29)$$

In a Monte Carlo calculation one evaluates the ratio of eq. (28) to eq. (29) by selecting a distribution function, say $p(x)$, rewrites the ratio of eq. (28) to (29) as

$$\langle\hat{H}\rangle = \frac{\sum_x p(x)E_0[\rho(x) + \delta(x)]/p(x)}{\sum_x p(x)\rho(x)/p(x)} \quad (30)$$

and then evaluates the numerator and the denominator with important sampling using $p(x)$ as a distribution. In eq. (30), as a shorthand notation, we denoted as $\rho(x)$ the term in the sum over x in eq. (29), and as $\rho(x) + \delta(x)$ the coefficient of E_0 in eq. (28), after it is factored out. Since we assumed small $c_{k>0}$, $\delta(x)$ is generally small compared to $\rho(x)$, and if $p(x)$ is large when $|\rho(x)|$ is large, the numerator is nearly proportional to the numerator. Therefore the Monte Carlo error of the energy is the error of a ratio of the type a/b, where a is a random variable almost proportional to the random variable b, hence the statistical error would be small. If this condition of almost proportionality is met, the statistical error can be small even in presence of sign fluctuations in the functional integral. This is true to the extent that the HFB wave functions are a good approximation to the eigenstates of the Hamiltonian, and provided, of course, that the distribution used in the sampling does not sample regions where $|\rho(x)|/p(x)$ is small and $|\delta(x)|/p(x)$ is large. In the limit of exact wave functions, the statistical error goes to zero.

The probabilities of the exact yrast wave functions in the HFB wave functions for a given J are given by, for sufficiently large β,

$$C_J = \frac{\langle\psi|\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle^2}{\langle\psi|\hat{P}\mathrm{e}^{-2\beta\hat{H}}|\psi\rangle}. \quad (31)$$

Ideally, eq. (31) can be evaluated using the differential equation $\mathrm{d}\ln\mathcal{N}/\mathrm{d}\beta = -E(\beta)$, for the norm $\mathcal{N}(\beta) = \langle\psi|\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle$, where $E_J(\beta)$ is given by

$$E_J(\beta) = \frac{\langle\psi|\hat{P}_{JJ}\hat{H}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle}{\langle\psi|\hat{P}_{JJ}\mathrm{e}^{-\beta\hat{H}}|\psi\rangle}. \quad (32)$$

Equation (31) can then be rewritten as (we explicitly insert the argument β in C_J)

$$C_J(\beta) = \exp\left[\int_0^{2\beta} E_J(t)\mathrm{d}t - 2\int_0^{\beta} E_J(t)\mathrm{d}t\right]. \quad (33)$$

If a given value of β is not deemed sufficiently large so that $E_J(\beta)$ is identified with the energy of the yrast level, but 2β is, the following approximate formula gives the size of the correction with respect to higher values of β:

$$\frac{C_J(2\beta)}{C_J(\beta)} = \mathrm{e}^{-\beta[E_J(\beta) - E_J(2\beta)]}. \quad (34)$$

For very large β, if $E^\star(\beta) = E(\beta) - E(\infty)$, eq. (33) becomes

$$C_J(\infty) = \exp\left[-\int_0^{\infty} E^\star(\beta)\mathrm{d}\beta\right]. \quad (33')$$

Instead of using eq. (33) or (33′) to evaluate C_J, which requires the computationally expensive evaluation of the energies for several β values, we evaluate directly eq. (31) in the following way. First we write the functional integral expressions for the numerator and the denominator appearing in eq. (31). Then we evaluate the ratio of the functional integrals with the Metropolis method (ref. [4]) using the same probability distribution, for both the numerator and the denominator. This method is computationally less expensive, although statistically not very accurate since the matrix elements in the numerator and in the denominator in eq. (31) have different values of β. Before proceeding, let us rewrite eq. (31) as

$$C_J = \frac{\langle\psi|\hat{P}_{JJ}\mathrm{e}^{-\beta[\hat{H} - \omega(\beta)\hat{J}_z - \mu_n(\beta)\hat{N}_n - \mu_p(\beta)\hat{N}_p]}|\psi\rangle^2}{\langle\psi|\hat{P}_{JJ}\mathrm{e}^{-2\beta[\hat{H} - \omega(2\beta)\hat{J}_z - \mu_n(2\beta)\hat{N}_n - \mu_p(2\beta)\hat{N}_p]}|\psi\rangle} K \quad (35)$$

with

$$K = \frac{\mathrm{e}^{2\beta[\omega(2\beta)J + \mu_n(2\beta)N + \mu_p(2\beta)Z]}}{\mathrm{e}^{2\beta[\omega(\beta)J + \mu_n(\beta)N + \mu_p(\beta)Z]}}. \quad (36)$$

