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Microscopic justification of the equal filling approximation

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The equal filling approximation, a procedure widely used in mean-field calculations to treat the dynamics of odd nuclei in a time-reversal invariant way, is justified as the consequence of a variational principle over an average energy functional. The ideas of statistical quantum mechanics are employed in the justification. As an illustration of the method, the ground and lowest-lying states of some octupole deformed radium isotopes are computed.

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I. INTRODUCTION

The Hartree-Fock-Bogoliubov (HFB) approximation is the cornerstone of the microscopic description of the atomic nucleus as it encompasses in the same approximation the concept of mean-field orbits needed to understand the extra stability associated with magic numbers as well as the concept of pairing correlations needed to understand, among others, why the ground state of all even-even nuclei always have the $J^\pi = 0^+$ quantum numbers. The HFB approximation has widely been used over the past decades with great success both to describe known properties of nuclei and to predict the properties of unknown or yet to be experimentally studied nuclei [1,2].

Another nice feature of the mean-field approximation is that it allows for the "spontaneous symmetry breaking" (SSB) mechanism in which the approximate (mean-field) solution of the problem breaks the underlying symmetries of the nuclear Hamiltonian. By the SSB mechanism many correlations can be incorporated into the mean-field wave function while maintaining the simplicity of the mean field description. A minor (mainly practical) drawback of the SSB mechanism is that the breaking of symmetries naturally leads to the appearance of "full matrices" in the numerical implementation of the method. Those full matrices are a direct consequence of the mixing of quantum numbers that otherwise could be used to bestow a block structure to the matrices considered. The increase of the effective size of the matrices leads to an increase in the number of operation needed to accomplish the numerical implementation of the method and therefore leads to an increase in the computational cost of the problem. Depending on the type of problem and the symmetry broken, the computational cost can increase so dramatically as to prevent the large-scale calculations needed to describe stellar nucleosynthesis or the stability of superheavy nuclei, just to mention a couple of physical situations of interest nowadays. A typical case of a computationally demanding application is the study of fission barriers allowing for time-reversal symmetry breaking, which is characteristic of high-spin states or odd-mass nuclei that have to be treated in the framework of the standard blocking method. In the treatment of odd-mass systems we have an additional source of computational complexity and it is the self-consistent character of the HFB equations that does not grant that blocking the quasiparticle with lowest excitation energy will yield the lowest energy self-consistent solution. As a consequence, several blocking possibilities have to be considered multiplying the computing time by the number of the possibilities considered (typically three or four times for each possible J_z and parity value).

However, the description of odd-A nuclei has started to receive the attention it deserves (three-quarters of all accessible nuclei are odd-A ones) as the typical odd-even effects, which are not well understood, are intimately related to pairing properties and can also serve as more stringent guidelines to the development of new energy functionals (see, for instance, Refs. [3,4] for recent discussions on this issue). As a consequence, any attempt to reduce the computational cost in the theoretical evaluation of odd-A nuclei properties is very important as it will eventually allow for a systematic and routinely evaluation of the required properties all over the periodic table.

A way to reduce the computational cost of mean-field calculations when dealing with odd-mass nuclei is to try to keep time-reversal symmetry facilitating in this way the imposition of axial symmetry. To keep time-reversal symmetry when dealing with odd-mass nuclei one is forced to adopt phenomenological approaches in which the unpaired nucleon is treated in an equal footing with its time-reversed companion. From a practical point of view this phenomenological approach amounts to look at the unpaired nucleon as siting half in a given orbital and the other half in the time-reversed partner [in the case of preserving spherical symmetry where the orbitals have the $2j + 1$ degeneracy the unpaired nucleon is distributed among all possible angular momentum projections $m = -j, \ldots, j$ with equal probability $1/(2j + 1)$]. The above procedure is usually referred in the literature as the equal (or uniform) filling approximation (EFA) and has been used quite often in the description of odd nuclei at the mean-field level and with different interactions—see Refs. [5–8] for recent applications of the method. This procedure is used because it is considered as an "intuitive" and "reasonable" approach but it is phenomenological in character and lacks a solid foundation as there is no product wave function that can

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reproduce the density matrix and pairing tensor of the EFA. The purpose of this article is to show that the EFA can be described in terms of a mixed state (in the sense of quantum statistical mechanics) density operator and the equations to be solved are a direct consequence of the variational principle over the energy of such mixed state. As a consequence of this microscopic justification it is now possible to introduce numerical procedures like the gradient method to solve the EFA equations facilitating enormously the procedure specially in the case of many constraints. Another consequence is that now other methods beyond mean field like the calculation of collective masses or the generator coordinate method itself can be consistently implemented in the EFA framework.

Obviously, the EFA is an approximation to the correct treatment of odd-A nuclei in the context of the mean field (the blocking procedure, see Ref. [2] for a detailed explanation). To discuss the possible differences between them it is convenient to look at the odd-A systems as made of an even-even core plus an unpaired nucleon (or quasiparticle). The interaction between the unpaired nucleon and the even-even core will induce polarization effects in the core of three types [3,4,9–11]; namely the mass polarization, the deformation polarization, and the spin polarization effects. The only one associated to the breaking of time-reversal invariance is the spin polarization and it is obvious that it is not included in the EFA. The other two effects (mass and shape polarizations) are obviously included in the EFA to some extent but it is not easy to estimate the possible impact of spin polarization effects on them. It is clear that a deeper understanding of the interrelationship between the three effects is needed and hopefully the present justification of the EFA will help to clarify the issue.

II. THE EQUAL FILLING APPROXIMATION

In the standard HFB method [2] quasiparticle operators β_μ^+ are introduced as linear combinations of the creation and annihilation single-particle operators corresponding to an arbitrarily chosen (usually a harmonic oscillator) basis

$$\beta_\mu^+ = \sum_m U_{m\mu} c_m^+ + V_{m\mu} c_m. \tag{1}$$

The HFB ground-state wave function is defined by the condition of being the vacuum of all the quasiparticle annihilation operators, that is, $\beta_\mu|\phi\rangle = 0$. A more concise definition is given by $|\phi\rangle = \prod_\mu \beta_\mu|0\rangle$, where the index μ run over all the quasiparticle annihilation operators that do not annihilate the true vacuum $|0\rangle$. The previous results will describe the ground state of an even-even nucleus as it can be shown that a paired HFB wave function is a linear combination of product wave functions with an even number of particles. However, odd-particle systems are handled by the "blocked" HFB wave functions

$$|\tilde{\phi}\rangle_{\mu_B} = \beta_{\mu_B}^+|\phi\rangle, \tag{2}$$

where μ_B is any of the quasiparticle indexes compatible with the symmetries of the odd-particle system as, for instance, the K quantum number (eigenvalue of J_z) or the parity. As the "blocked" HFB wave function is a product of quasiparticle operators, Wick's theorem applies and the energy is given in the usual way in terms of the "blocked" normal and abnormal densities $\rho^{(\mu_B)}$ and $\kappa^{(\mu_B)}$

$$E^{(\mu_B)} = \mathrm{Tr}\,[t\rho^{(\mu_B)}] + \tfrac{1}{2}\,\mathrm{Tr}\,[\Gamma^{(\mu_B)}\rho^{(\mu_B)}] - \tfrac{1}{2}\,\mathrm{Tr}\,[\Delta^{(\mu_B)}\kappa^{(\mu_B)*}]. \tag{3}$$

The normal and abnormal densities are given by

$$\begin{aligned}\rho_{kk'}^{(\mu_B)} &= \langle\phi|\beta_{\mu_B} c_{k'}^+ c_k \beta_{\mu_B}^+|\phi\rangle \\ &= (V^*V^T)_{kk'} + \left(U_{k'\mu_B}^* U_{k\mu_B} - V_{k'\mu_B} V_{k\mu_B}^*\right)\end{aligned} \tag{4}$$

and

$$\begin{aligned}\kappa_{kk'}^{(\mu_B)} &= \langle\phi|\beta_{\mu_B} c_{k'} c_k \beta_{\mu_B}^+|\phi\rangle \\ &= (V^*U^T)_{kk'} + \left(U_{k\mu_B} V_{k'\mu_B}^* - U_{k'\mu_B} V_{k\mu_B}^*\right).\end{aligned} \tag{5}$$

