BEYOND MEAN-FIELD BOSON–FERMION DESCRIPTION OF ODD NUCLEI*

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We develop a novel theoretical method for calculating spectroscopic properties of those nuclei with odd number of nucleons that is based on the nuclear density functional theory and the particle–boson coupling scheme. A self-consistent mean-field calculation based on the DFT is performed to provide microscopic inputs to build the Hamiltonian of the interacting boson–fermion systems, which gives excitation spectra and transition rates of odd-mass nuclei. The method is successfully applied to identify the quantum shape phase transitions and the role of octupole correlations in odd-mass nuclei, and is further extended to odd–odd nuclear systems.

1. Introduction

Microscopic description of the low-lying states in those nuclei with odd numbers of nucleons is one of the challenging problems in nuclear structure physics. Primary reason is that, as compare to the even–even nuclei where nucleons are coupled pairwise and they determine to a large extent the low-lying nuclear structure, in the odd-A and odd–odd nuclei, one has to consider both the single-particle (unpaired nucleon) and collective degrees of freedom on the same footing.

Here, we specially focus on a recently developed theoretical method [1] for calculating spectroscopic properties of the odd nuclei that is based on the nuclear energy density functional theory (DFT) [2, 3] and the particle–(boson-) core coupling scheme. In this framework, the constrained self-consistent mean-field (SCMF) calculation based on the nuclear DFT is performed to compute potential energy surface (PES) in the relevant collective coordinates for the even–even core nucleus, and the spherical single-particle energies and occupation probabilities of odd particles. These quantities are used as a microscopical input to build the interacting boson–fermion model (IBFM) [4]

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Hamiltonian. At the cost of having to determine a few coupling constants for the boson–fermion interaction empirically, this method has allowed for a detailed, systematic, and computationally feasible description of spectroscopy of those nuclei with odd nucleon numbers. Here, the recent applications of this method are highlighted, *i.e.*, the effect of an odd particle on the nature of quantum shape phase transitions [5], the octupole correlations in odd-A neutron-rich nuclei [6], and the extension of the method to odd–odd nuclei [7].

2. Theoretical framework

The IBFM for a given odd-A system consists of the interacting boson model (IBM) [8] Hamiltonian $\hat{H}_B$ for the even–even core nucleus, single-particle (either neutron $\rho = \nu$ or proton π) Hamiltonian $\hat{H}_F^\rho$, and the interaction $\hat{H}_{BF}^\rho$ between the odd neutron (proton) and the boson core

$$\hat{H}_{\mathrm{IBFM}} = \hat{H}_B + \hat{H}_F^\nu + \hat{H}_F^\pi + \hat{H}_{BF}^\nu + \hat{H}_{BF}^\pi \,. \tag{1}$$

The IBM Hamiltonian is typically of the form of

$$\hat{H}_B = \epsilon(\hat{n}_{d_\nu} + \hat{n}_{d_\pi}) + \kappa \hat{Q}_\nu^{\chi_\nu} \cdot \hat{Q}_\pi^{\chi_\pi} + \kappa' \hat{L} \cdot \hat{L} \,, \tag{2}$$

where the first and second terms are the d-boson number operator and quadrupole–quadrupole interaction between the neutron and proton bosons, respectively, and the third term is the rotational term. The strength parameters ϵ, κ, χ_ν, and χ_π are determined by following the procedure of Ref. [9]: the total mean-field energy obtained from the EDF calculation at each (β, γ) deformation, *i.e.*, $E_{\mathrm{EDF}}(\beta, \gamma)$, is equated to the expectation value of the IBM Hamiltonian in the intrinsic wave function for the boson system at the corresponding configuration, $E_{\mathrm{IBM}}(\beta, \gamma)$. Only the parameter κ' for the rotational term is determined separately from the other parameters, in such a way that the SCMF cranking moment of inertia at the equilibrium minimum, be equal to the IBM counterpart [10].