Let us write the functional integrals in the schematic form, as in sect. 2, as

$$\mathrm{e}^{-\beta(\hat{H} - \mu_n\hat{N}_n - \mu_p\hat{N}_p - \omega\hat{J}_z)} = \int \mathrm{d}\vec{x} G\beta(\vec{x})\hat{W}, \quad (37)$$

$$\mathrm{e}^{-2\beta(\hat{H} - \mu_n\hat{N}_n - \mu_p\hat{N}_p - \omega\hat{J}_z)} = \int \mathrm{d}\vec{x}_2\mathrm{d}\vec{x}_1 G_{2\beta}(\vec{x}_2, \vec{x}_1)\hat{W}(\vec{x}_2)\hat{W}(\vec{x}_1). \quad (37')$$

The integration vector $\vec{x}$ in eq. (37) denotes all the integration variables at the time intervals $n = 1, 2, \ldots, N_t$ while in eq. (37′) the integration vectors $\vec{x}_1$ and $\vec{x}_2$ are the integration variables at $n = 1, 2, \ldots, N_t$ and $n = N_t + 1, \ldots, 2N_t$, respectively. The meaning of the functions G_β and $G_{2\beta}$ is the same as in sect. 2.

The time interval ϵ, implicit in eqs. (37) and (37′), is the same. The propagator in eq. (37′) was explicitly

$$C_J = K\frac{\int \mathrm{d}\vec{x}_2\mathrm{d}\vec{x}_1\rho(\vec{x}_2,\vec{x}_1)G_\beta(\vec{x}_2)G_\beta(\vec{x}_1)\frac{\langle\psi|\hat{P}\hat{W}(\vec{x}_2)|\psi\rangle\langle\psi|\hat{P}\hat{W}(\vec{x}_1)|\psi\rangle}{\rho(\vec{x}_2,\vec{x}_1)}}{\int \mathrm{d}\vec{x}_2\mathrm{d}\vec{x}_1\rho(\vec{x}_2,\vec{x}_1)G_{2\beta}(\vec{x}_2,\vec{x}_1)\frac{\langle\psi|\hat{P}\hat{W}(\vec{x}_2)\hat{W}(\vec{x}_1)|\psi\rangle}{\rho(\vec{x}_2,\vec{x}_1)}} \tag{39}$$

written as the product of the propagator from 0 to β and of the propagator from β to 2β.

Equation (35) can now be rewritten as

$$C_J = K\frac{\int \mathrm{d}\vec{x}_2\mathrm{d}\vec{x}_1 G_\beta(\vec{x}_2)G_\beta(\vec{x}_1)\langle\psi|\hat{P}\hat{W}(\vec{x}_2)|\psi\rangle\langle\psi|\hat{P}\hat{W}(\vec{x}_1)|\psi\rangle}{\int \mathrm{d}\vec{x}_2\mathrm{d}\vec{x}_1 G_{2\beta}(\vec{x}_2,\vec{x}_1)\langle\psi|\hat{P}\hat{W}(\vec{x}_2)\hat{W}(\vec{x}_1)|\psi\rangle}. \tag{38}$$

For the purpose of the evaluation of this expression with Monte Carlo methods, eq. (38) is further rewritten as

see equation (39) *above*

with

$$\rho(\vec{x}_2,\vec{x}_1) = G_{2\beta}(\vec{x}_2,\vec{x}_1)|\langle\psi|\hat{W}(\vec{x}_2)\hat{W}(\vec{x}_1)|\psi\rangle| \tag{40}$$

being the absolute value of the angular-momentum unprojected integrand appearing in eq. (37′) at the inverse temperature 2β [3]. Since $\rho(\vec{x}_2,\vec{x}_1)$ contains the cranking frequency (and the chemical potentials), it generates, with higher probability, states with $M_z = J$ and the appropriate number of particles and it can be used as a density distribution in the Metropolis method.

