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Ground-state properties of even and odd Magnesium isotopes in a symmetry-conserving approach

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A B S T R A C T

We present a self-consistent theory for odd nuclei with exact blocking and particle number and angular momentum projection. The demanding treatment of the pairing correlations in a variation-after-projection approach as well as the explicit consideration of the triaxial deformation parameters in a projection after variation method, together with the use of the finite-range density-dependent Gogny force, provides an excellent tool for the description of odd–even and even–even nuclei. We apply the theory to the Magnesium isotopic chain and obtain an outstanding description of the ground-state properties, in particular binding energies, odd–even mass differences, mass radii and electromagnetic moments among others.

In the last years there has been an important development in the description of even–even nuclei with effective interactions, in particular with the Skyrme, Gogny and relativistic [1–3] ones. The breakthrough has been possible by means of the beyond-mean-field theories (BMFT), namely by the recovery of the symmetries broken in the mean-field approach (MFA) and by the explicit consideration of large-amplitude fluctuations around the most probable mean-field values. The shape parameters (β, γ) [4–6] (and pairing gaps [7–9]) were used as coordinates in the framework of the generator-coordinate method (GCM) and the particle-number (PN) and angular-momentum (AM) symmetries were recovered by means of projectors. These developments are called symmetry-conserving configuration mixing (SCCM) approaches and have been applied to even–even nuclei. Methods based on the Bohr collective Hamiltonian have also made large progress lately [10–12].

Odd nuclei, on the other hand, are far more complicated to deal with. Even at the mean-field level like in the Hartree–Fock–Bogoliubov (HFB) or BCS theories, odd nuclei are numerically cumbersome and to calculate ground states one must try several spins, parity, etc. Furthermore, the blocked structure of the wave function entail the breaking of the time-reversal symmetry and triaxial calculations must be performed. The SCCM developments have taken place for even–even nuclei and it seems natural to extend these approaches to odd–even and odd–odd nuclei. As a matter of fact angular-momentum projected calculations for odd-A nuclei started long ago, though they have been mostly performed on HF or HFB states in small valence spaces [13–17]. More recently a GCM mixing based on parity and AM-projected Slater determinants in a model space of antisymmetrized Gaussian wave packets has been carried out in the frameworks of fermionic [18] and antisymmetrized [19,20] molecular dynamics. In the latter calculations, however, the pairing correlations are not treated properly. A first extension of BMFT from even to odd nuclei with the Skyrme force has been done recently in Ref. [21].

The purpose of this Letter is to report on the first systematic description of the odd and even nuclei of an isotopic chain in a symmetry-conserving approach with the Gogny force in a BMFT considering the (β, γ) degrees of freedom explicitly and dealing optimally with the pairing correlations. Our approach considers exact triaxial self-consistent blocking and exact particle number and angular momentum conservation. As an illustration of our approach we have chosen the Magnesium isotopic chain for which there is abundant experimental data. Basic properties like odd–even mass differences, magnetic and quadrupole moments as well as mass radii, among others, are investigated.

Our starting approach is the HFB theory [22]. As a mean-field approximation the HFB wave function $|\phi\rangle$ is a product of quasiparticles α_ρ defined by the general Bogoliubov transformation

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$$\alpha^\dagger_\rho = \sum_\mu U_{\mu\rho} c^\dagger_\mu + V_{\mu\rho} c_\mu, \tag{1}$$

where $c^\dagger_\mu, c_\mu$ are the particle-creation and -annihilation operators in the reference basis, in our case the Harmonic Oscillator one. U and V are the Bogoliubov matrices to be determined by the Ritz variational principle.