These two matrices obviously violate time-reversal invariance. As a consequence, the HF field

$$\Gamma_{ll'}^{(\mu_B)} = \sum_{qq'} \overline{v}_{lq'l'q} \rho_{qq'}^{(\mu_B)} \tag{6}$$

as well as the pairing field

$$\Delta_{ll'}^{(\mu_B)} = \frac{1}{2} \sum_{qq'} \overline{v}_{ll'qq'} \kappa_{qq'}^{(\mu_B)} \tag{7}$$

both violate time-reversal invariance making the numerical calculation much more computationally expensive to carry out. A way to preserve time-reversal invariance is to use the EFA that amounts to use the "average" density

$$\begin{aligned}\rho_{kk'}^{\mathrm{EFA}} = (V^*V^T)_{kk'} + \tfrac{1}{2}\big(&U_{k'\mu_B} U_{k\mu_B}^* - V_{k'\mu_B}^* V_{k\mu_B} \\ &+ U_{k'\overline{\mu}_B} U_{k\overline{\mu}_B}^* - V_{k'\overline{\mu}_B}^* V_{k\overline{\mu}_B}\big)\end{aligned} \tag{8}$$

and the "average" pairing tensor

$$\begin{aligned}\kappa_{kk'}^{\mathrm{EFA}} = (V^*U^T)_{kk'} + \tfrac{1}{2}\big(&U_{k\mu_B} V_{k'\mu_B}^* - U_{k'\mu_B} V_{k\mu_B}^* \\ &+ U_{k\overline{\mu}_B} V_{k'\overline{\mu}_B}^* - U_{k'\overline{\mu}_B} V_{k\overline{\mu}_B}^*\big)\end{aligned} \tag{9}$$

that now preserve time-reversal invariance as both expressions involve and average with equal weights of the blocked level μ_B and its time-reversed and degenerate partner $\overline{\mu}_B$ (see below for higher order degeneracy). Intuitively, the above densities should correspond to an occupancy of $1/2$ for the states μ_B and $\overline{\mu}_B$. In the next step of the EFA framework, it is assumed without proof that the energy is given by the standard HFB expression but using ρ^{EFA} and κ^{EFA} instead of the corresponding densities, i.e.,

$$E_{\mathrm{EFA}} = \mathrm{Tr}\,[t\rho^{\mathrm{EFA}}] + \tfrac{1}{2}\,\mathrm{Tr}\,[\Gamma^{\mathrm{EFA}}\rho^{\mathrm{EFA}}] - \tfrac{1}{2}\,\mathrm{Tr}\,[\Delta^{\mathrm{EFA}}\kappa^{\mathrm{EFA}*}]. \tag{10}$$

Finally, it is assumed that the U and V amplitudes of the Bogoliubov transformation are given as the solution of the standard HFB equation

$$\begin{pmatrix} h^{\mathrm{EFA}} & \Delta^{\mathrm{EFA}} \\ -\Delta^{\mathrm{EFA}*} & -h^{\mathrm{EFA}*} \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \tag{11}$$

where E are the quasiparticle energies. To our knowledge, the two previous assumptions of the EFA, namely that the energy

is given by Eq. (10) and that the U and V amplitudes are given by Eq. (11), lacked a foundation and were just considered as a plausible quantity (the energy) and equation. Here we will show that both assumptions are well founded in terms of standard quantum mechanic procedures and therefore we are giving more credit to the approximation.

A. Justification of the EFA expression for the energy

In the standard HFB theory the density matrix and pairing tensor are the components of a bipartite generalized density matrix

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix} = W\mathbb{R}W^+, \quad (12)$$

where the generalized quasiparticle density matrix

$$\mathbb{R}_{\nu\mu} = \begin{pmatrix} \langle\phi|\,\beta^\dagger_\mu\beta_\nu\,|\phi\rangle & \langle\phi|\,\beta_\mu\beta_\nu\,|\phi\rangle \\ \langle\phi|\,\beta^\dagger_\mu\beta^\dagger_\nu\,|\phi\rangle & \langle\phi|\,\beta_\mu\beta^\dagger_\nu\,|\phi\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (13)$$

and the Bogoliubov super-matrix

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad (14)$$

have been introduced. In the EFA case we can also introduce a generalized density matrix

$$\mathcal{R}^{\rm EFA} = \begin{pmatrix} \rho^{\rm EFA} & \kappa^{\rm EFA} \\ -\kappa^{\rm EFA*} & 1-\rho^{\rm EFA*} \end{pmatrix} \quad (15)$$

that again can be written as

$$\mathcal{R}^{\rm EFA} = W\mathbb{R}^{\rm EFA}W^+ \quad (16)$$

with

$$\mathbb{R}^{\rm EFA}_{\nu\mu} = \begin{pmatrix} f_\mu & 0 \\ 0 & 1-f_\mu \end{pmatrix} \quad (17)$$

and the f_μ is given by

$$f_\mu = \begin{cases} \frac{1}{2} & \mu = \mu_B \text{ or } \overline{\mu}_B \\ 0 & \text{otherwise.} \end{cases} \quad (18)$$

The above result immediately remind us of the finite-temperature HFB formalism [12], where the quasiparticle density matrix has exactly the same form as above but with the statistical occupancies

$$f_\mu = \frac{1}{e^{\beta E_\mu}+1}. \quad (19)$$

Therefore, the EFA can be viewed as a finite-temperature HFB formalism with the statistical factors of Eq. (18). The finite-temperature formalism is nothing but a quantum mechanics statistical formalism where instead of pure states a statistical admixture of them is considered weighted with given probabilities. In the finite-temperature formalism the probabilities are obtained according to the statistical "ensemble" considered but in the EFA they are just fixed by the requirements of the approximation. For this reason we will not use in the following the language of finite temperature but instead the one of statistical quantum mechanics. The two relevant concepts in statistical quantum mechanics are the one of the "density matrix operator" and the other is the concept of trace. In the present context the trace is taken over the whole Fock space in such a way that given a set of quasiparticle creation and annihilation operators β^+_μ and β_μ and the corresponding vacuum $|\phi\rangle$ [see Eq. (1)] we have the following expression for the trace of an arbitrary operator

$$\mathrm{Tr}\,[\hat{O}] = \langle\phi|\hat{O}|\phi\rangle + \sum_\mu \langle\phi|\beta_\mu\hat{O}\beta^\dagger_\mu|\phi\rangle + \frac{1}{2!}\sum_{\nu\mu}\langle\phi|\beta_\mu\beta_\nu\hat{O}\beta^\dagger_\nu\beta^\dagger_\mu|\phi\rangle\ldots \quad (20)$$

The density operator $\hat{\mathcal{D}}$ can be chosen in such a way that $\hat{\mathcal{D}}|\phi\rangle = |\phi\rangle$ and $\hat{\mathcal{D}}\beta^\dagger_\mu = p_\mu\beta^\dagger_\mu\hat{\mathcal{D}}$, where p_μ is the probability of the one-quasiparticle excitation $\beta^+_\mu|\phi\rangle$. In this formalism the statistical mean value of an operator is given by

$$\langle\hat{O}\rangle_S = \frac{\mathrm{Tr}\,[\hat{O}\hat{\mathcal{D}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}]} = \frac{1}{Z}\Big(\langle\phi|\hat{O}|\phi\rangle + \sum_\mu p_\mu\langle\phi|\beta_\mu\hat{O}\beta^\dagger_\mu|\phi\rangle + \frac{1}{2!}\sum_{\nu\mu}p_\mu p_\nu\langle\phi|\beta_\mu\beta_\nu\hat{O}\beta^\dagger_\nu\beta^\dagger_\mu|\phi\rangle\ldots\Big) \quad (21)$$

with

$$\mathrm{Tr}\,[\hat{\mathcal{D}}] = Z = 1 + \sum_\mu p_\mu + \sum_{\nu<\mu} p_\mu p_\nu \ldots = \prod_\mu (1+p_\mu). \quad (22)$$

It is also easy to show that

$$\langle\beta_\rho\beta_\sigma\rangle_S = \langle\beta^+_\rho\beta^+_\sigma\rangle_S = 0 \quad (23)$$

and also

$$\langle\beta^+_\rho\beta_\sigma\rangle_S = \delta_{\rho\sigma}\frac{p_\sigma}{1+p_\sigma} = \delta_{\rho\sigma}f_\sigma;\ \langle\beta_\rho\beta^+_\sigma\rangle_S = \delta_{\rho\sigma}\left(1-\frac{p_\sigma}{1+p_\sigma}\right) = \delta_{\rho\sigma}(1-f_\sigma) \quad (24)$$

and therefore we recover the EFA's density matrix of Eq. (15) by using the above formalism with

$$p_\mu = \begin{cases} 1 & \mu = \mu_B \text{ or } \overline{\mu}_B \\ 0 & \text{otherwise.} \end{cases} \quad (25)$$

Here we are implicitly assuming that the single-particle levels are doubly degenerate (Kramer's degeneracy) but in those cases where spherical symmetry is preserved in the mean-field procedure we will have to populate with the same probability all the states with different $m = -j, \ldots, j$ (third component of the angular momentum) for a given orbital labeled with the j quantum number. The formalism being developed here apply equally well in this case and the reader is referred to Appendix A for technical details in the spherical case.