5 Calculations of yrast levels

In this section we discuss the calculations performed so far for the yrast states of ^{166}Er. Some of them have already been presented in ref. [3], for $J^\pi = 0^+, 2^+, 4^+, 6^+$ and 12^+. We completed the calculations up to $J^\pi = 18^+$. The strength of *n-n*, *p-p*, and *n-p* quadrupole force (cf. eq. (4′)) and the oscillator length for neutrons and protons are as in ref. [8], *i.e.* $b^2_{n,p} = b^2/c_{n,p}$ and $\chi b^4 = 70$ MeV/$A^{1.4}$. The cranking frequencies used in the calculations were obtained in the following way. Instead of fixing the cranking frequencies with the requirement that

$$\frac{\langle\psi NZ|\hat{J}_z\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle}{\langle\psi NZ|\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle} = J, \tag{41}$$

we fix these frequencies only using the mean-field propagator. The results for the energies do not depend on these values, since they do not affect the angular-momentum projected matrix elements, but they do affect the probability distribution $p(x)$ used in eq. (16), that is, the values of ω affect the Monte Carlo error. In practice this approximate recipe works reasonably well, although it tends to underestimate the values of ω at large values of β. The chemical potentials have been determined with the same method used in ref. [7].

Instead of considering the full angular-momentum projector in eq. (1), one could consider instead the projector to the good z-component of the angular momentum $J_z = J$ and then test whether the Monte Carlo expectation values of $\hat{J}^2$ are statistically consistent with $J(J+1)$. This method is not expected to be very accurate at low angular momentum because of contamination of nearby states with the same J_z but different J; however it leads to values of $\hat{J}^2$ consistent with $J(J+1)$ at large values of J_z. The calculations at large angular momenta have been performed in this way.

Quantities which are revealing with respect of the goodness of the substitution of projected probability distributions with the cranked unprojected ones are the following ratios of overlaps:

$$\mathcal{O}_J = \frac{\langle\psi NZ|\hat{P}^{(J)}_{JJ}\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle}{\langle\psi NZ|\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle}, \tag{42}$$

$$\mathcal{O}_{J_z} = \frac{\langle\psi NZ|\hat{P}(J_z = M)\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle}{\langle\psi NZ|\mathrm{e}^{-\beta(\hat{H}-\omega\hat{J}_z)}|\psi NZ\rangle}, \tag{43}$$

which, depending on the projector used, give the amount of depletion caused by the angular-momentum projection, whether full or J_z only. If the cranking recipe well approximates the projector we expect the above quantity to be close to unity, if not it should be small. Typical values are between 0.1 and 0.2, with a slight tendency to decrease for larger values of β at large angular momentum. This is probably an indication that the cranking frequencies are off their ideal values.

The numerical results obtained so far for the energies, inclusive of the partial ones of ref. [3], are summarized in table 1. The calculations reported in table 1 have been performed at $\beta = 1$ MeV^{-1} and $\beta = 2$ MeV^{-1}. The values of the energies indicate that the values of β are sufficiently large. The 4th column in table 1 indicates the type of angular-momentum projector used in the calculation. Also shown are the expectation values of $\langle\hat{J}^2\rangle$ with their statistical error. In the case the full angular-momentum projector is used, these values are only their nominal values.

The calculations proceed as follows. After the chemical potentials and the cranking frequencies have been selected, the cranked unprojected probability distribution $p(x)$, given by

$$p(x) = |\mathrm{Re}[G(x)\langle\psi NZ|W^{(n)}\hat{W}^{(p)}|\psi NZ\rangle]| \tag{44}$$

(cf. eq. (15)), is generated with the Metropolis method. We keep typically one every 50 or 60 of the integration points.

[3] The use of this function is optimal at 2β but less so in the evaluation of the numerator of eq. (35). However, the smaller inverse temperatures should suppress fluctuations.

Table 1. Monte Carlo results for selected yrast states of ^{166}Er. The column labeled $\hat{P}$ identifies the type of projection. If only the z-component of the angular momentum is projected, the expectation values of J^2 are given with the statistical error. If J^2, J_z are projected $\langle J^2 \rangle$ is the nominal value. N_s is the number of samples, and "ac" is the autocorrelation of the energy samples. $\mathcal{O}$ is given by eq. (42) or eq. (43).

