GROUND STATE OF NUCLEI
IN THE BARIUM REGION WITHIN
THE HIGHLY TRUNCATED DIAGONALIZATION APPROACH

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Abstract: The ground state of some barium isotopes has been investigated in the framework of the parity-symmetry projection of the Highly Truncated Diagonalization Approach (HTDA), which is suited to treat the correlations in an explicitly particle-number conserving microscopic approach. A Skyrme energy-density function using the SkM∗ interactions has been considered to treat the particle-hole channel, whereas a density-independent δ force has been adopted for the residual interaction. The obtained results are compared with the previous calculations using the Woods-Saxon potentials.

Keywords: HTDA, parity-symmetry projection, octupole deformation

1   Introduction

It is well known that the nuclear structure of doubly-closed shell nuclei is well described by the mean-field approximations. However, many correlations (e.g. pairing correlations) must be taken into account when the nuclear system is far from the stability on the nuclear chart. One simple and useful way to deal with this problem is to use the Bardeen-Cooper-Schrieffer (BCS) approximation. The latter was firstly designed for the system of about 10^{23} fermions in solid-states physics. Unfortunately, this approximation breaks the particle-number symmetry in the nuclear finite systems. The Highly Truncated Diagonalization Approach (HTDA) has been developed to overcome this difficulty [1]. This approximation produces the realistic correlated wave functions in an approach which explicitly conserves the particle number and does not violate the Pauli principle. It consists in performing intrinsic shell-model like calculations using single-particle states deduced from a mean-field potential. The nucleon-nucleon effective interactions (Skyrme-type interactions [2]) have been used to define the mean field while the zero-range δ force has been used to simulate the residual interactions. Recently a parity-symmetry projection of correlated

microscopic solutions for HTDA approach has been extensively used to study the octupole deformation for [240]Pu (at second fission barrier region) [3] and [194]Pb (normal deformed and superdeformed states) [4] where the strong octupole correlations can arise when nucleons near the Fermi surface occupy states of opposite parity with orbital and total angular momenta differing by $3\hbar$.

In this work, we extend the latter calculations for the barium isotopes region which have been successfully performed by using the semi-microscopic approach [5]. The paper is organized as follows. In Sec. 2, we present the formalism of the parity-symmetry projection for the HTDA solutions. The analysis of the numerical results is presented in Sec. 3. The main conclusions of our study are drawn in the last section.

2   Theoretical formalism

The HTDA approach solves the Schrödinger equation in a highly truncated space. This space contains the excitations beyond 1p–1h excitations. Hence, the HTDA wave function is a superposition of Slater determinants built from np-nh excitations on the ground-state obtained from a converged Hartree-Fock+BCS (HF+BCS) calculations.

The Hamiltonian of the many-body nuclear system reads

$$H = \sum_{ik} t_{ik} \hat{a}_i^\dagger \hat{a}_i + \frac{1}{4} \sum_{ikxy} \tilde{v}_{ikxy} \hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_x \hat{a}_y \ . \tag{1}$$

We define the independent quasiparticles Hamiltonian

$$\hat{H} = E_{HF} + \hat{H}_{IQP} + \hat{V}_{res} \ , \tag{2}$$

with

$$E_{HF} = \langle \phi_0 | \hat{H} | \phi_0 \rangle = \langle \phi_0 | \hat{H}_{HF} | \phi_0 \rangle \ , \tag{3}$$

and

$$\hat{H}_{IQP} = \sum_i \zeta_i \eta_i^\dagger \eta_i \ , \tag{4}$$

where

$\eta_i^\dagger$ is the creation operator $a_i^\dagger$ (unoccupied states),

η_i is the annihilation operator a_i (occupied states),

$\zeta_i = e_p^i$ or $\zeta_i = -e_t^i$; e^i are the energy of single-particle states,

and the residual interaction $\hat{V}_{res}$

$$\hat{V}_{res} = \hat{V} - \hat{V}_{HF} = \left(\hat{K} + \hat{V} \right) - \left(\hat{K} + \hat{V}_{HF} \right) = \hat{H} - \hat{H}_{HF} \ . \tag{5}$$