In our approach we have imposed three discrete self-consistent symmetries on our basis states $\{c^\dagger_\mu, c_\mu\}$: spatial parity, $\hat{P}$, simplex, $\Pi_1 = \hat{P} e^{-i\pi J_x}$ and the $\Pi_2\mathcal{T}$ symmetry, with $\Pi_2 = \hat{P} e^{-i\pi J_y}$ and $\mathcal{T}$ the time reversal operator. The first two symmetries provide good parity and simplex quantum numbers and the third allows to use only real quantities. The simplex symmetry furthermore allows to characterize the blocking structure of odd and even nuclei [23,24]. Our basis is symmetrized in such a way that

$$\Pi_1 c^\dagger_k \Pi^\dagger_1 = +i c^\dagger_k, \quad \Pi_1 c^\dagger_{\bar{k}} \Pi^\dagger_1 = -i c^\dagger_{\bar{k}}, \tag{2}$$

with $k = 1, ..., M$ and $2M$ the dimension of the configuration space. We use Latin indices to distinguish the levels according to their simplex, $\{k, l, m\}$ for simplex $+i$ and $\{\bar{k}, \bar{l}, \bar{m}\}$ for simplex $-i$. The Greek indices μ, ρ, on the other hand, do not distinguish simplex and run therefore over the whole configuration space. If we further assume that the intrinsic wave function is an eigenstate of the simplex operator, then, for a paired even–even nucleus half of the quasiparticle operators $\alpha^\dagger_\mu$, have simplex $+i$ and the other half have simplex $-i$, i.e., Eq. (1) separates in two blocks:

$$\alpha^\dagger_m = \sum_{k=1}^{M} U^+_{km} c^\dagger_k + V^+_{km} c_{\bar{k}},$$
$$\alpha^\dagger_{\bar{m}} = \sum_{k=1}^{M} U^-_{km} c^\dagger_{\bar{k}} + V^-_{km} c_k, \tag{3}$$

with $m = 1, ..., M$ in an obvious notation.

The wave function of the ground state of an even–even nucleus is given by[1]

$$|\phi\rangle = \prod_{\mu=1}^{2M} \alpha_\mu |-\rangle, \tag{4}$$

with $|-\rangle$ the particle vacuum. The quasiparticle vacuum $|\phi\rangle$ is obviously defined by

$$\alpha_\mu |\phi\rangle = 0, \;\; \mu = 1, ..., 2M. \tag{5}$$

The ground state of an even–even nucleus has simplex +1. The quasiparticle excitations

$$|\tilde{\phi}\rangle = \alpha^\dagger_{\rho_1} |\phi\rangle \tag{6}$$

correspond to odd–even nuclei. They can be written as vacuum to the quasiparticle operators $\tilde{\alpha}_\rho$,

$$\tilde{\alpha}_\rho |\tilde{\phi}\rangle = 0, \;\; \rho = 1, ..., 2M. \tag{7}$$

The $2M$ operators $\{\tilde{\alpha}^\dagger_\rho\}$ are obtained from the set $\{\alpha^\dagger_\mu\}$ by replacing the creation operator $\alpha^\dagger_{\rho_1}$ by the annihilation operator α_{ρ_1}, the other $2M-1$ operators remain unchanged. The simplex of the state $|\tilde{\phi}\rangle$ is given by $\Pi_1|\tilde{\phi}\rangle = i^n|\tilde{\phi}\rangle$, where we have introduced the blocking number n. It is $n = 1$ if $\alpha^\dagger_{\rho_1}$ has simplex $+i$ and $n = -1$ if $\alpha^\dagger_{\rho_1}$ has simplex $-i$. The unblocked wave function $|\phi\rangle$ is vacuum to M operators with simplex $+i$ and to M with simplex $-i$. The blocked wave function $|\tilde{\phi}\rangle$ is vacuum to $M_+ = M - n$ operators $\tilde{\alpha}^\dagger_m$ with simplex $+i$ and to $M_- = M + n$ operators $\tilde{\alpha}^\dagger_{\bar{m}}$ with simplex $-i$.

$$\tilde{\alpha}^\dagger_m = \sum_{k=1}^{M} \tilde{U}^+_{km} c^\dagger_k + \tilde{V}^+_{km} c_{\bar{k}}, \quad m = 1, ..., M_+,$$
$$\tilde{\alpha}^\dagger_{\bar{m}} = \sum_{k=1}^{M} \tilde{U}^-_{km} c^\dagger_{\bar{k}} + \tilde{V}^-_{km} c_k, \quad m = 1, ..., M_-. \tag{8}$$