β	State	$\langle J^2 \rangle$	$\hat{P}$	N_s	ac	$\mathcal{O}$	E (MeV)
1	0^+	0	J^2, J_z	97	0.02	0.080 ± 0.009	-112.860 ± 0.052[a]
2	0^+	0	J^2, J_z	108	-0.028	0.27 ± 0.1	-112.876 ± 0.119[a]
1	2^+	6	J^2, J_z	93	0.12	0.119 ± 0.009	-112.532 ± 0.033[a]
2	2^+	6	J^2, J_z	93	-0.05	0.16 ± 0.02	-112.643 ± 0.061[a]
1	2^+	10.4 ± 1.3	J_z	83	0.07	0.17 ± 0.02	-112.399 ± 0.064[a]
2	2^+	6.7 ± 2.4	J_z	102	-0.009	0.22 ± 0.03	-112.602 ± 0.140[a]
1	4^+	20	J^2, J_z	104	0.14	0.133 ± 0.009	-112.165 ± 0.052[a]
2	4^+	20	J^2, J_z	98	0.0008	0.12 ± 0.02	-112.146 ± 0.121[a]
1	4^+	25 ± 1	J_z	120	0.03	0.16 ± 0.01	-112.014 ± 0.059[a]
2	4^+	22 ± 4	J_z	91	-0.03	0.18 ± 0.03	-112.132 ± 0.086[a]
1	6^+	42	J^2, J_z	89	0.25	0.114 ± 0.007	-111.626 ± 0.041[a]
2	6^+	42	J^2, J_z	97	-0.07	0.14 ± 0.01	-111.656 ± 0.040[a]
1	6^+	45 ± 1	J_z	180	0.02	0.121 ± 0.006	-111.583 ± 0.033[a]
2	6^+	40.1 ± 2.4	J_z	102	0.03	0.13 ± 0.01	-111.701 ± 0.076[a]
1	8^+	76.3 ± 1.5	J_z	114	-0.01	0.124 ± 0.016	-111.026 ± 0.032
2	8^+	73.3 ± 1.9	J_z	97	0.03	0.098 ± 0.015	-111.035 ± 0.056
1	10^+	119 ± 1	J_z	89	0.05	0.099 ± 0.007	-110.462 ± 0.040
2	10^+	117 ± 2	J_z	137	-0.008	0.063 ± 0.006	-110.535 ± 0.039
1	12^+	162 ± 1	J_z	115	0.008	0.101 ± 0.006	-110.164 ± 0.052[a]
2	12^+	158 ± 4	J_z	107	0.06	0.1 ± 0.01	-110.283 ± 0.097[a]
1	14^+	216 ± 1	J_z	111	0.05	0.16 ± 0.01	-110.082 ± 0.035
2	14^+	214 ± 1	J_z	102	-0.02	0.13 ± 0.02	-110.116 ± 0.057
1	16^+	275 ± 1	J_z	124	-0.03	0.14 ± 0.02	-109.709 ± 0.041[b]
2	16^+	275 ± 2	J_z	111	0.03	0.11 ± 0.02	-109.669 ± 0.049[b]
2	18^+	346 ± 1	J_z	99	-0.02	0.12 ± 0.02	-109.156 ± 0.049

([a]) Levels up to $J = 6$ and the $J = 12$ level were evaluated in ref. [3].
([b]) From ref. [9].

This subset of integration points is then tested for the presence of correlation in the energy (at this stage we use the J_z projected values). If the absolute value of the autocorrelation in the energy is larger 0.1, we keep more distant (in the sense of Monte Carlo time) integration points. Typically we end up keeping one integration point every few hundreds. The numbers below the column labeled "ac" give the residual autocorrelation of the projected energy (fully angular-momentum projected or only partial, depending on the projector used in the evaluation of eq. (1)).

The starting HFB wave functions were determined up to a certain amount of accuracy. An indication of the accuracy, with respect to the adopted minimization method, is the gradient of the energy functional. The values of the angular-momentum projected energy after variation of the input HFB wave functions as well as the highest value of the gradient of the energy functional are shown in table 2. Better wave functions are expected to improve the performance of the Monte Carlo method.

