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Monte Carlo spectroscopy with Hartree-Fock-Bogoliubov wave functions

G. Puddu
Dipartimento di Fisica dell'Università di Milano, I-20133 Milano, Italy
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We propose a simple method to evaluate the lowest energy levels of a given angular momentum using exact Monte Carlo methods. The method relies on an efficient evaluation of quantities such as $\langle \psi NZ|\hat{P}^{(J)}_{JJ}\hat{H}e^{-\beta\hat{H}}|\psi NZ\rangle$ where the wave functions are particle number projected Hartree-Fock-Bogoliubov wave functions and $\hat{P}^{(J)}_{JJ}$ is the angular momentum projector with $J_z=J$. The method has been applied to the evaluation of 0^+, 2^+, 4^+, 6^+ levels of ^{166}Er within the pairing+quadrupole model and we show that energy eigenvalues can be obtained for small β values.

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The exact evaluation of energy levels in nuclei so far has relied on the nuclear shell model, where few valence nucleons are assumed to contribute to the low-energy part of the spectrum. The two-body shell model Hamiltonian as well as the single-particle states are fixed by reproducing selected experimental information (Ref. [1]). The shell model approach, which is based on the exact diagonalization of the many-body Hamiltonian, has the fundamental limitation that the dimension of the Hamiltonian matrix grows extremely fast with the number of valence nucleons and with the size of the single-particle basis. In particular, rare earth nuclei are outside of the reach of the exact shell model approach. For example, in the case of ^{166}Er, if we consider the single-particle states between $82\leqslant N\leqslant 126$ and $50\leqslant Z\leqslant 82$ neutron and proton major shells, the dimension of the Hamiltonian matrix is about 10^{16} for the angular momentum and parity $J^\pi=0^+$, and it increases with the angular momentum. Clearly a description of these nuclei, even with simplified many-body Hamiltonians, has to rely on Monte Carlo methods, which are not based on the diagonalization of the many-body Hamiltonian matrix and therefore are independent on the dimension of the shell model space. So far, Monte Carlo methods have been applied only to the determination of ground state properties and to thermal properties of nuclei but not to levels other than the ground state. The methods which have been used are based on the evaluation in the large β limit of quantities such as $\langle\psi|\hat{H}e^{-\beta\hat{H}}|\psi\rangle$ or $\mathrm{Tr}[\hat{H}e^{-\beta\hat{H}}]$, $\hat{H}$ being the many-body Hamiltonian, and on the evaluation with Monte Carlo methods of the functional integrals of these quantities (Refs. [2,3]). In the past, in order to remove this limitation, quantities like $\langle\psi J|\hat{H}e^{-\beta\hat{H}}|\psi J\rangle$, J being the angular momentum, have been considered (Ref. [4]), but were applied only to the lowest 0^+ state or to oversimplified schematic models. The application of the technique of Ref. [4] to $J\neq 0$ levels presents numerical accuracy problems and it seems reasonable only for low angular momentum. Ideally we would like to evaluate quantities like

$$E(\beta,N,Z,J)=\frac{\langle\psi NZJM|\hat{H}e^{-\beta\hat{H}}|\psi NZJM\rangle}{\langle\psi NZJM|e^{-\beta\hat{H}}|\psi NZJM\rangle}, \qquad (1)$$

where the wave function is the neutron number, proton number, and angular momentum projected variational Hartree-Fock-Bogoliubov (HFB) wave function. N and Z are the number of valence neutrons and valence protons, respectively.

For $\beta=0$, $E(\beta,N,Z,J)$ gives the Hartree-Fock-Bogoliubov approximation for the lowest energy level of angular momentum J and it decreases as β is increased leading to the exact lowest energy eigenstate having angular momentum J. This quantity is ideal to improve and to test the validity of the projected HFB approximation, which is very successful when applied to problems where the shell model diagonalization method is applicable (Ref. [5]).