The matrices $(\tilde{U}^+, \tilde{V}^+, \tilde{U}^-, \tilde{V}^-)$ are rectangular with M rows and M_+ or M_- columns and according to the transformation $\alpha^\dagger_{\rho_1} \to \alpha_{\rho_1}$, they are obtained, from the $M \times M$ squared matrices (U^+, V^+, U^-, V^-) from Eq. (3) by the corresponding columns exchange.

Though the state $|\tilde{\phi}\rangle$ has the right blocking structure, since the Bogoliubov transformation mixes creator and annihilator operators and states with different angular momenta, $|\tilde{\phi}\rangle$ is not an eigenstate of the PN or the AM operators. As with even–even nuclei, to recover the particle-number symmetry one has to project to the right quantum numbers, see [22]. The *easiest* way would be to minimize the HFB energy, i.e., determine $(\tilde{U}, \tilde{V})$ and then perform the projections, i.e. the so-called projection-after-variation (PAV). The *optimal* way is to determine $(\tilde{U}, \tilde{V})$ directly from the minimization of the projected energy, i.e., the variation-after-projection (VAP) method. From even–even nuclei one knows that PN-VAP is feasible while AM-VAP is very CPU-time consuming. The approach of solving the PN-VAP variational equation to find the self-consistent minimum and afterwards to perform an AM-PAV is not very good because the AMP is not able to exploit any degree of freedom of the HFB transformation and self-consistency with respect to the AMP is not guarantied. An intermediate way is to perform an approximate AM-VAP approach by solving the variational PN-VAP equation for a large set of relevant physical situations as to cover the sensitive degrees of freedom. Afterwards an AM-PAV to this set of wave functions will determine the absolute minimum among these states for different angular momenta. Usually it is believed that the strongest energy dependence of the nuclear interaction is related to the deformation parameters (β, γ) and we will consider them as the additional degrees of freedom. Notice that this method guarantees, at least, AM-VAP self-consistency with respect to these relevant quantities. Therefore, in order to obtain a grid of wave functions we solve the PN-VAP constrained equations

$$E'[\tilde{\phi}] = \frac{\langle\tilde{\phi}|\hat{H}\hat{P}^N|\tilde{\phi}\rangle}{\langle\tilde{\phi}|\hat{P}^N|\tilde{\phi}\rangle} - \langle\tilde{\phi}|\lambda_{q_0}\hat{Q}_{20} + \lambda_{q_2}\hat{Q}_{22}|\tilde{\phi}\rangle, \tag{9}$$

with the Lagrange multiplier λ_{q_0} and λ_{q_2} being determined by the constraints

$$\langle\tilde{\phi}|\hat{Q}_{20}|\tilde{\phi}\rangle = q_0, \quad \langle\tilde{\phi}|\hat{Q}_{22}|\tilde{\phi}\rangle = q_2. \tag{10}$$

The relation between (β, γ) and (q_0, q_2) is given by $\beta = \sqrt{20\pi(q_0^2 + 2q_2^2)}/3r_0^2 A^{5/3}$, $\gamma = \arctan(\sqrt{2}q_2/q_0)$ with $r_0 = 1.2$ fm and A the mass number.

In this work we are interested in the odd–even Magnesium isotopes. We therefore consider wave functions of the form

$$|\tilde{\phi}^\pi\rangle = \alpha^\dagger_{\rho_1} \prod_{\mu=1}^{2M} \alpha_\mu |-\rangle. \tag{11}$$

According to the isospin and parity we have four blocking channels: protons (neutrons) of positive or negative parity. Since Magnesium isotopes have $Z = 12$, we restrict ourselves to the neutron

[1] The quasiparticle operators that annihilate trivially the particle vacuum are to be omitted from the product.