The Monte Carlo calculations were performed with constant $\epsilon = \beta/N_t = 0.0625$ MeV^{-1}. In the case of the ground state, a calculation, not shown in the table, was performed at $\beta = 0.625$ MeV^{-1}. The result for the energy is $E = (-112.869 \pm 0.066)$ MeV. This result was obtained with 99 samples of the energy with a residual autocorrelation of 0.07. Keeping in mind that the results of the calculations are of probabilistic nature, we notice that this value for the ground state is nearly the same as the one obtained with $\beta = 2$ MeV^{-1}. This constancy for the ground-state energy obtained with the Monte Carlo calculation, as well as the relatively small discrepancy ((567 ± 119) KeV) between the Monte Carlo value and the HFB energy, together with eq. (33′), which gives the probability of the ground state in the HFB wave function, suggests a rather large overlap between the ground state and the HFB wave function, although this last one was far from being the best possible HFB wave function. A determination of the probability using eq. (33′) is time

Table 2. Values for the input HFB wave functions for ^{166}Er. The column labeled $\hat{P}$ identifies the type of projection used in the variational calculation. The column labeled max. grad. gives the maximum value of the gradient of the energy functional. The energies are angular-momentum projected values after variation for the purpose of comparison with the corresponding Monte Carlo values.

State	$\hat{P}$	max. grad.	E (MeV)
0^+	none	9×10^{-5}	-112.309
2^+	J_z	0.004	-112.133
4^+	J_z	0.014	-111.726
6^+	J_z	0.003	-111.264
8^+	J_z	0.009	-110.690
10^+	J_z	0.006	-110.195
12^+	J_z	0.03	-109.832
14^+	J_z	0.01	-109.715
16^+	J_z	0.02	-109.327
18^+	J_z	0.008	-108.860

Table 3. Monte Carlo results for the probability C_J of eq. (39) for some yrast states of ^{166}Er. The column labeled $\hat{P}$ identifies the type of projection. N_s is the number of decorrelated samples used in the evaluation of C_J.

State	$\hat{P}$	N_s	β	C_J
0^+	J^2, J_z	174	1	0.31 ± 0.11
0^+	J^2, J_z	97	0.5	0.68 ± 0.19
2^+	J^2, J_z	282	1	0.47 ± 0.19
4^+	J^2, J_z	128	1	0.85 ± 0.28
6^+	J^2, J_z	101	1	0.34 ± 0.06
6^+	J^2, J_z	98	0.5	0.63 ± 0.11
8^+	J_z	97	1	0.84 ± 0.23
10^+	J_z	130	1	0.95 ± 0.22
12^+	J_z	130	1	0.95 ± 0.23
14^+	J_z	102	1	0.81 ± 0.20
16^+	J_z	111	1	0.63 ± 0.26
18^+	J_z	99	1	0.61 ± 0.25

consuming, and, in order to have an idea of this quantity, we performed a calculation of these probabilities using the method sketched in sect. 4 (cf. eq. (39)). Equation (33′) requires the calculation of the function $E(\beta)$ at several values of β for the yrast states, while eq. (39) requires only one extra Monte Carlo calculation for every yrast state.

It should be kept in mind that a Monte Carlo evaluation of eq. (39) may fail to properly sample the numerator, since the integration points were obtained by sampling the denominator of eq. (39), which has a different value of β from the numerator. Therefore the calculations performed using eq. (39) should be regarded as a rough estimate of the probability of having the yrast state in the corresponding HFB wave function and statistical uncertainties are expected to be large and eq. (39) probably underestimates actual values. The results are shown in table 3. As expected from the above considerations these probabilities are close to unity, especially at large angular momentum.

Table 4. Monte Carlo excitation energies and the experimental values.

State	$E^\star$ (MeV)	Exp.
2^+	0.233 ± 0.134	0.081
4^+	0.730 ± 0.170	0.265
6^+	1.220 ± 0.126	0.545
8^+	1.841 ± 0.132	0.911
10^+	2.341 ± 0.125	1.350
12^+	2.593 ± 0.154	1.847
14^+	2.760 ± 0.132	2.389
16^+	3.207 ± 0.129	2.970
18^+	3.724 ± 0.129	–

The excitation energies obtained with the Monte Carlo method are larger than the experimental excitation energies (ref. [10]), as shown in table 4.