If the HFB approximation is accurate, only small values of β are necessary in order to converge to the yrast levels. However, using the functional integral expression of $e^{-\beta\hat{H}}$, Eq. (1) becomes a formidable numerical problem with standard angular momentum projectors.

The purpose of this Rapid Communication is to point out that a reasonably simple and efficient Monte Carlo method can be devised which still gives the exact Monte Carlo estimate for the yrast level and it converges at small β values. To our knowledge, calculations of this type are presented for the first time. Since all calculations discussed in this Rapid Communication have been performed with XP+1600 and XP +1800 personal computers (each level takes about a couple of weeks of CPU) we decided to evaluate only $J=0,2,4,6$ positive parity levels. Instead of Eq. (1) we consider the following quantity:

$$E(\beta,N,Z,J)=\frac{\langle\psi NZ|\hat{P}^{(J)}_{JJ}\hat{H}e^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}{\langle\psi NZ|\hat{P}^{(J)}_{JJ}e^{-\beta(\hat{H}-\omega\hat{J}_z-\mu_n\hat{N}_n-\mu_p\hat{N}_p)}|\psi NZ\rangle}, \qquad (2)$$

which contains the same physical information as Eq. (1). In Eq. (2) ω is the cranking frequency, μ_n and μ_p are the neutron and proton chemical potentials, and $\hat{N}_{n,p}$ are the neutron (proton) particle number operators, $\hat{J}_z$ is the z component of the angular momentum operator and $\hat{P}^{(J)}_{JJ}$ is the angular momentum projector to angular momentum J and z component $J_z=J$. In the above equation, we select $|\psi NZ\rangle$ with the following prescription: it is a HFB particle number projected wave function and it is such that, if we call $\hat{P}(J_z=M)$ the

projector operator to a definite value of the z component of the angular momentum, $J_z=M$, it minimizes the energy functional

$$\frac{\langle \psi NZ|\hat{P}(J_z=J)\hat{H}|\psi NZ\rangle}{\langle \psi NZ|\hat{P}(J_z=J)|\psi NZ\rangle}. \tag{3}$$

In the case of the ground state, the first we performed, in the energy functional (3) we did not apply $\hat{P}(J_z=0)$.

A better choice for $|\psi NZ\rangle$ would be the one that minimizes the energy functional

$$\frac{\langle \psi NZ|\hat{P}^{(J)}_{JJ}\hat{H}|\psi NZ\rangle}{\langle \psi NZ|\hat{P}^{(J)}_{JJ}|\psi NZ\rangle},$$

which is the $\beta=0$ limit of Eq. (2). Since the determination of these last wave functions is computationally expensive, we preferred to minimize the energy functional (3).

We shall give the formulas for one type of particles for brevity of the equations and since the generalization to two types of particles is straightforward. The Hamiltonian is pairing+quadrupole Hamiltonian,

$$\hat{H}=\hat{H}_0-k/2\sum_{a=-2}^{2}(-1)^a\hat{Q}^{(2)}_{-a}\hat{Q}^{(2)}_{a}-G\hat{P}^{\dagger}\hat{P}, \tag{4}$$

where $\hat{Q}^{(2)}_a$ is the quadrupole operator, $\hat{P}$ is the pair destruction operator, k and G are the coupling constants, and $\hat{H}_0$ is the independent particle Hamiltonian. The functional integral expression for $e^{-\beta(\hat{H}-\mu\hat{N}-\omega\hat{J}_z)}$ is given by (Ref. [4])

$$e^{-\beta(\hat{H}-\mu\hat{N}-\omega\hat{J}_z)}=e^{-\beta G\Omega/2}\mathcal{N}\times\int\prod_{n=1}^{N_t}\left(d\phi_{xn}d\phi_{yn}\prod_{a=-2}^{2}d\sigma_{an}\right)\times e^{-1/2\Sigma_{an}\sigma^2_{an}-1/2\Sigma_n(\phi^2_{xn}+\phi^2_{yn})}\hat{U}, \tag{5}$$