Additional microscopic inputs from the DFT are the single-particle energies ϵ_{j_ρ} (for $\hat{H}_F^\rho$) and occupation probabilities $v_{j_\rho}^2$ (for $\hat{H}_{BF}^\rho$) for the odd nucleon at the orbital j_ρ. These quantities are obtained from the SCMF calculation at zero deformation and the particle number of either neutrons or protons constrained to odd number [1]. The boson–fermion interaction $\hat{H}_{BF}^\rho$ is composed of the three essential terms, *i.e.*, dynamical quadrupole, exchange, and monopole terms [4]. Hence, there are three strength parameters for $\hat{H}_{BF}^\rho$ for odd-N or odd-Z system. They are the only phenomenological parameters and are fixed so as to reasonably reproduce the experimental low-lying levels for each odd-A nucleus. For the detailed account of the whole procedure, the reader is referred to Ref. [1].

3. Signatures of quantum phase transitions in odd-*A* nuclei

Even–even Sm isotopes are a well-known example where the phase transition from spherical vibrational to deformed rotational states is suggested to occur by addition/subtraction of only a few nucleons [11]. The triaxial quadrupole (β, γ) PESs for a set of Sm isotopes are depicted in Fig. 1, which are obtained by the constrained relativistic Hartree–Bogoliubov (RHB) method [3] with the DD-PC1 EDF [12]. One sees near-spherical minimum
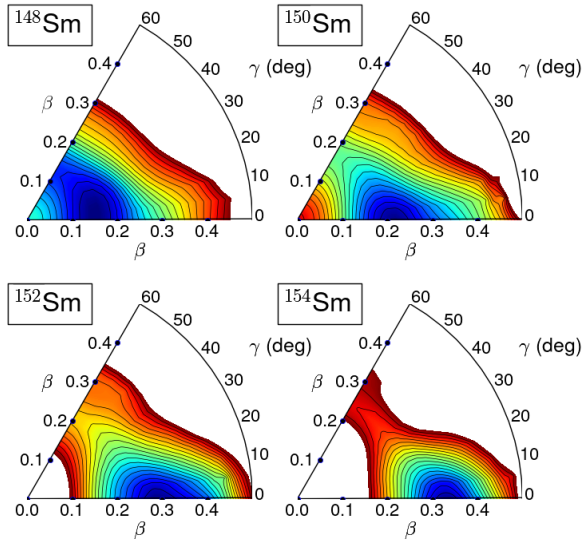

Fig. 1. Potential energy surfaces for the Sm isotopes computed with the constrained RHB method [3] using the DD-PC1 EDF [12]. Energy difference between neighboring contours is 250 keV.