The discrepancy between the Monte Carlo excitation energies and the experimental values is especially large for the $J = 8$ and $J = 10$ states and it decreases at larger angular momentum, showing a too strong backbending behaviour, not seen experimentally. Moreover at low angular momentum, the excitation energies are larger than a factor of 3–2. This last feature is primarily due to the full angular-momentum projection and it is enhanced in the Monte Carlo calculation, since excitation energies evaluated within the HFB approximation with J_z projection only, give values in better agreement with the experimental ones. We cannot rule out that these discrepancies with the experimental data have their origin in the restriction to one major shell with the parameter values normally used, rather than to the Hamiltonian itself. The analogy of behaviour of the excitation energies as a function of the angular momentum of the HFB approximation and the Monte Carlo calculation, suggests a redetermination of the Hamiltonian, using the HFB method, since the determination of the Hamiltonian and of its parameters with Monte Carlo methods is computationally expensive.

A final comment about the computational time. The computational effort is mostly due to the evaluation of the angular-momentum projected matrix elements for the Hamiltonian of eq. (15) (for $\mathcal{O} = \hat{H}$). On a XP1800+ processor each evaluation of a projected energy sample takes about 2 hours, independent of the value of β. The computational effort for the J_z projected energies is negligible compared to the above. Roughly, depending on the value of β, the generation of statistically decorrelated integration points takes about one half or less than the evaluation of each angular-momentum projected energy sample. On the same processor, the evaluation of each decorrelated ratio of overlaps in eq. (39) takes about one hour.

In conclusion, we have presented a scheme that allows the evaluation of the energies of the yrast states using Monte Carlo methods. This scheme makes full use, and also allows to assess the validity, of the HFB wave

functions. The scheme seems to require relatively small values of the inverse temperature. The method discussed in this work bypasses entirely the basic difficulty of the standard shell model method, which is inapplicable in this mass region because of the prohibitively large dimensionality of the Hilbert space. Moreover this method allows one to treat excited states explicitly rather than as a statistical average.

Appendix A.

In order to evaluate the matrix elements for one particle species $\mathcal{O}_1(\hat{M})$ of eq. (17), we shall use the algebra of quadratic forms in the creation and annihilation operators of ref. [11]. The method consists in the following properties (eqs. (A.1)-(A.9) below) of exponentials of quadratic forms in the creation and destruction operators of the type

$$\hat{W} = \exp\left[\frac{1}{2}(a^\dagger a)\begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22}\end{pmatrix}\begin{pmatrix} a \\ a^\dagger\end{pmatrix}\right] \tag{A.1}$$

with the restriction of R_{12} and R_{21} to be skew-symmetric matrices and $R_{22} = -\tilde{R}_{11}$. The dimensionality of the matrices R_{ij} equals the dimensionality of the single-particle space N_s. Operators as in eq. (A.1) satisfy a group property, that is, the product of any two operators of this form is an operator of the same form and they are identified by the following associated matrix (which we denote with the same symbol without the caret), written in terms of $N_s \times N_s$ submatrices,

$$W \equiv \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22}\end{pmatrix} = \exp\left[\begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22}\end{pmatrix}\right]. \tag{A.2}$$

Thus, if $\hat{W}_3 = \hat{W}_2\hat{W}_1$ then $W_3 = W_2W_1$. From eq. (A.2) the following properties can be derived (ref. [11]). Provided $|W_{22}| \neq 0$, any operator $\hat{W}$ can be written as a product of the form

$$\hat{W} = \hat{\tau}_c\hat{\tau}_0\hat{\tau}_d \tag{A.3}$$

with

$$\begin{aligned}
&\hat{\tau}_c = \mathrm{e}^{\frac{1}{2}a^\dagger C a^\dagger}, && \tau_c = \begin{pmatrix} 1 & C \\ 0 & 1\end{pmatrix}, \\
&\hat{\tau}_0 = \exp\left[\frac{1}{2}(a^\dagger a)\begin{pmatrix} t & 0 \\ 0 & -\tilde{t}\end{pmatrix}\begin{pmatrix} a \\ a^\dagger\end{pmatrix}\right], && \\
&\tau_0 = \begin{pmatrix} \mathrm{e}^{t} & 0 \\ 0 & \mathrm{e}^{-\tilde{t}}\end{pmatrix} = \begin{pmatrix} \tilde{W}_{22}^{-1} & 0 \\ 0 & W_{22}\end{pmatrix}, && \\
&\hat{\tau}_d = \mathrm{e}^{\frac{1}{2}aDa}, && \tau_d = \begin{pmatrix} 1 & 0 \\ D & 0\end{pmatrix}
\end{aligned} \tag{A.4}$$

with the matrices D, t and C given by

$$D = W_{22}^{-1}W_{21}, \quad C = W_{12}W_{22}^{-1}, \quad \mathrm{e}^{-\tilde{t}} = W_{22}\,. \tag{A.5}$$