$$\hat{U}=\hat{U}_{N_t}\hat{U}_{N_t-1}\ldots\hat{U}_1, \tag{6}$$

$$\hat{U}_n=e^{-\epsilon\hat{H}'_0-\sqrt{\epsilon k}\Sigma_a\sigma_{an}\hat{Q}_a-\sqrt{\epsilon G/2}(\phi_n\hat{P}+\phi^{\star}_n\hat{P}^{\dagger})}], \tag{7}$$

and $\phi_n=(\phi_{xn}+i\phi_{yn})$. In Eq. (7), $\hat{H}'_0=\hat{H}_0-\omega\hat{J}_z-\mu'\hat{N}$ and $\mu'=\mu+G/2$ and Ω is one-half of the number of single particle states. $\mathcal{N}$ is the normalization constant

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

The operators $\hat{Q}_a$ are the Cartesian components of the quadrupole tensor operator, N_t is the number of intervals in which the interval $[0,\ \beta]$ is divided, and $\epsilon=\beta/N_t$. Schematically we write the functional integral as

$$e^{-\beta(\hat{H}-\mu\hat{N}-\omega\hat{J}_z)}=\int d\vec{x}G(\vec{x})\hat{U}, \tag{8}$$

with the obvious meaning of the symbols. Using the expression

$$\hat{P}^{(J)}_{JJ}=\frac{2J+1}{8\pi^2}\int d\Omega_E D^{(J)*}_{JJ}(\Omega_E)\hat{R}(\Omega_E), \tag{9}$$

for the angular momentum projection operator, where $\Omega_E=(\theta_1\theta_2\theta_3)$ is the collection of the three Euler angles, $d\Omega_E=d\theta_1\sin\theta_2\,d\theta_2 d\theta_3$, $D^{(J)}_{JJ}$ is the Wigner function, and

$$\hat{R}(\Omega_E)=e^{i\theta_3\hat{J}_z}e^{i\theta_2\hat{J}_y}e^{i\theta_1\hat{J}_z} \tag{10}$$

is the rotation operator, we have

$$E(\beta,N,J)=\frac{\int d\vec{x}G(\vec{x})\int d\Omega_E D^{(J)*}_{JJ}\langle\psi N|\hat{R}(\Omega_E)\hat{H}\hat{U}|\psi N\rangle}{\int d\vec{x}G(\vec{x})\int d\Omega_E D^{(J)*}_{JJ}\langle\psi N|\hat{R}(\Omega_E)\hat{U}|\psi N\rangle}. \tag{11}$$

Rather than evaluating $E(\beta,N,J)$ by sampling the distribution

$$G(\vec{x})\left|\int d\Omega_E D^{(J)*}_{JJ}\langle\psi N|\hat{R}(\Omega_E)\hat{U}|\psi N\rangle\right|,$$

using the Metropolis method (Ref. [6]), we first rewrite Eq. (11) as

$$E(\beta,N,J)=\frac{\int d\vec{x}G(\vec{x})|\langle\psi N|\hat{U}|\psi N\rangle|\dfrac{\int d\Omega_E D^{(J)*}_{JJ}\langle\psi N|\hat{R}(\Omega_E)\hat{H}\hat{U}|\psi N\rangle}{|\langle\psi N|\hat{U}|\psi N\rangle|}}{\int d\vec{x}G(\vec{x})|\langle\psi N|\hat{U}|\psi N\rangle|\dfrac{\int d\Omega_E D^{(J)*}_{JJ}\langle\psi N|\hat{R}(\Omega_E)\hat{U}|\psi N\rangle}{|\langle\psi N|\hat{U}|\psi N\rangle|}}, \tag{12}$$

and then we evaluate both functional integrals with the Metropolis method by sampling the unprojected distribution

$$G(\vec{x})|\langle\psi N|\hat{U}|\psi N\rangle|. \tag{13}$$

The energies $E(\beta,N,J)$ are then evaluated and we assign a statistical error to the ratio of Eq. (12), which we write schematically as $E=a/b$, with the formula

$$\Delta E = \frac{1}{\langle b\rangle\sqrt{N_s}}\sqrt{\left\langle\left(a-\frac{\langle a\rangle}{\langle b\rangle}b\right)^2\right\rangle}, \tag{14}$$

where N_s is the number of decorrelated samples.