Thanks to the existence of a statistical Wick's theorem (see, for instance, the proof given by Gaudin [13] and also Ref. [14] for a more recent account) it is possible to compute any statistical mean value of a product of creation and annihilation operators in terms of the corresponding contractions and

therefore it is possible to express the statistical mean value of the energy $\langle \hat{H} \rangle_S = \mathrm{Tr}\,[\hat{H}\hat{\mathcal{D}}]/\mathrm{Tr}\,[\hat{\mathcal{D}}]$ by using the standard expression

$$\langle \hat{H} \rangle_S = \mathrm{Tr}\,[t\rho] + \tfrac{1}{2}\,\mathrm{Tr}\,[\Gamma\rho] - \tfrac{1}{2}\,\mathrm{Tr}\,[\Delta\kappa^*], \tag{26}$$

where the density matrix and pairing tensor are given by the contractions

$$\rho_{kk'} = \frac{\mathrm{Tr}\,[c_{k'}^+ c_k \hat{\mathcal{D}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}]}; \quad \kappa_{kk'} = \frac{\mathrm{Tr}\,[c_{k'} c_k \hat{\mathcal{D}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}]}. \tag{27}$$

Applying this result to the EFA case, we conclude that the energy of Eq. (10) can be written as $E_{\mathrm{EFA}} = \mathrm{Tr}\,[\hat{H}\hat{\mathcal{D}}^{\mathrm{EFA}}]/\mathrm{Tr}\,[\hat{\mathcal{D}}^{\mathrm{EFA}}]$. This result justifies the, otherwise ad hoc, expression of the EFA energy and gives a physical interpretation to it as the statistical mean value of the Hamiltonian taken with the EFA density operator. The EFA energy E_{EFA} can also be written in a more transparent way by using Eq. (21) together with Eq. (25) as

$$\begin{aligned} E_{\mathrm{EFA}} = \tfrac{1}{4}\big(&\langle\phi|\hat{H}|\phi\rangle + \langle\phi|\beta_{\mu_B}\hat{H}\beta^\dagger_{\mu_B}|\phi\rangle + \langle\phi|\beta_{\overline{\mu}_B}\hat{H}\beta^\dagger_{\overline{\mu}_B}|\phi\rangle \\ &+ \langle\phi|\beta_{\mu_B}\beta_{\overline{\mu}_B}\hat{H}\beta^\dagger_{\overline{\mu}_B}\beta^\dagger_{\mu_B}|\phi\rangle\big) \end{aligned} \tag{28}$$

showing that it is simply an average with equal weights of the energy of the reference even-even wave function $|\phi\rangle$, the energies of one quasiparticle excitations with quantum numbers μ_B and $\overline{\mu}_B$ and the energy of the two quasiparticle excitation with the same quantum numbers. This result, which was to the knowledge of the authors previously unknown[1], is very illustrative of the nature of the EFA as a statistical theory. The same kind of arguments can be applied to compute mean values of any kind of operators in the EFA framework. A curious result that can be easily derived is that the EFA mean values of any one-body operator, which according to the general result can be written as

$$\begin{aligned} \langle\hat{O}\rangle_{\mathrm{EFA}} = \tfrac{1}{4}(&\langle\phi|\hat{O}|\phi\rangle + \langle\phi|\alpha_{\mu_B}\hat{O}\alpha^\dagger_{\mu_B}|\phi\rangle + \langle\phi|\alpha_{\overline{\mu}_B}\hat{O}\alpha^\dagger_{\overline{\mu}_B}|\phi\rangle \\ &+ \langle\phi|\alpha_{\mu_B}\alpha_{\overline{\mu}_B}\hat{O}\alpha^\dagger_{\overline{\mu}_B}\alpha^\dagger_{\mu_B}|\phi\rangle), \end{aligned} \tag{29}$$

can also be written in a more compact way as

$$\begin{aligned} \langle\hat{O}\rangle_{\mathrm{EFA}} &= \tfrac{1}{2}(\langle\phi|\alpha_{\mu_B}\hat{O}\alpha^\dagger_{\mu_B}|\phi\rangle + \langle\phi|\alpha_{\overline{\mu}_B}\hat{O}\alpha^\dagger_{\overline{\mu}_B}|\phi\rangle) \\ &= \tfrac{1}{2}(\langle\phi|\hat{O}|\phi\rangle + \langle\phi|\alpha_{\mu_B}\alpha_{\overline{\mu}_B}\hat{O}\alpha^\dagger_{\overline{\mu}_B}\alpha^\dagger_{\mu_B}|\phi\rangle). \end{aligned} \tag{30}$$

This allows us to write the density matrix and pairing tensor as an average over one-quasiparticle excitations

$$\rho^{\mathrm{EFA}}_{kk'} = \tfrac{1}{2}(\langle\phi|\alpha_{\mu_B}c^+_{k'}c_k\alpha^+_{\mu_B}|\phi\rangle + \langle\phi|\alpha_{\bar{\mu}_B}c^+_{k'}c_k\alpha^+_{\bar{\mu}_B}|\phi\rangle) \tag{31}$$

and

$$\kappa^{\mathrm{EFA}}_{kk'} = \tfrac{1}{2}(\langle\phi|\alpha_{\mu_B}c_{k'}c_k\alpha^+_{\mu_B}|\phi\rangle + \langle\phi|\alpha_{\bar{\mu}_B}c_{k'}c_k\alpha^+_{\bar{\mu}_B}|\phi\rangle), \tag{32}$$

which is a very intuitive result according to the expressions of Eqs. (8) and (9). This result, however, does by no means imply that the energy, which is the average of a two-body operator, could be written as $\frac{1}{2}(\langle\phi|\alpha_{\mu_B}H\alpha^+_{\mu_B}|\phi\rangle + \langle\phi|\alpha_{\bar{\mu}_B}H\alpha^+_{\bar{\mu}_B}|\phi\rangle)$.

[1] In Ref. [3] it is mentioned that the EFA in the zero pairing limit can be described by the density operator of a mixed state but no further development of the idea was pursued there.

B. Variational derivation of the EFA-HFB equation

Another interesting feature of the results obtained so far is that the variational principle can be applied now to the E_{EFA} energy. As it will be shown below the variational principle leads naturally to the HFB equation of the EFA mentioned in Eq. (11), justifying thereof its use to determine the coefficients of the Bogoliubov transformation. This result is also advantageous from a practical point of view as the variational origin of the HFB-EFA equations allows the use of "gradient-like" methods to solve it and also makes the treatment of constraints much easier.

The first step in the application of the variational principle is to establish the variational space by defining the most general Bogoliubov transformation. This is a common procedure that the interested reader can consult in the standard literature [2,15] and we will give here only the most relevant formulas just to establish the notation. Given a reference HFB wave function $|\phi\rangle$ the most general HFB wave function $|\phi(\mathbb{Z})\rangle$ not orthogonal to it is given by $|\phi(\mathbb{Z})\rangle = \exp(i\hat{Z})|\phi\rangle$, where $\hat{Z}$ is a Hermitian (to preserve the unitarity of the transformation) one-body operator $\hat{Z} = \frac{1}{2}\sum_{\mu\nu}\mathbb{Z}_{\mu\nu}\alpha^+_\mu\alpha_\nu$ that is here written in terms of the generalized quasiparticle operators $\alpha_\mu = (\beta_1, \ldots, \beta_N, \beta^+_1, \ldots, \beta^+_N)$, its Hermitian conjugate α^+_μ, and the bipartite Hermitian matrix [15]

$$\mathbb{Z} = \begin{pmatrix} Z^{11} & Z^{20} \\ -Z^{20*} & -Z^{11*} \end{pmatrix}, \tag{33}$$

where Z^{11}_{mn} $(m, n = 1, \ldots, N)$ is a Hermitian matrix (N^2 free parameters, complex Z^{11}_{mn} with $m > n$ plus real Z^{11}_{mm}), whereas Z^{20} is skew-symmetric ($N^2 - N$ free parameters, complex Z^{20}_{mn} with $m > n$). The matrix elements of Z^{11}_{mn} with $m > n$ plus Z^{11}_{mm} and those of Z^{20}_{mn} with $m > n$ constitute the complex variational parameters of our model. The complex variational parameters are also denoted by the vector z_ρ of dimension $2N^2 - N$ (see Appendix B for details). The coefficients of the Bogoliubov transformation of the quasiparticle operators associated to $|\phi(\mathbb{Z})\rangle$ are given by the matrix $W(\mathbb{Z}) = W(0)\exp(i\mathbb{Z})$ that is written in terms of the exponential of $\mathbb{Z}$ and the Bogoliubov transformation coefficients $W(0)$ of the reference HFB wave function $|\phi\rangle$. To determine the dependence of the generalized density with the variational parameters we will use Eq. (16) to write