at ^{148}Sm, which is typical of the vibrational nucleus. For ^{150,152}Sm, the minimum becomes soft both in β and γ deformations, and these nuclei are supposed to be the transitional nuclei. A distinct prolate minimum is seen in ^{154}Sm, indicating that the deformed rotational structure appears. Figure 2 depicts the excitation spectra for the low-lying states of the odd-*A* $_{63}$Eu and $_{62}$Sm isotopes resulting from the IBFM Hamiltonian. Our calculation reproduces the experimental spectra quite nicely, even though there are only three free parameters. A signature of the nuclear structure evolution is identified in the change of the ground-state spin at $N \approx 90$. Around this neutron number, the corresponding even–even system undergoes a rapid shape transition. We have further computed several mean-field and spectroscopic properties for the odd-*A* systems, that can be considered order parameters for the phase transition: $\overline{\beta}$ (average β deformation), $\Delta\beta$ (variance of β), $\overline{B(\text{E2})}$ (average $B(\text{E2})$ value between the band-head of a given
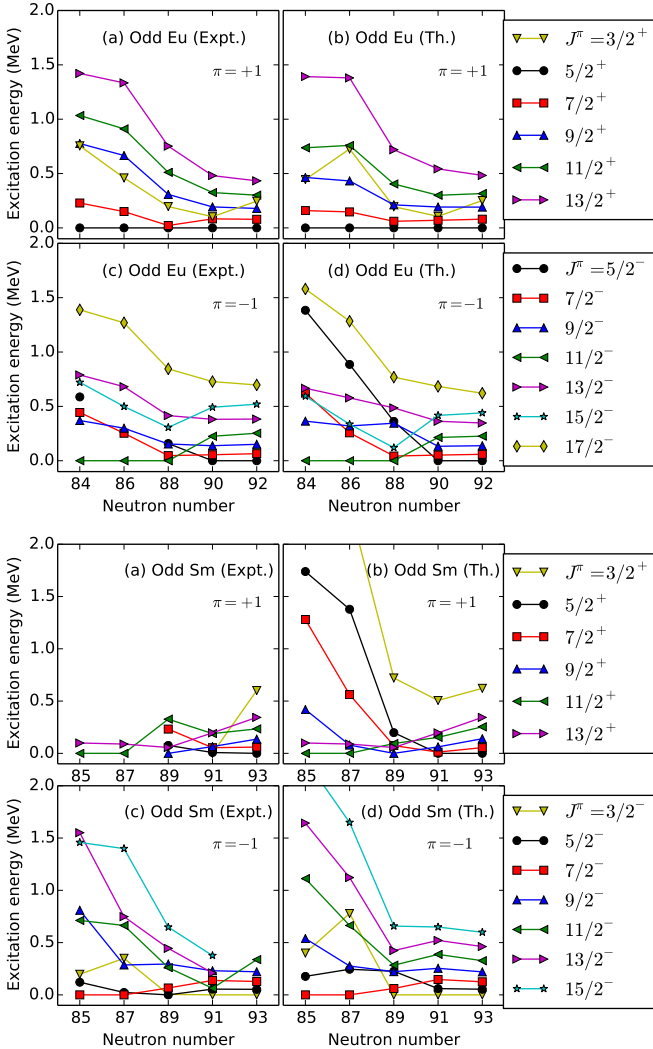
Fig. 2. Excitation spectra for the low-lying positive- ($\pi = +1$) and negative-parity ($\pi = -1$) states for the odd-A Eu and Sm isotopes.

band with spin J_0 and the lowest five states with $J_0 + \Delta J$, with $\Delta = 1, 2$), $E(J_1, J_0)$ (energy of the first excited state J_1 in a given band with respect to the band-head J_0), and $R(J_2, J_1, J_0)$ (energy ratio of the second J_2 to first J_1 excited states with respect to the band-head J_0 in a given band). Figure 3 depicts the differentials of these quantities between the neighboring isotopes, $\delta\mathcal{O} = \sum_i^n |\mathcal{O}_{i,A} - \mathcal{O}_{i,(A-2)}|/n$, which is averaged over the lowest $n(\approx 5)$ bands. One realizes, in most of these calculated quantities, a kink around $N \approx 90$ that can be considered a signature of phase transition.
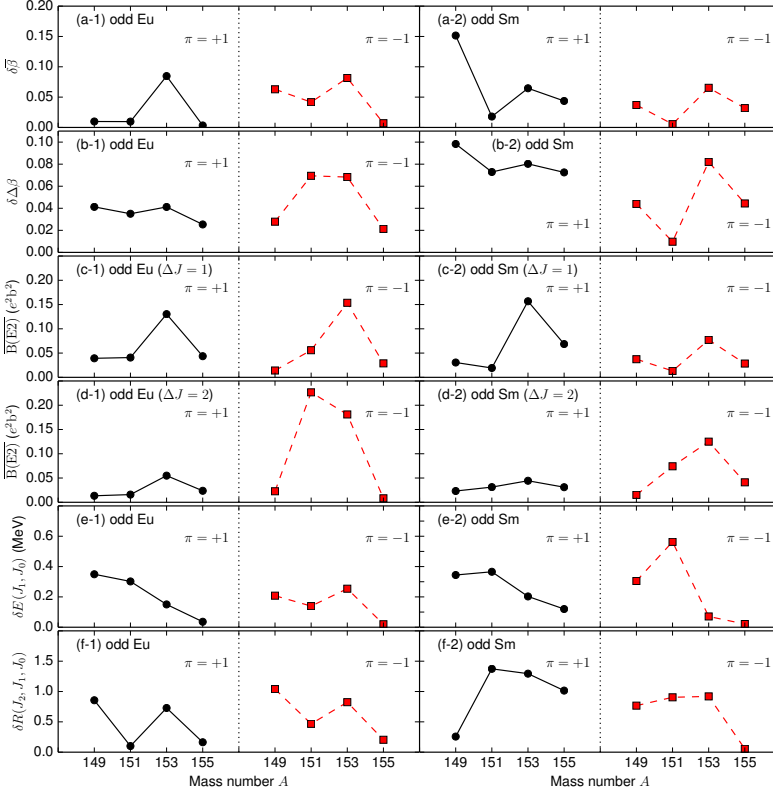
Fig. 3. Differentials of several calculated mean-field and spectroscopic properties of the odd-A Eu and Sm for both parities.