The reason why we select the distribution (13) which does not contain the angular momentum projector (but does contain the particle number projector) is because it is prohibitively expensive to sample the angular momentum projected matrix elements. Incidentally an appropriate selection of the cranking frequency ω, does precisely this, although approximately. In principle there are several things which could prevent the application of this scheme. First of all both the numerator and denominator in Eq. (12) could become very small because of strong sign oscillations in both functional integrals, that is

$$P = \frac{\int d\Omega_E D^{(J)}_{JJ}{}^{*}\langle\psi N|\hat{R}(\Omega_E)\hat{U}|\psi N\rangle}{|\langle\psi N|\hat{U}|\psi N\rangle|} \tag{15}$$

could strongly oscillate in sign as the sampling proceeds. Or each value of the above ratio could be very small, and therefore it would be very sensitive to the numerical accuracy achievable in the computation of the matrix elements. Moreover for some angular momenta, the cranking recipe might not work. In fact, selecting ω so that $J_z = J$ is lowest in energy might give predominance to other values of J; this could be, for example, the case of the 3^+ state (no calculation has actually been performed for this level), since the first 4^+ state could dominate the unprojected distribution (13).

In practice we found for the angular momenta we considered, that P increases as we increase β and that the smallest values of P are obtained for small values of β for which the evaluation of the various matrix elements is numerically rather stable. As shown below, for the cases considered in this paper, the angular momentum projection gives an average value of P of about 0.1. The reason for this behavior at nonzero angular momentum is the presence of the cranking term that moves at higher energies the components having the value of J_z different from the desired one.

We found that the terms inside the square root of the error formula in Eq. (14) are not small, but cancel out each other almost completely, giving small statistical errors. To achieve good separation of the energy levels above the statistical uncertainty we need statistical errors at the most of 100 KeV; in the applications discussed below we achieve errors smaller or of about this amount with only about 100 samples.

If good wave functions are used, we need to evaluate Eq. (12) at small β values and therefore we expect sign oscillations, if there are any, to be caused only by the angular momentum projection. However, since $\hat{U}$ is not very large, we do not expect a large effect in the statistical error. In fact the statistical error becomes 0 as $\beta\to 0$. Up to now, in order to obtain the ground-state energy, large values of β had to be used. With this method instead, we rely more on the angular momentum projection and on the optimal character of the HFB wave function since both aspects deplete excited states from the wave function $\hat{P}^{(J)}_{JJ}e^{-\beta\hat{H}}|\psi NZ\rangle$.

Although less interesting, we could substitute the angular momentum projector with the J_z projector in Eq. (2) and then check whether the expectation values of J^2 have the desidered value. Since the evaluation of the J_z projected matrix elements is inexpensive, we have also performed calculations of J_z projected energies.

Having discussed the essential elements of the method we now discuss the actual calculation for ^{166}Er.

The single-particle space consists of the $0h9/2$, $1f7/2$, $1f5/2$, $2p3/2$, $2p1/2$, $0i13/2$ neutron levels and of the $0g7/2$, $1d5/2$, $1d3/2$, $2s1/2$, $1h11/2$ proton levels. The matrix elements of the quadrupole operator are the same as Ref. [7] (without renormalizing the quadrupole matrix elements of the $0i13/2$ and the $1h11/2$ states) as well as the strengths of the interactions and the single-particle levels. The calculations have been performed with $\beta=1$ and $\beta=2$. The results are summarized in the table, where we also report a J_z projected calculation for $M=12$ at $\beta=2$. In the table we also show the overlaps