$$\mathcal{R}^{EFA}(\mathbb{Z}) = W(\mathbb{Z})\mathbb{R}^{EFA}W^+(\mathbb{Z}), \tag{34}$$

where we have kept $\mathbb{R}^{EFA}$ fixed as in Eq. (17), according to its definition. For infinitesimal variational parameters (i.e., infinitesimal $\mathbb{Z}$) we have

$$\begin{aligned} \mathcal{R}^{EFA}(\mathbb{Z}) &= \mathcal{R}^{EFA}(0) + iW(0)[\mathbb{Z}, \mathbb{R}^{EFA}]W^+(0) + O(\mathbb{Z}^2) \\ &= \mathcal{R}^{EFA}(0) + i[\mathcal{Z}, \mathcal{R}^{EFA}] + O(\mathbb{Z}^2), \end{aligned} \tag{35}$$

where $\mathcal{Z} = W(0)\mathbb{Z}W^+(0)$. Now to facilitate the manipulation of different quantities we write the energy as

$$E_{EFA} = \tfrac{1}{4}\,\mathrm{Tr}_2\,[(\mathcal{H} + \mathcal{T})\mathcal{S}] \tag{36}$$

in terms of the Hamiltonian matrix

$$\mathcal{H} = \begin{pmatrix} t + \Gamma & \Delta \\ -\Delta^* & -(t + \Gamma)^* \end{pmatrix},$$

the kinetic energy matrix

$$\mathcal{T} = \begin{pmatrix} t & 0 \\ 0 & -t^* \end{pmatrix}$$

and the matrix

$$\mathcal{S} = \mathcal{R} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & -\rho^* \end{pmatrix}$$

derived from the generalized density. The trace is taken over the double size space where bipartite matrices are defined. To arrive at the above expression we made use of the properties $\mathrm{Tr}\,[\Gamma_2\rho_1] = \mathrm{Tr}\,[\Gamma_1\rho_2]$ and $\mathrm{Tr}\,[\Delta_2\kappa_1^*] = \mathrm{Tr}\,[\Delta_1\kappa_2^*]^*$ where Γ_i and Δ_i stand for the Hartree-Fock and pairing fields computed with the density matrix ρ_i and pairing tensor κ_i, respectively. The two previous relations can be written using bipartite matrices as

$$\mathrm{Tr}_2[(\mathcal{H}_1 - \mathcal{T})\mathcal{S}_2] = \mathrm{Tr}_2[(\mathcal{H}_2 - \mathcal{T})\mathcal{S}_1], \tag{37}$$

This result allows to write the variation of the energy in a more compact way, namely

$$\begin{aligned} \delta E_{\mathrm{EFA}} &= \tfrac{1}{4}\{\mathrm{Tr}_2\,[(\mathcal{H} + \mathcal{T})\delta\mathcal{S}] + \mathrm{Tr}_2\,[(\delta\mathcal{H} - \mathcal{T})\mathcal{S}]\} \\ &= \tfrac{1}{2}\,\mathrm{Tr}_2\,[\mathcal{H}\delta\mathcal{S}] = \tfrac{i}{2}\mathrm{Tr}_2\,[[\mathcal{R}, \mathcal{H}]\mathcal{Z}] + O(\mathbb{Z}^2), \end{aligned} \tag{38}$$

where we have made use of Eq. (35) and the fact that $\delta\mathcal{S} = \delta\mathcal{R}$. The variational condition $\delta E_{\mathrm{EFA}} = 0$ has to be handled with care as not all the parameters of the bipartite matrix $\mathcal{Z}$ are variational parameters but as it is shown in Appendix B the variational condition can be written as $[\mathcal{R}, \mathcal{H}] = 0$ that is the standard form of the HFB equation. It has to be emphasized again that the previous form of the HFB equation in the EFA was just an assumption and now we are able to justify it in our framework by simply invoking the variational principle. The HFB equation could be solved using iterative methods as it is customary with the standard HFB equations but we have found it more convenient to take advantage of the variational origin of the equation to use other methods to find its minimum, like the gradient method. To implement the gradient method it is more convenient to write the variation of the EFA energy in the "quasiparticle" basis as

$$\delta E_{\mathrm{EFA}} = \tfrac{i}{2}\mathrm{Tr}_2\,[[\mathbb{R}, \mathbb{H}]\mathbb{Z}] + O(\mathbb{Z}^2) \tag{39}$$

with

$$\mathbb{H} = W^+(0)\mathcal{H}W(0) = \begin{pmatrix} H^{11} & H^{20} \\ -H^{20\,*} & -H^{11\,*} \end{pmatrix}.$$

Using this form and the definitions of Appendix B we can finally write $\delta E_{\mathrm{EFA}} = \sum_{\rho=1}^{2N^2-N}(g_E)_\rho z_\rho + O(z^2)$, where $(g_E)_\rho$ are the components of the gradient of the energy with respect to the variational parameters z_ρ. In the spirit of the gradient method, by choosing $z_\rho = -\eta(g_E^*)_\rho$ we make sure we gain energy at least to first order in z if the scaling parameter (or step size) η is always chosen to be positive. The previous election implies that $\mathbb{Z} = i\eta[\mathbb{R}, \mathbb{H}]$. The step size η is estimated in each iteration as to make second-order terms smaller enough compared with first-order ones so that the energy always decreases. Once the $\mathbb{Z}$ parameters have been determined the wave function $W(\mathbb{Z})$ is computed by evaluating the exponential $e^{i\mathbb{Z}}$ by means of a Padé approximation to the exponential of the form $e^x = N_{pp}(x)/N_{pp}(-x)$ with $N_{pp}(x) = \sum_{k=0}^{p} c_k^{(p)} x^k$ (that is, the polynomials in both the numerator and denominator have the same degree; the coefficients $c_k^{(p)}$ are determined by the standard recurrence relation $c_k^{(p)} = c_{k-1}^{(p)} \frac{p+1-k}{(2p+1-k)k}$) that has the nice feature of preserving the unitarity of the exponential when used with anti-Hermitian exponents as it is the case. Usually, a Padé approximation of order $p = 1$ suffices and in our numerical implementation we have taken $e^{i\mathbb{Z}} \approx (\mathbb{1} + \frac{i}{2}\mathbb{Z})(\mathbb{1} - \frac{i}{2}\mathbb{Z})^{-1}$.

C. Dealing with constraints

In dealing with constraints, we face the numerical problem of minimizing a given function of the variational parameters $E_{\mathrm{EFA}}(\mathbb{Z})$ subject to some constraints of the kind

$$\frac{\mathrm{Tr}\,[\hat{Q}_i\hat{\mathcal{D}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}]} = q_i, \tag{40}$$

where $\hat{Q}_i$ are one-body operators that can be usually written as $\hat{Q}_i = \sum_{kk'}(Q_i)_{kk'}c_k^+ c_{k'}$ (extending the results below to the case of operators not commuting with the particle number one is straightforward). Introducing the bipartite matrix

$$\mathcal{Q}_i = \begin{pmatrix} Q_i & 0 \\ 0 & -Q_i^* \end{pmatrix}$$

we can write

$$q_i = \tfrac{1}{2}\mathrm{Tr}\,[\mathcal{Q}_i\mathcal{S}] \tag{41}$$

that yields, in analogy to Eq. (38), to the following expression for the variation of q_i

$$\begin{aligned} \delta q_i &= \tfrac{i}{2}\mathrm{Tr}_2\,[[\mathcal{R}, \mathcal{Q}_i]\mathcal{Z}] + O(\mathcal{Z}^2) \\ &= \tfrac{i}{2}\mathrm{Tr}_2\,[[\mathbb{R}, \mathbb{Q}_i]\mathbb{Z}] + O(\mathbb{Z}^2). \end{aligned} \tag{42}$$