4. Octupole correlations in neutron-rich odd-A nuclei

Octupole degree of freedom is expected to play an important role in several specific mass regions. Figure 4 depicts the axially-symmetric quadrupole β_{20}–octupole β_{30} PESs for $^{140-150}$Ba, where the octupole correlation is suggested to be particularly relevant. The PESs indicate pronounced octupole deformation with the non-zero β_{30} value for $^{144-150}$Ba. For studying the octupole collective states, we included the negative-parity f bosons with $L^{\pi} = 3^{-}$ in the IBM space, in addition to the positive-parity s ($L^{\pi} = 0^{+}$) and d ($L^{\pi} = 2^{+}$) bosons. The sdf-IBM Hamiltonian is fixed by mapping the (β_{20}, β_{30}) SCMF PES onto the bosonic one. As for the odd-A Ba, we have implemented the f-boson degrees of freedom in the IBFM [6], and the sdf-IBFM Hamiltonian has been fixed by a similar procedure to the one in the case of sd-IBFM. The resultant sdf-IBM and sdf-IBFM spectra for even–even ^{144}Ba and odd-A ^{145}Ba are compared to the experimental counter-
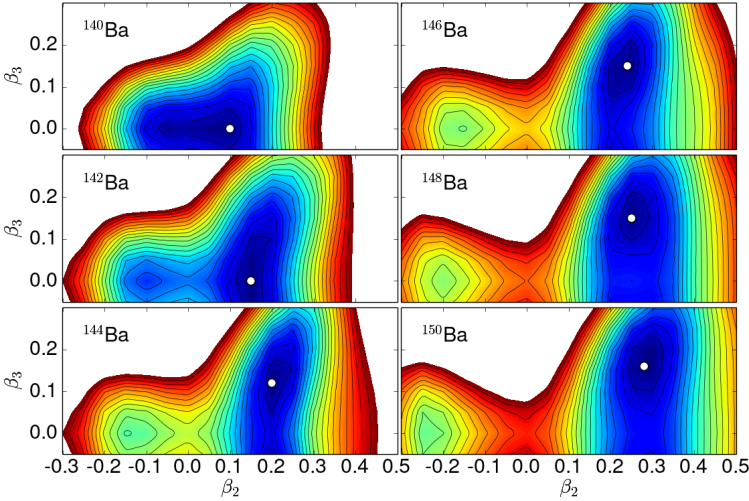
Fig. 4. Axially-symmetric (β_{20}, β_{30}) PESs for the $^{140-150}$Ba isotopes, computed with the RHB method with DD-PC1 EDF.

parts in Fig. 5. Our calculation describes very nicely the experimental data [13] for the excitation spectra and B(E3) transition rates in the even–even ^{144}Ba nucleus. For the odd-A ^{145}Ba nucleus, the band-head energies of those bands that are empirically suggested [14] to be the octupole bands (shown in thick lines in Fig. 5) are reproduced by the calculation (the corresponding theoretical bands composed of one-f-boson configuration are indicated also as thick lines in the figure). We have also predicted the B(E3) values to be approximately 20–30 W.u., for the transitions from the octupole to the ground state bands in odd-A Ba, which are comparable to the calculated $B(\text{E3}; 3_1^- \to 0_1^+) = 23$ W.u. for the even–even neighbor.
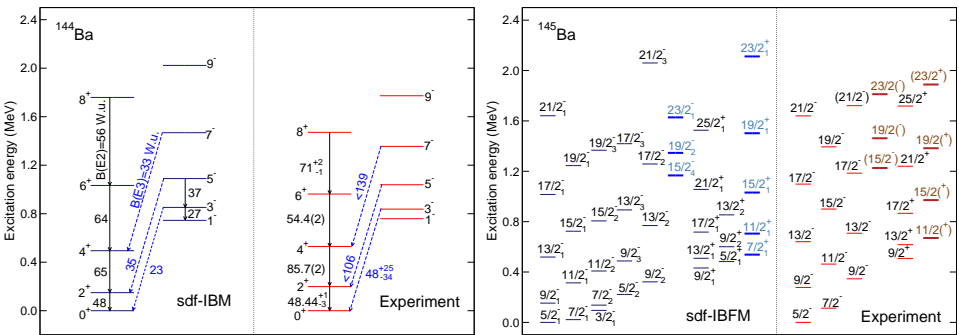