The matrices C and D are skew-symmetric. Moreover, the column vector of the destruction and creation operators $\begin{pmatrix} a \\ a^\dagger\end{pmatrix}$ satisfies the relation

$$\hat{W}^{-1}\begin{pmatrix} a \\ a^\dagger\end{pmatrix}\hat{W} = W\begin{pmatrix} a \\ a^\dagger\end{pmatrix}. \tag{A.6}$$

The particle vacuum matrix elements of $\hat{W}$ are given by

$$\langle 0|\hat{W}|0\rangle = |W_{22}|^{1/2}\,. \tag{A.7}$$

This last expression leaves the sign undetermined. The inverse of the representive matrix W satisfies the relation

$$W^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\tilde{W}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix} \tag{A.8}$$

which gives the following relation for W_{11} in terms of W_{22}, C and D:

$$W_{11} = \tilde{W}_{22}^{-1} + W_{12}D\,. \tag{A.9}$$

In order to proceed, let us also define exponentials of particle number operators $\hat{P}(z)$ as

$$\mathrm{e}^{\alpha\hat{N}} \equiv z^{N_s/2}\hat{P}(z) = z^{N_s/2}\exp\left[\frac{\alpha_p}{2}(a^\dagger a)\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}\begin{pmatrix} a \\ a^\dagger\end{pmatrix}\right] \tag{A.10}$$

with $z = \mathrm{e}^\alpha$. To obtain expressions for the particle number projected matrix elements of eq. (17) for one type of particles, we consider quantities like

$$\mathcal{O}_1(M, z_p, z_q) = (z_pz_q)^{N_s/2}\langle 0|\hat{V}^\dagger\hat{P}(z_p)\hat{R}\hat{M}\hat{W}\hat{P}(z_q)\hat{V}|0\rangle \tag{A.11}$$

which are functions of the fugacities $z_{p,q} = \mathrm{e}^{\alpha_{p,q}}$ and $\hat{M}$ is a polynomial of the creation and destruction operators. The operator $\hat{V}$ in eq. (A.11) is the one that connects the vacuum to the HFB state in eq. (2) and its associated matrix is

$$V = \begin{pmatrix} 1 & X \\ 0 & 1\end{pmatrix}. \tag{A.12}$$

We now evaluate eq. (A.11). Let us define the operator

$$\hat{W}' = \hat{W}\hat{P}(z_q)\hat{V}\,, \tag{A.13}$$

then the group property gives

$$W' = \begin{pmatrix} z_qW_{11} & z_qW_{11}X + \frac{1}{z_q}W_{12} \\ z_qW_{21} & z_qW_{21}X + \frac{1}{z_q}W_{22}\end{pmatrix}. \tag{A.14}$$

The decomposition theorem applied to $\hat{W}'$ gives

$$\hat{W}'|0\rangle = \langle 0|\hat{W}'|0\rangle\tau_c'|0\rangle \tag{A.15}$$

with τ_c' of the type as in eq. (A.5) having as associated matrix

$$\tau_c' = \begin{pmatrix} 1 & C' \\ 0 & 1\end{pmatrix}. \tag{A.16}$$

From eqs. (A.5), (A.14) and (A.9), one obtains the following expression for C':

$$C' = C + z_q^2 \tilde{W}_{22}^{-1} X (1 + z_q^2 DX)^{-1} W_{22}^{-1}\,; \qquad \text{(A.17)}$$

moreover eqs. (A.7), (A.14) and eq. (A.15) give

$$z_q^{N_s/2} \hat{W}' |0\rangle = |W_{22}|^{1/2} |1 + z_q^2 DX|^{1/2} \hat{\tau}'_c |0\rangle\,. \qquad \text{(A.18)}$$