To consider the constrained minimization procedure we will proceed in the standard way by introducing Lagrange multipliers λ_i and a new functional to be minimized, namely $E'_{\mathrm{EFA}}(\mathbb{Z}) = E_{\mathrm{EFA}}(\mathbb{Z}) - \sum_i \lambda_i q_i(\mathbb{Z})$. The Lagrange multipliers are determined as to make the gradient of $E'_{\mathrm{EFA}}(\mathbb{Z})$ orthogonal to the ones of the $q_i(\mathbb{Z})$'s that will be denoted by $(g_{q_i})_\rho$. Taking into account that the gradient of $E'_{\mathrm{EFA}}(\mathbb{Z})$ is given by the vector $(g_{E'})_\rho = (g_E)_\rho - \sum_j \lambda_j (g_{q_j})_\rho$ the orthogonality condition yields

$$\lambda_i = \sum_j S_{ij}^{-1} d_j \tag{43}$$

where

$$S_{ij} = \sum_\rho \left(g_{q_i}\right)_\rho^* \left(g_{q_j}\right)_\rho \tag{44}$$

and

$$d_i = \sum_\rho (g_E)_\rho^* \left(g_{q_j}\right)_\rho \tag{45}$$

Using the explicit form of the corresponding gradients (see Appendix B) we can finally write the two quantities above as

$$S_{ij} = \tfrac{1}{4}\,\mathrm{Tr}_2\,[[\mathbb{Q}_i, \mathbb{R}][\mathbb{Q}_j, \mathbb{R}]] \tag{46}$$

and

$$d_i = \tfrac{1}{4}\,\mathrm{Tr}_2\,[[\mathbb{Q}_i, \mathbb{R}][\mathbb{H}, \mathbb{R}]]. \tag{47}$$

It is also convenient to establish a procedure to readjust the constraints as it is customary that in the iterative process their values q_i slightly depart from the desired ones $q_i^{(0)}$, that is, $q_i = q_i^{(0)} + \delta q_i$. In the context of the gradient method such a procedure is elemental and we only have to replace the chemical potentials λ_j by $\lambda_j + \delta\lambda_j$ and impose that the variation of the values of the constraints δq_i given by Eq. (42) yields the desired value. The result is $\eta\delta\lambda_j = \sum_i S_{ij}^{-1}\delta q_i$, where the matrix elements S_{ij} are the same as in Eq. (46).

D. Density-dependent interactions

For density-dependent interactions, like the Gogny force [16] used in the next section to illustrate the whole procedure, we have to define the explicit form of the density-dependent part of the interaction for statistical averages. It seems natural that, if for a pure state (an HFB mean-field wave function in this case) the DD part of the interaction is a function of the density of the pure state, then for a statistical average the DD should be the same function but of the density of the statistical average; that is, a function of

$$\begin{aligned}\rho(\vec{R}) &= \frac{\mathrm{Tr}\,[\hat{\rho}(\vec{R})\hat{\mathcal{D}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}]} \\ &= \frac{1}{Z}\Bigg(\langle\phi|\hat{\rho}(\vec{R})|\phi\rangle + \sum_{\mu} p_\mu \langle\phi|\beta_\mu\hat{\rho}(\vec{R})\beta_\mu^\dagger|\phi\rangle \\ &\quad + \frac{1}{2!}\sum_{\nu\mu} p_\mu p_\nu \langle\phi|\beta_\mu\beta_\nu\hat{\rho}(\vec{R})\beta_\nu^\dagger\beta_\mu^\dagger|\phi\rangle\ldots\Bigg) \quad (48)\end{aligned}$$

(see Eq. (22) for the definition of Z). This prescription has been the one used in previous calculations with the Gogny force at finite temperature [17,18] as well as by other authors with other density dependent interactions like several variants of the Skyrme one [19]. This prescription has the right limit when the probabilities go to zero (pure state) and also produces consistent results when the one-quasi-particle energies are computed as partial derivatives of the energy with respect to the probabilities: when the above prescription is used the expression for the one-quasiparticle energies includes the rearrangement term present in all the HF or HFB calculations with density dependent interactions [16]. It is obvious that for a consistent treatment of the problem, the variation of the energy with respect to the variational parameters has to take into account also that the Hamiltonian depends on them via the DD term and the corresponding rearrangement terms have to be considered (see Refs. [16,20] for details). To summarize this section, in the EFA case we use the density

$$\begin{aligned}\rho^{\mathrm{EFA}}(\vec{R}) = \frac{\mathrm{Tr}\,[\hat{\rho}(\vec{R})\hat{\mathcal{D}}^{\mathrm{EFA}}]}{\mathrm{Tr}\,[\hat{\mathcal{D}}^{\mathrm{EFA}}]} &= \frac{1}{4}(\langle\phi|\hat{\rho}(\vec{R})|\phi\rangle \\ &+ \langle\phi|\beta_{\mu_B}\hat{\rho}(\vec{R})\beta_{\mu_B}^\dagger|\phi\rangle + \langle\phi|\beta_{\bar{\mu}_B}\hat{\rho}(\vec{R})\beta_{\bar{\mu}_B}^\dagger|\phi\rangle \\ &+ \langle\phi|\beta_{\mu_B}\beta_{\bar{\mu}_B}\hat{\rho}(\vec{R})\beta_{\bar{\mu}_B}^\dagger\beta_{\mu_B}^\dagger|\phi\rangle) \quad (49)\end{aligned}$$

for the density-dependent part of the Gogny interaction.

III. RESULTS

To show an example of the proposed method we have computed the spectrum of several odd-A isotopes of the radium in the range of A between 221 and 231. As it is well known, some isotopes of Ra are known to display octupole deformation [21] in their ground state and therefore, to study their spectrum, we will carry out calculations constraining the octupole moment to locate the different minima and to check their depths as they are relevant for the stability of the configuration against octupole fluctuations. We will limit the calculation to axially symmetric (but reflection symmetry breaking) configurations and therefore each of the blocked levels will be characterized (and labeled) by its J_z value (but not parity). The calculations are performed in the framework of the EFA with the finite range and effective interaction of Gogny [16]. As it is customary in all the mean-field calculations with the Gogny force, we have subtracted the kinetic energy of the center-of-mass motion from the Routhian to be minimized to ensure that the center-of-mass is kept at rest. We have also dealt with the exchange Coulomb energy in the Slater approximation and neglected the contribution of the Coulomb interaction to the pairing field. For the Gogny force we have used the parameter set known as D1S that was adjusted more than 20 years ago [22,23] to reproduce basic nuclear matter properties and the binding energies of several magic nuclei. The HFB wave functions have been expanded in a harmonic oscillator (HO) basis containing 14 major shells that is enough as to grant convergence in the excitation spectra obtained.

Due to the self-consistent nature of our procedure it is by no means granted that starting the iterative procedure by blocking the quasiparticle of lowest energy the minimization process in going to end up in the lowest-energy solution. For this reason one has to repeat the minimization process several times using different quasiparticle configurations each time (usually ones with the lowest one-quasiparticle energy) for the initial blocking. In our case we have repeated each calculation three times implying a computational cost 18 times higher (6 values of J_z times 3 starting configurations) than the corresponding calculation in an even-even neighbor. By following this procedure we can be pretty sure to have reached the lowest-energy solution for all values of the octupole moment and mass number.

In Fig. 1 we show the potential energy surfaces (PES) as a function of the octupole moment for the six radium isotopes considered and corresponding to the blocking of the lowest quasiparticles with J_z values ranging from 1/2 to 11/2. Higher J_z values are not considered here as the corresponding single-particle levels lie too far away from the Fermi surface as to be relevant for the lowest-energy configurations. By looking at the PES for different isotopes we learn that the response to octupole deformation strongly depends on the J_z value of the level blocked as it is, for instance, the case in ^{231}Ra, where the PES of some levels show a minimum at $Q_3 = 0$, whereas others (like the ones with $J_z = 3/2$ and $J_z = 7/2$) have an octupole deformed minimum at $Q_3 = 3b^{3/2}$. Another

interesting fact is that breaking reflection symmetry implies energy gains of up to 2 MeV in some cases as compared to the symmetry preserving mean-field configuration and this amount of energy cannot be disregarded in the evaluation of masses. In all the cases, the potential energy wells are not very deep indicating the relevance of considering fluctuations on the octupole degree of freedom. This fact was already observed in calculations of the same kind and the same interaction but for even-even nuclei [24,25] and the conclusion reached there was that a treatment of the octupole fluctuations was needed. One of the advantages of the present formulation of the EFA is the fact that the standard methods to incorporate correlations (as, for instance, the collective Schroedinger equation, see Refs, [24,25] for details) can be now generalized to the present case [26]. Another improvement to the present treatment is to consider parity projection in the manner discussed in Ref. [27] for even-even nuclei; work along this lines is in progress and will be reported in the near future [26].