Fig. 5. Low-energy level schemes for ^{144}Ba and ^{145}Ba.

5. Odd–odd nuclei

In the cases of odd–odd systems, one single neutron and one single proton degrees of freedom are explicitly considered in the framework of the interacting boson–fermion–fermion model (IBFFM) [4]. The coupling constants of the interactions between single neutron (proton) to the boson space are fixed to reproduce low-energy levels of the neighboring odd-N (odd-Z) nucleus, using the prescription mentioned in Sec. 2. Furthermore, the residual neutron–proton interaction should be considered, and the parameters for the interaction are determined so as to reasonably reproduce the lowest-lying levels in the odd–odd nucleus [7]. As an example, we show in Fig. 6 the IBFFM spectra for the odd–odd nuclei ^{194,196}Au. Microscopic inputs have been provided by the Gogny-EDF SCMF calculation. The even–even core ^{194,196}Hg isotopes exhibit weakly deformed oblate shapes in the Gogny PESs. The description of the excitation spectra for the considered odd–odd nuclei is fairly good. Their electromagnetic properties have been also described reasonably well [7]. We also mention another relevant application of the EDF-based IBFFM calculation of Ref. [15], where we explored chiral band structure in a number of odd–odd Cs isotopes, that is mainly composed of the $(\nu h_{11/2})^{-1} \otimes \pi h_{11/2}$ neutron–proton pairs coupled to γ-soft even–even Xe cores.
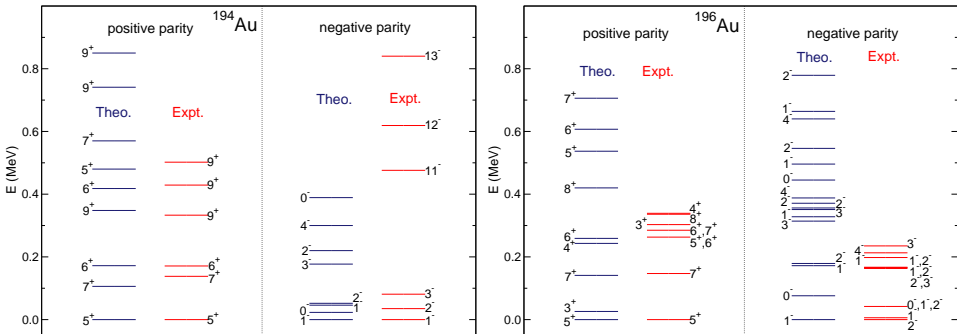

Fig. 6. Low-energy excitation spectra for the odd–odd nuclei ^{194,196}Au.

6. Conclusions

We introduced a recently developed theoretical method for calculating spectroscopic properties of those nuclei with odd nucleon numbers that is based on the nuclear DFT and the particle–boson coupling scheme. The boson-core Hamiltonian, and the spherical single-particle energies and occupation probabilities of the odd nucleons are determined from fully microscopic SCMF calculations, whereas there are only a few free parameters that are fixed empirically. Successful applications of the employed theoret-

ical method to study the shape QPT and octupole correlations in odd-A systems, and the structure of odd–odd nuclei (as well as other examples not covered in this contribution) indicate that the method is promising for studying spectroscopic properties of even–even, odd-A, and odd–odd nuclear systems in a systematic and computationally feasible way.

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