If we denote the associated matrix of the rotation operator as

$$R = \begin{pmatrix} r & 0 \\ 0 & \tilde{r}^{-1} \end{pmatrix}, \qquad \text{(A.19)}$$

where r is the collection of the Wigner D-matrices in the single-particle space, and define the operator product

$$\hat{W}'' = \hat{V}^\dagger \hat{P}(z_p) \hat{R} \qquad \text{(A.20)}$$

which has as associated matrix

$$W'' = \begin{pmatrix} z_p r & 0 \\ -z_p X^\star r & \frac{1}{z_p} \tilde{r}^{-1} \end{pmatrix}, \qquad \text{(A.21)}$$

then the decomposition theorem (eqs. (A.5), (A.5)) gives

$$z_p^{N_s/2} \langle 0 | \hat{W}'' = \langle 0 | \hat{\tau}''_d \qquad \text{(A.22)}$$

with τ'' given by (cf. eq. (A.5))

$$\tau''_d = \begin{pmatrix} 1 & 0 \\ D'' & 0 \end{pmatrix}, \qquad D'' = -z_p^2 \tilde{r} X^\star r. \qquad \text{(A.23)}$$

Combining eqs. (A.13)-(A.23) we obtain

$$\mathcal{O}_1(\hat{M}, z_p, z_q) = |W_{22}|^{1/2} |(1 + z_q^2 DX)|^{1/2} \langle 0 | \hat{\tau}''_d \hat{M} \hat{\tau}'_c | 0 \rangle \qquad \text{(A.24)}$$

We shall consider the cases where $\hat{M} = 1$, $\hat{M} = a_i^\dagger a_j$ and $\hat{M} = a_i^\dagger a_j^\dagger a_r a_s$.

For $\hat{M} = 1$, using the group property and eq. (A.7), and eqs. (A.17) and (A.23) for the associated matrices of $\hat{\tau}''_d$ and $\hat{\tau}'_c$, we obtain

$$\mathcal{O}_1(\hat{M} = 1, z_p, z_q) = |W_{22}|^{1/2} |(1 + z_q^2 DX)|^{1/2} |1 + D'' C'|^{1/2}. \qquad \text{(A.25)}$$

For the case where $\hat{M} = a_i^\dagger a_j$ using eq. (A.6) we obtain, after exchanging a_j with $\hat{\tau}'_c$,

$$\mathcal{O}_1(\hat{M} = a_i^\dagger a_j, z_p, z_q) = \mathcal{O}_1(\hat{M} = 1, z_p, z_q) \rho_{ji} \qquad \text{(A.26)}$$

with the matrix ρ given by

$$\rho = 1 - (1 + C' D'')^{-1}\,. \qquad \text{(A.27)}$$

Finally for the case where $\hat{M} = a_i^\dagger a_j^\dagger a_r a_s$, again using eq. (A.6) in order to exchange the destruction operators with $\hat{\tau}'_c$, we obtain

$$\mathcal{O}_1(\hat{M} = a_i^\dagger a_j^\dagger a_r a_s, z_p, z_q) = \mathcal{O}_1(\hat{M} = 1, z_p, z_q) \times [D'''_{ji} C''_{sr} + \rho_{si} \rho_{rj} - \rho_{ri} \rho_{sj}] \qquad \text{(A.28)}$$

and the matrices D''' and C''' are given by

$$D''' = D''(1 + C' D'')^{-1}, \qquad C'' = (1 + C' D'')^{-1} C'\,. \qquad \text{(A.29)}$$

From these equations the formulas in sect. 3 immediately follow. The matrix W associated to the propagator $\hat{W}$, can be evaluated by using the group property of the operators $\hat{W}_m$ of eq. (9) and eq. (A.2) to construct the representative matrices for each $\hat{W}_m$ of eq. (8). With the substitution $\hat{V}^\dagger \to \hat{V}'^\dagger$ one can obtain formulas for off-diagonal matrix elements, simply by replacing $X^\star$ with $X'^\star$ (but not X with X') everywhere in the results. Although not used in this work, using this method one can obtain compact expressions in the case $\hat{M}$ in eq. (A.11) is replaced with $\hat{U}\hat{M}$, where $\hat{U}$ is another operator of the form given by eq. (A.1).

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