The HTDA Hamiltonian could be re-written as follows

$$\hat{H} = \hat{H}_{MF} + \hat{V}_{res}.$$ (6)

The total energy E_{HTDA} is defined as the average value of $\hat{H}$ for the correlated state $|\Psi\rangle$

$$\langle\Psi|\hat{H}|\Psi\rangle = E_{HTDA},$$ (7)

where $|\Psi\rangle$ is the eigenvector of lowest energy. It conserves the particle-number symmetry

$$|\Psi\rangle = \sum_i \chi_i |\Phi_i\rangle = \chi_0 |\Phi_0\rangle + \sum_{1p1h} \chi_1 |\Phi_1\rangle + \sum_{2p2h} \chi_2 |\Phi_2\rangle + \cdots,$$ (8)

where the real coefficient $|\chi_i\rangle$ ensures the normalization of the correlated state $|\Psi\rangle$

$$\sum_i \chi_i^2 = 1.$$ (9)

Finally, the projected energy reads

$$E_p = \langle\Psi_p|H|\Psi_p\rangle = \frac{\langle\Psi|\hat{H}|\Psi\rangle + p\langle\Psi|\hat{H}|\tilde{\Psi}\rangle + p\langle\tilde{\Psi}|\hat{H}|\Psi\rangle + \langle\tilde{\Psi}|\hat{H}|\tilde{\Psi}\rangle}{2(1 + p\langle\Psi|\tilde{\Psi}\rangle)}.$$ (10)

where $|\tilde{\Psi}\rangle = \Pi|\Psi\rangle$, Π is the parity operator and $p = \pm 1$.

Numerical aspects

The numerical procedure could be divided into 3 steps. The parity-asymmetry HF + BCS calculations have been performed to obtain the ground state and the mean-field potential. The effective phenomenological Skyrme SkM* interaction has been chosen. The intensity of the seniority force is fixed for ^{148}Ba and for the remaining isotopes. The strengths g_q (where q is a charge state index) of the seniority force are $g_q = \dfrac{G_0^{(q)}}{11 + N_q}$ (MeV) with $G_0^{(n)} = 15.21$ (MeV) and $G_0^{(p)} = 12.95$ (MeV) and where N_q is the nucleon number. The cut-off energy window around the Fermi level is 6 MeV. For the HTDA calculations, the many-body basis comprises only one-pair-transfer states and the ground state. A valence space of 6 MeV around the Fermi level has been introduced with a diffusivity parameter of $\mu = 0.2$ MeV. The intensities of δ interaction are fixed at $\delta_n = -407.5$ MeV.fm^3 and $\delta_p = -228.5$ MeV.fm^3. These strengths have been fitted to reproduce the Fermi-surface diffuseness of the corresponding HF + BCS calculations for the same isotopes. Then, a projection after variation (PAV) has been performed to get the parity-projected HTDA ground state energy at a fixed quadrupole and octupole deformation.

Numerical integrations have made use of a Gauss–Laguerre and Gauss–Hermite approximations scheme with 16 and 50 mesh points, respectively.