Another consequence of the different responses to octupole deformation of the different J_z blocked configurations is that the spectrum corresponding to the minimum energy is rather different from the one obtained by restricting the system to reflection symmetric configurations showing the relevance of the octupole degree for freedom for the ordering of the spectrum of these and other odd-A nuclei in the region of the actinide. The different theoretical spectra allowing and not allowing octupole deformation are depicted in Fig. 2 along with the experimental data. The inclusion of octupole deformation improves the spectrum for several nuclei like ^{221}Ra, ^{225}Ra, and ^{227}Ra and makes it to look much closer to the experimental one. In fact, the inclusion of octupole deformation on these nuclei allows for a correct prediction of the spin of the ground state. For the other cases the inclusion of the octupole degree of freedom leaves the spectra more or less unchanged as compared to the $Q_3 = 0$ results. However, it has to be kept in mind that when the octupole moment is allowed to take values different from zero, parity mixing is also allowed in the wave functions and therefore the different levels lose parity as a quantum number. To restore parity symmetry a projection onto good parity is required that would lead to the appearance of two levels with opposite parity for each one of the levels breaking the parity symmetry. The energy splitting between the two levels strongly depends on the octupole deformation but we can state as a rule of thumb that the energy splitting is going to be rather small (a few tens of keV at most) in most of the cases and it will hardly exceed 0.5 MeV. Fortunately, the formalism developed in this article can be extended to the situation of symmetry restoration by means of parity projection and the results as well as the whole formalism will be published elsewhere. For the present purposes the only relevant information needed is that parity projection will lead to a parity doublet with a not so big energy splitting. A bigger splitting could eventually be obtained by fully treating octupole fluctuations as mentioned above and again one of the advantages of the present formulation is that the collective masses needed for such a task can be consistently evaluated in the present framework. Concerning the comparison with the experiment, we have to keep in mind the strong sensitivity

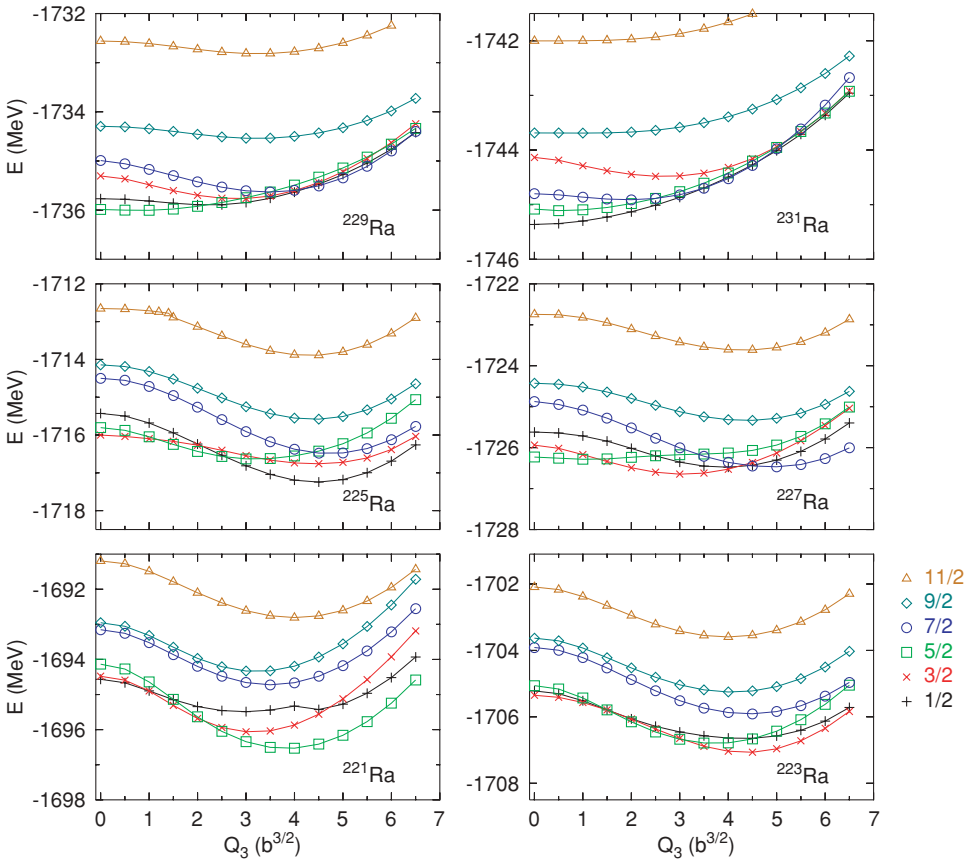

FIG. 1. (Color online) Potential energy surfaces as a function of the octupole moment Q_3 (in units of $b^{3/2} \equiv 10^3$ fm^3) for the odd-mass isotopes of Ra considered and blocking in each of the relevant J_z channels from 1/2 to 11/2.

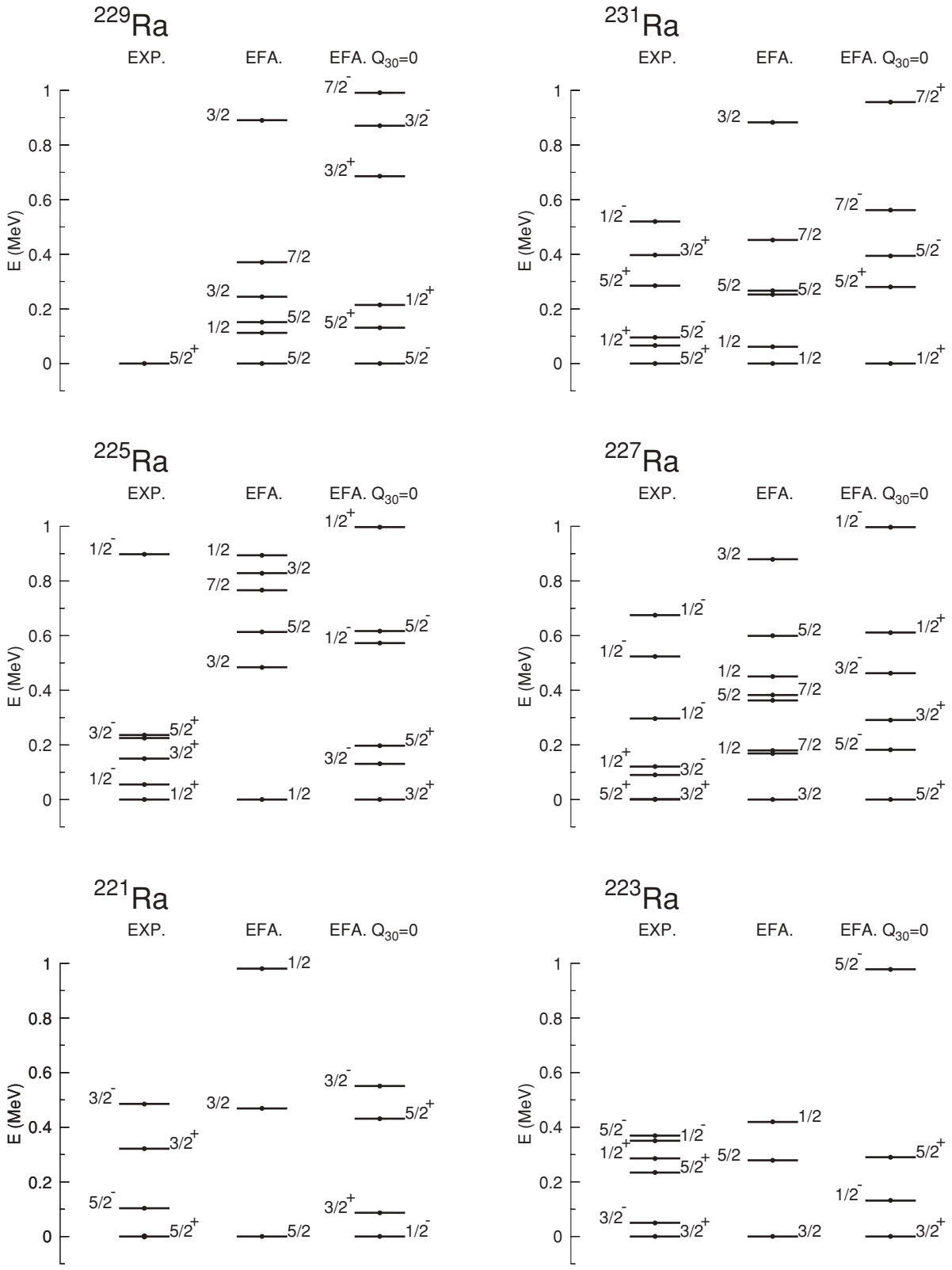

FIG. 2. Lowest lying excitation spectrum for the six isotopes of radium considered. In each panel three spectra are included: the one to the left is the experimental one, the other two are theoretical predictions (including octupole deformation effect in the middle and not including it, that is $Q_3 = 0$, to the right).