$$\mathcal{O}_J = \frac{\langle\psi NZ|\hat{P}^{(J)}_{JJ}e^{-\beta\hat{H}}|\psi NZ\rangle}{\langle\psi NZ|e^{-\beta\hat{H}}|\psi NZ\rangle}, \tag{16}$$

$$\mathcal{O}_{J_z} = \frac{\langle\psi NZ|\hat{P}(J_z=M)e^{-\beta\hat{H}}|\psi NZ|\rangle}{\langle\psi NZ|e^{-\beta\hat{H}}|\psi NZ\rangle}, \tag{17}$$

depending on the type of projection. The above quantities give an indication of the depletion of excited states caused by projecting the wave vector $e^{-\beta\hat{H}}|\psi NZ\rangle$. That is, the smaller the overlap the larger the depletion.

We performed the integration over the Euler angles using a mesh of $25\times10\times25$, with a ten-point Gauss-Legendre integration formula over the angle θ_2 and with 25 equidistant points for the θ_1 and θ_3 integrals. Only in the case of $M=12$ we used a mesh of 35 points. In the calculation we took $N_t=16$ and $N_t=32$ time intervals for $\beta=1$ and $\beta=2$, respectively. The values of the cranking frequency ω and of the chemical potentials were adjusted only by considering the mean field of the functional integral associated with the propagator of Eq. (8) (as done in Ref. [4]). The value of ω was determined by fixing the desired value of the mean-field expectation value of J_z. The statistical errors are rather small, especially for $\beta=1$. Parity was fixed by selecting parity conserving HFB wave functions of the type $|\psi,N,Z\rangle = |\psi N\rangle|\psi Z\rangle$, each term being the parity conserving neutron and proton part. The particular form of the functional integral of Eqs. (5)–(7) does not change the parity of the HFB wave function.

In Table I, we also show the residual autocorrelation of the decorrelated energy samples [the energy sample is the value of the fraction in the numerator of Eq. (12)] and the number N_s of the decorrelated samples. The Monte Carlo calculation was performed by discarding the first few thousand samples to ensure independence from the initial start (the ''thermalization'' step) and then collecting the data once every 120–250 samples to have statistically independent values (the ''decorrelation'' step). Only in the case of the 6^+

TABLE I. 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, which gives an indication of the statistical independence of the samples. $\mathcal{O}$ is given by Eq. (16) or Eq. (17).

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
2	0^+	0	J^2, J_z	108	-0.028	0.27 ± 0.1	-112.876 ± 0.119
1	2^+	6	J^2, J_z	93	0.12	0.119 ± 0.009	-112.532 ± 0.033
2	2^+	6	J^2, J_z	93	-0.05	0.16 ± 0.02	-112.643 ± 0.061
1	2^+	10.4 ± 1.3	J_z	83	0.07	0.17 ± 0.02	-112.399 ± 0.064
2	2^+	6.7 ± 2.4	J_z	102	-0.009	0.22 ± 0.03	-112.602 ± 0.140
1	4^+	20	J^2, J_z	104	0.14	0.133 ± 0.009	-112.165 ± 0.052
2	4^+	20	J^2, J_z	98	0.0008	0.12 ± 0.02	-112.146 ± 0.121
1	4^+	25 ± 1	J_z	120	0.03	0.16 ± 0.01	-112.014 ± 0.059
2	4^+	22 ± 4	J_z	91	-0.03	0.18 ± 0.02	-112.132 ± 0.086
1	6^+	42	J^2, J_z	89	0.25	0.114 ± 0.007	-111.626 ± 0.041
2	6^+	42	J^2, J_z	97	-0.07	0.14 ± 0.01	-111.656 ± 0.040
1	6^+	44 ± 1	J_z	89	-0.02	0.111 ± 0.006	-111.655 ± 0.057
2	6^+	40.1 ± 2.4	J_z	102	0.03	0.13 ± 0.01	-111.701 ± 0.076
2	12^+	157 ± 4	J_z	107	0.06	0.097 ± 0.010	-110.283 ± 0.097

state, for $\beta = 2$, we had to take one sample every 300. In the case of the 6^+ evaluated at $\beta = 1$ there seems to be a strong residual correlation; in this case we took one sample every 180. The size of the decorrelation steps were estimated from the J_z-projected samples and then verified in the case of the fully projected calculations.