3   Results

The HTDA solutions have been projected on the good parity state for each value of octupole moments Q_{30}. The obtained results (see Fig. 1) show that the positive-parity curve is always below the un-projected HTDA curve whereas the negative-parity curve is always above it. At zero octupole deformation, the un-projected HTDA solution and the projection on positive-parity states have the same energy. The projection energy on the negative-parity state is not defined. At large octupole moment, the three curves merge.
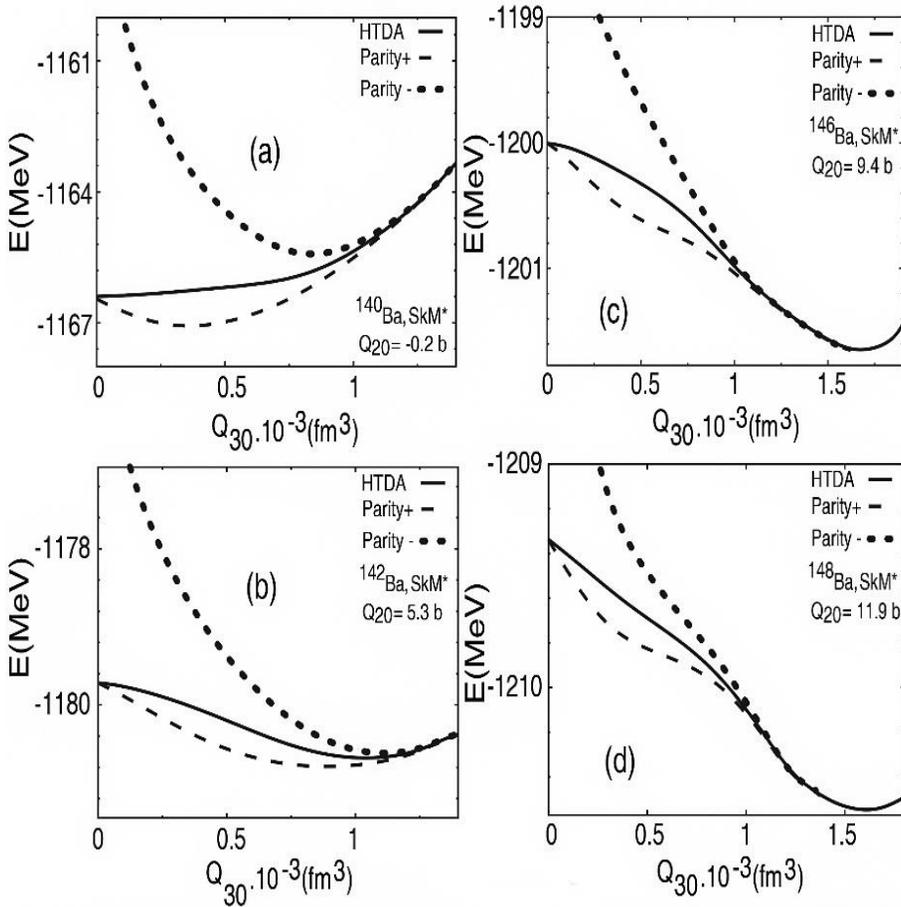
Fig. 1. Octupole deformation properties of the ground state of some Barium isotopes. The solid, dash and dotted curves correspond to asymmetrical un-projected HTDA solutions, the positive-parity projection states energies and negative-parity ones, respectively

Different behaviors could be observed from the intrinsic energy curve $E(Q_{30}, Q_{20}^{eq})$ and positive-parity curve $E^+(Q_{30}, Q_{20}^{eq})$. One has an equilibrium intrinsic solution which is symmetrical ($Q_{30} = 0$) in the axial octupole mode so that the projection is not able to create the positive-parity minimum for a finite value of Q_{30}. Such a projection reduces the stiffness with respect to the axial octupole mode which possibly creates the dynamical instability. In contrast, if the symmetrical

equilibrium solution has a sufficiently small deformation, the parity-projection could create a minimum at a non-vanishing value of the octupole moment. This situation was also observed in the calculations of intrinsic super-deformed state of [194]Pb [4]. A static instability away from symmetry, (which was not available with the intrinsic solutions), appears. For the situation where the intrinsic equilibrium solution is not symmetrical but corresponds to a not-too-large absolute value of $|Q_{30}|$, the positive-parity projection emphasizes the instability already present at the intrinsic level, yielding possible the corresponding equilibrium $|Q_{30}|$ values. Beyond a certain critical value of $|Q_{30}|$, the projection does not have any effects.

4   Conclusion

We have studied the octupole deformation properties of nuclei in the barium region by using the microscopic self-consistent HTDA approach. Four even-even neutron rich nuclei are considered. The obtained results confirm the calculations of W. Nazarewicz *et al.* which predicted a significant octupole deformation in the barium region. Note that the latter calculations were performed by using the Woods-Saxon potentials.

Acknowledgments

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