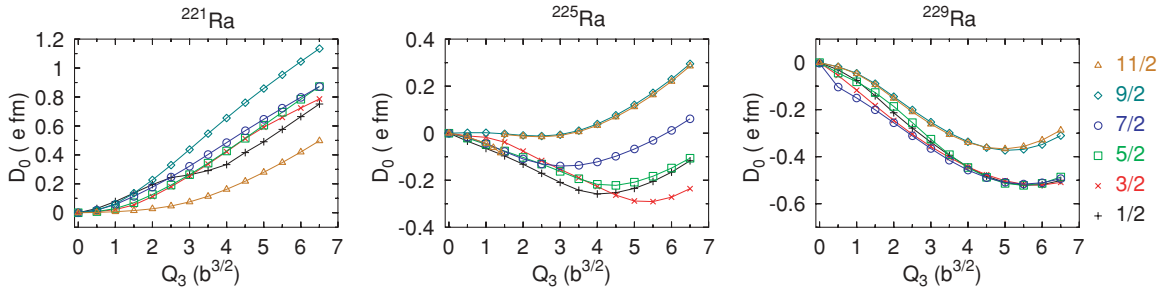

FIG. 3. (Color online) Dipole moments as a function of Q_3 for three representative nuclei and all the J_z values considered.

of the spectra to tiny details of the underlying single-particle states that makes quite difficult to obtain the experimental spectrum in the right order. The accuracy of modern effective interaction only entitle to look for an agreement in the number of levels and J_z values in a range of 1 or 1.5 MeV above the ground state but it does not entitle whatsoever to sought for an agreement in the ordering of the levels. However, the inclusion of the octupole degree of freedom allows for a correct description of the spin of the ground state in five of the six considered nuclei. With this in mind we can conclude that the agreement with experiment is quite good in the whole isotopic chain.

A procedure that is sometimes used to describe odd-A nuclei is to neglect explicitly all kind of polarization effects and treat the quasiparticle excitations in a perturbative fashion [3]. To this end, a reference HFB wave function $|\varphi_R\rangle$ is computed assuming that is fully paired (that is, is a linear combination of wave functions with even number of particles) but the number of particles is constrained to be odd on the average. The wave functions of the ground state and excitations of the odd nucleus are built as one-quasiparticle excitations built on top of the reference HFB wave function ($\beta_\mu^+|\varphi_R\rangle$). The excitation energies are then given by the corresponding one-quasiparticle energies E_μ computed as the mean value of the Routhian $E_\mu = \langle\varphi_R|\beta_\mu(\hat{H} - \lambda\hat{N})\beta_\mu^+|\varphi_R\rangle$ in an attempt to correct those energies perturbatively for the fact that particle number differs from the right value by the quantity $N_{\mu\mu}^{11} = \langle\varphi_R|\beta_\mu\hat{N}\beta_\mu^+|\varphi_R\rangle$. The perturbative correction works well when $N_{\mu\mu}^{11}$ is small but it is not so reliable when this quantity is large, as the chemical potential is usually a few MeV. In Table I we present the results of such perturbative calculation for the nuclei ^{223}Ra and ^{225}Ra. The spectrum looks rather similar to the self-consistent one obtained in the EFA framework (see Fig. 2) but the perturbative one is much more compressed. In this table we also include the values of $N_{\mu\mu}^{11}$ and we observe very big values of the order of 1 in absolute value. These large values together with the neutron chemical potential energies (-5.24 MeV for ^{223}Ra and -4.97 MeV for ^{225}Ra) make a too-big perturbative correction. It has to be mentioned that the value of $N_{\mu\mu}^{11}$ for the ground state is rather small in agreement with the motivation for the introduction of $|\varphi_R\rangle$ given in Ref. [3]. We can conclude that the polarization effects accounted for by the EFA are rather strong and the perturbative treatment, although a reasonable qualitative approximation, is not good at the quantitative level. No other mean values and/or physical quantities are considered in this comparison as it would imply the evaluation of the perturbative correction due to particle number departures from the physical values (that is the evaluation of "chemical potential" like quantities for mean values of arbitrary observables) and this is out of the scope of the present work.

TABLE I. Perturbative results for the nuclei ^{223}Ra and ^{225}Ra. The lowest five states in each case have been included.

^{223}Ra			^{225}Ra		
J_z	E_μ (MeV)	$N_{\mu\mu}^{11}$	J_z	E_μ (MeV)	$N_{\mu\mu}^{11}$
3/2	0.000	0.06	1/2	0.000	−0.09
5/2	0.059	−0.56	3/2	0.211	−0.62
1/2	0.216	0.64	5/2	0.410	−0.81
7/2	0.695	0.94	7/2	0.484	0.89
1/2	1.077	0.93	1/2	0.573	0.89

Another relevant physical quantity for octupole deformed nuclei is the intrinsic dipole moment D_0 that is directly related to the strong $E1$ transition probabilities observed in these nuclei. It is given as the mean value of the dipole operator

$$D_0 = e\frac{NZ}{A}(\langle\hat{z}\rangle_{\text{prot}} - \langle\hat{z}\rangle_{\text{neut}}), \tag{50}$$

in terms of the mean value of the z coordinate for protons and neutrons. The theoretical results for such quantity and for each blocked configuration and as a function of Q_3 are presented in Fig. 3 for three representative nuclei. In the first nucleus ^{221}Ra the global tendency for D_0 is to increase with increasing octupole moment for all possible configurations with different J_z. However, for the nucleus ^{225}Ra the dipole moment D_0 first decreases going to negative values and afterward increases to reach positive values (or negative but rather small) as the octupole moment increases. Finally, for the nucleus ^{229}Ra the dipole moments steadily decrease with increasing octupole moment and reaching absolute values greater than in the previous case. The behavior is rather similar to the one of the neighboring even-even radium isotopes as can be observed in Ref. [25]. This behavior was related in Ref. [25] to the increasing occupancy of the neutron $j_{15/2}$ orbital with increasing number of neutrons and leads to the prediction of a minimum in the absolute value of the dipole moment $|D_0|$ for the nucleus ^{224}Ra. As a consequence, we expect substantially lower values of $|D_0|$ for the nuclei ^{223}Ra and ^{225}Ra as is indeed the case.

TABLE II. Dipole moments D_0 in e fm for the six nuclei considered and obtained for the configuration corresponding to the minimum of each blocked configuration with varying J_z value. Only the J_z values up to 7/2 have been considered as this is the maximum value of that quantity for all the low lying states.

J_z	^{221}Ra	^{223}Ra	^{225}Ra	^{227}Ra	^{229}Ra	^{231}Ra
$\frac{1}{2}$	0.331	0.056	−0.253	−0.413	−0.226	0.000
$\frac{3}{2}$	0.255	0.175	−0.263	−0.275	−0.357	−0.374
$\frac{5}{2}$	0.427	0.050	−0.162	−0.053	−0.077	−0.057
$\frac{7}{2}$	0.403	0.254	−0.098	−0.471	−0.415	−0.279

The numerical values of the dipole moments obtained at the minima of the potential energy curves of Fig. 1 are given in Table II. The values are given not only for the theoretical ground state but also for other close lying configurations as our theoretical prediction not necessarily coincides with the experimental assignments. Experimental values taken from the compilation of Ref. [21] and also from Ref. [28] tell us that for ^{221}Ra the J^π of the ground state is $5/2^+$ with a value of $D_0 = 0.36 \pm 0.10e$ fm that is in good agreement with the D_0 value of the lowest lying $5/2^+$ theoretical state. For the ^{223}Ra nucleus there are values not only for the ground state but also for some excited ones; the values of D_0 are $0.129 \pm 0.009e$ fm, $0.035 \pm 0.005e$ fm and $0.076 \pm 0.004e$ fm for the $3/2^+$(ground state), $5/2^+$ and $1/2^+$states, respectively. As it can be checked in Table II the agreement between theory and experiment is very satisfactory for the three states. In the nucleus ^{225}Ra the experimental D_0 value is $0.14 \pm 0.02e$ fm that corresponds in reality to the absolute value of that quantity (D_0 is extracted from $B(E1)$ values where it enters squared and therefore the sign cannot be determined in that way). Taking this in account, we can say that there is a reasonable agreements with the theoretical prediction which, however, can be quite strongly affected by fluctuations in the octupole degree of freedom [25]. Finally, for the ^{227}Ra isotope the experimental value is $0.099 \pm 0.003e$ fm for the $3/2^+$ ground state and this value again agrees reasonably well with the theoretical prediction. The agreement between theory and experiment can be considered as quite good, especially taking into account the fact that no information on this kind of physics was included in the fitting procedure of the force afterwards.