The determination of the energies was done using Eq. (12) rather than the method used in Ref. [4], which consists of taking the derivative with respect to β of the effective action, since statistical errors are much smaller especially for small values of β. As can be seen from the table, the energies at $\beta = 1$ and $\beta = 2$ are consistent with each other within the statistical error implying that these values of β are sufficiently large to give the yrast energies. Also the J_z projected energies and the corresponding values of the expectation values of J^2 imply that convergency has been reached. A reliable criterion for convergency to the yrast level is that the energy does not change as β is increased. From the table we see that convergency is reached already at $\beta = 1$, and it is conceivable that smaller values of β are sufficient for convergency, if better HFB wave functions (that is angular momentum projected before variation) are used. This could potentially mitigate the sign problem in the evaluation of functional integrals with the Monte Carlo methods, in the case of more complicated Hamiltonians.

In the table, we omitted the calculation of J_z projected energy for the ground state, because of the contamination of the nearby 2^+ state.

The calculation for $J_z = 12$ was carried out for the purposes of testing the statistical error at large angular momentum. Although only the z component of the angular momentum has been projected, the expectation value of J^2 evaluated at $\beta = 2$ indicates convergency to $J = 12$ levels within the statistical error.

It is instructive to compare the energies shown in the table with the ones evaluated at $\beta = 0$. For the states considered in this work, the angular momentum projected energies are $E(\beta = 0, 0^+) = -112.309$ Mev, $E(\beta = 0, 2^+) = -112.133$, $E(\beta = 0, 4^+) = -111.726$ Mev, $E(\beta = 0, 6^+) = -111.264$ Mev, and $E(\beta = 0, 12^+) = -109.832$ Mev. To some extent, the discrepancy between the Monte Carlo results and the angular momentum projected energies is roughly the same for different states. The size of the discrepancy could be due to the fact that the HFB wave functions were not determined by varying the angular momentum projected energy functional.

Although for a comparison with the experimental level spacings it would be more appropriate to increase the number of time intervals, the indication that emerges from these calculations is that the model, with the parameters and the single-particle space employed in these calculations, overestimates the experimental level spacings. The experimental value for the excitation energy of the first 2^+ state is 0.081 MeV, for the first 4^+ state is 0.265 MeV, for the first 6^+ state is 0.545 MeV, and for the first 12^+ state is 1.847 MeV (Ref. [8]). The corresponding Monte Carlo values, evaluated at $\beta = 2$, are instead, $E^*(2^+) = (0.233 \pm 0.134)$ MeV, $E^*(4^+) = (0.730 \pm 0.170)$ MeV, $E^*(6^+) = (1.220 \pm 0.126)$ MeV, and $E^*(12^+) = (2.593 \pm 0.154)$ MeV. The theoretical excitation energies are too large compared to the experimental ones.

It should be mentioned that in the past few years other methods have been developed to evaluate low-lying energy levels of fermionic systems. Most notably the methods of Ref. [9]. The major differences between the method of Ref. [9] and the method proposed in this paper, can be summarized as follows. In Ref. [9], a many-body basis is constructed stochastically with the requirement that the energies obtained by diagonalizing the Hamiltonian matrix are the lowest. Hence this method lacks a central limit theorem

which gives the statistical uncertainty of the energy levels. Moreover it considers a limited, although optimized, many-body basis, while the approach proposed in this paper is entirely independent on the many-body basis necessary to reach reasonable convergency and its uncertainty is solely given by the statistical error.

In conclusion, we have evaluated for the first time the energies of excited states entirely with Monte Carlo methods with very reasonable statistical uncertainties, that allow us to perform spectroscopic studies on many-body Hamiltonians in mass regions unaccessible with standard shell model techniques.

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