IV. CONCLUSIONS

A prescription for the treatment of odd-mass nuclei in a time-reversal preserving mean-field (HFB) framework usually known as the EFA has been justified in terms of standard procedures of quantum statistical mechanics. It turns out that the EFA can be described as a mixed state where the blocked one-quasiparticle state and its time-reversed counterpart have probability one, whereas the others have zero probability. As a consequence, the EFA energy is given by an average involving the energy of the underlying even-even system, the energy of the blocked one-quasiparticle configurations and the two-quasiparticle excitation built out of them. As the energy now has a well-defined expression in terms of the HFB wave functions it is possible to invoke the variational principle to obtain the standard EFA-HFB equation and allow for the use of more sophisticated numerical techniques, like the gradient method, for its numerical solution. The method has been applied to the study of odd-A radium isotopes as a function of octupole deformation and with the Gogny D1S force and the agreement obtained between theory and experiment is quite reasonable. One of the advantages of the present method is the preservation of time-reversal symmetry that reduces substantially the computational cost of mean-field calculations of odd-mass nuclei. Another advantage of the justification obtained in this article is that the procedure can be extended beyond mean field in a consistent way increasing its range of applicability.

ACKNOWLEDGMENTS

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APPENDIX A: HIGHER-ORDER DEGENERACY: THE SPHERICAL CASE

In the spherical case, the levels to be "blocked" are characterized by angular momentum quantum numbers j_B, m_B with $m_B = -j_B, \ldots, j_B$. In the spirit of the EFA each of these levels will be uniformly populated with a fraction $1/(2j_B + 1)$ of a nucleon what means that in this case the density matrix and pairing tensors in the EFA approximation are given by the "average" density

$$\rho^{\mathrm{EFA}}_{kk'} = (V^* V^T)_{kk'} + \frac{1}{2j_B+1} \sum_{m_B=-j_B}^{j_B} \left(U_{k'\mu_B, j_B, m_B} U^*_{k\mu_B, j_B, m_B} - V^*_{k'\mu_B, j_B, m_B} V_{k\mu_B, j_B, m_B} \right) \tag{A1}$$

and the "average" pairing tensor

$$\kappa^{\mathrm{EFA}}_{kk'} = (V^* U^T)_{kk'} + \frac{1}{2j_B+1} \sum_{m_B=-j_B}^{j_B} \left(U_{k\mu_B, j_B, m_B} V^*_{k'\mu_B, j_B, m_B} - U_{k'\mu_B, j_B, m_B} V^*_{k\mu_B, j_B, m_B} \right). \tag{A2}$$

The EFA occupancies to be used in the density matrix operator are in this case

$$f_\mu = \begin{cases} \frac{1}{2j_B+1} & \mu = \mu_B, j_B, m_B \quad m_B = -j_B, \ldots, j_B \\ 0 & \text{otherwise,} \end{cases} \tag{A3}$$

where the index μ has been decomposed in the labels j_B corresponding to the total angular momentum, m_B, corresponding to the third component of the angular momentum and finally μ_B that represents the remaining quantum numbers. Once the value of the EFA occupancies are established the formalism developed in the main body of the article can be applied straightforwardly and all the formulas can be used verbatim.

APPENDIX B: VARIATIONAL PARAMETERS AND GRADIENTS

Given a reference HFB wave function $|\phi\rangle$ the most general HFB wave function $|\phi(\mathbb{Z})\rangle$, not orthogonal to it, is given by $|\phi(\mathbb{Z})\rangle = \exp(i\hat{Z})|\phi\rangle$, where $\hat{Z}$ is a Hermitian (to preserve the unitarity of the transformation) one-body operator $\hat{Z} = \frac{1}{2}\sum_{\mu\nu}\mathbb{Z}_{\mu\nu}\alpha^+_\mu\alpha_\nu$ that is written in terms of the generalized quasiparticle operators $\alpha_\mu = (\beta_1, \ldots, \beta_N, \beta^+_1, \ldots, \beta^+_N)$, its Hermitian conjugate α^+_μ, and the bipartite Hermitian matrix

$$\mathbb{Z} = \begin{pmatrix} Z^{11} & Z^{20} \\ -Z^{20*} & -Z^{11*} \end{pmatrix} \tag{B1}$$

that parametrizes the Bogoliubov transformation. Not all the $2\times(2N)^2$ parameters of this matrix are independent as the matrix Z^{11}_{mn} has to be a Hermitian matrix with N^2 free parameters, the complex numbers Z^{11}_{mn} with $m > n$ plus real Z^{11}_{mm}, i.e., $N^2 = 2\times[N(N-1)/2] + N$, whereas Z^{20} is a complex skew-symmetric matrix with $N^2 - N$ free parameters, the complex numbers Z^{20}_{mn} with $m > n$, i.e., $N^2 - N = 2\times[N(N-1)/2]$. As customary we will consider Z^{11} and Z^{11*} as independent parameters instead of the real and imaginary parts of Z^{11} and will apply the same consideration to Z^{20}. As a consequence, the variational parameters of the Bogoliubov transformation are Z^{11}_{mn} and Z^{11*}_{mn} with $m > n$, the real parameters Z^{11}_{mm} and finally Z^{20}_{mn} and Z^{20*}_{mn} with $m > n$. The variational parameters can be handled in a compact notation by introducing the vector z_ρ of dimension $2N^2 - N$

$$z_\rho = \begin{cases} Z^{11}_{mn} & m > n \\ Z^{11}_{mm} & \\ Z^{11*}_{mn} & m > n \\ Z^{20}_{mn} & m > n \\ Z^{20*}_{mn} & m > n \end{cases} \tag{B2}$$

As obtained in the body of the article, the variation of the mean value of an observable can be written as

$$\delta a = \tfrac{i}{2}\mathrm{Tr}_2\,[\mathbb{O}\mathbb{Z}] + O(\mathbb{Z}^2) \tag{B3}$$

where $\mathbb{O} = [\mathbb{R}, \mathbb{A}]$. Taking the most general form of the bipartite matrix

$$\mathbb{O} = \begin{pmatrix} O^{11} & O^{12} \\ O^{21} & O^{22} \end{pmatrix} \tag{B4}$$

a little algebra gives δa as a function of the variational parameters

$$\begin{aligned}\delta a = \frac{i}{2}\Bigg[&\sum_{m>n}(O^{11}_{nm} - O^{22}_{mn})Z^{11}_{mn} + (O^{11}_{mn} - O^{22}_{nm})Z^{11*}_{mn} \\ &+ (O^{21}_{nm} - O^{21}_{mn})Z^{20}_{mn} + (O^{12}_{mn} - O^{12}_{nm})Z^{20*}_{mn} \\ &+ \sum_m (O^{11}_{mm} - O^{22}_{mm})Z^{11}_{mm}\Bigg].\end{aligned} \tag{B5}$$

Taking now into account the expression of $\mathbb{O}$ and the fact that $\mathbb{A}$ is the quasiparticle representation of the operator given by

$$\mathbb{A} = \begin{pmatrix} A^{11} & A^{20} \\ -A^{20*} & -A^{11*} \end{pmatrix}, \tag{B6}$$

where A^{20} is a skew-symmetric and A^{11} is a Hermitian matrix if the operator is Hermitian (as it should be for any observable!) we obtain

$$\begin{aligned}\delta a = i\sum_{m>n} &A^{11}_{nm}(f_n - f_m)Z^{11}_{mn} \\ &- A^{20*}_{nm}(1 - f_n - f_m)Z^{20}_{mn} + \text{c.c.}\end{aligned} \tag{B7}$$

This expression can be written in a compact way $\delta a = \sum_\rho z_\rho (g_a)_\rho$ by introducing the vector $(g_a)_\rho$ that is the gradient of the mean value a with respect to the variational parameters

$$(g_a)_\rho = \begin{cases} iA^{11}_{nm}(f_n - f_m) & m > n \\ 0 & m = m \\ -iA^{11*}_{nm}(f_n - f_m) & m > n\,. \\ -iA^{20*}_{nm}(1 - f_n - f_m) & m > n \\ iA^{20}_{nm}(1 - f_n - f_m) & m > n \end{cases} \tag{B8}$$

Finally, it is important to point out that the requirement $(g_a)_\rho = 0$ is equivalent to $[\mathbb{R}, \mathbb{A}] = 0$, a fact that is used in the derivation of the EFA-HFB equation.

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