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Beyond-mean-field Boson-fermion Description of Odd-mass Nuclei

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Abstract: A recently developed method for calculating spectroscopic properties of medium-mass and heavy atomic nuclei with an odd number of nucleons is reviewed, that is based on the framework of nuclear energy density functional theory and the particle-core coupling scheme. The deformation energy surface of the even-even core, as well as the spherical single-particle energies and occupation probabilities of the odd particle(s), are obtained by a self-consistent mean-field calculation with the choice of the energy density functional and pairing properties. These quantities are then used as a microscopic input to build the interacting boson-fermion Hamiltonian. Only three strength parameters for the particle-core coupling are specifically adjusted to selected data for the low-lying states of a particular odd-mass nucleus. The method is illustrated in a systematic study of low-energy excitation spectra and electromagnetic transition rates of axially-deformed odd-mass Eu isotopes. Recent applications of the method, to the calculations of the signatures of shapes phase transitions in axially-deformed odd-mass nuclei, octupole correlations in neutron-rich odd-mass Ba isotopes, are discussed.

Key words: nuclear energy density functional; interacting boson-fermion model; odd-mass nuclei

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1 Introduction of BRIF

The interplay between single-particle and collective degrees of freedom plays a crucial role in atomic nuclei[1]. At low energy, in even-even nuclei, nucleons are coupled pairwise and this is manifest in low-lying rotational and vibrational collective excitations[1]. Many nuclear models have successfully been applied in studies of the structure of even-even nuclei[1–5]. The situation is, however, more complicated in nuclei with odd Z and/or N, because one has to consider unpaired fermions explicitly and treat the single-particle and collective degrees of freedom on the same level[1, 6]. Although most nuclear species have an odd Z or/and N, microscopic studies of their structure have not been pursued as extensively as in the case of even-even systems, especially for medium-heavy and heavy nuclei.

The energy density functional (EDF)[4, 7] method allows for a global description of low-energy properties of nuclei all over the chart of nuclides. Although not as common as in the even-even case, a number of calculations have been made within the EDF framework at the mean-field level for odd-mass systems. In the EDF framework, a proper description of excited states requires the inclusion of dynamical correlations associated with the restoration of broken symmetries and fluctuations via the symmetry-projected configuration mixing calculation. A significant extension of this type of calculation to odd-mass systems was made[8], by explicitly taking into account the breaking of time-reversal symmetry. Nevertheless, the practical applications of this approach to medium-heavy and heavy nuclei are computationally demanding, and so far have been limited to very light-mass systems[8–9].

Recently we have developed a novel theoretical method[10] for odd-mass nuclei, that is based on nuclear density functional theory and the particle-core coupling scheme. In this approach the even-even core is described in the framework of the interacting boson model (IBM)[3], and the particle-core coupling is modelled by the interacting boson-fermion model (IBFM)[11]. The deformation energy surface of an even-even nucleus as a function of the quadrupole shape variables (β, γ), as well as the single-particle energies and occupation probabilities of the odd nucleon, are obtained in a self-consistent mean-field calculation with a given EDF, and they determine the microscopic

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input for the parameters of the IBFM Hamiltonian. Only the strength parameters of the boson-fermion coupling terms in the IBFM Hamiltonian have to be adjusted to the data for the low-lying states in the considered odd-mass nucleus.

So far, the method has been applied to study (i) the spherical-to-axially-deformed[12–13] and (ii) spherical-to-γ-soft[14–15] shape phase transitions in odd-mass nuclei, (iii) the octupole correlations in neutron-rich Ba isotopes[16], (iv) the structure of neutron-rich Kr isotopes[17], and (v) the prolate-to-oblate shape transitions in the mass $A\approx 190$ region[18], and to address (vi) the robustness of the method by using both non-relativistic[13, 15] and relativistic[12, 14] EDFs. In this contribution, we focus on the topics (i) and (iii). The results reported here are based on the collaborations with D. Vretenar, T. Nikšić, R. Rodríguez-Guzmán, and L. M. Robledo.

In Sec. 2 the procedure to construct the IBFM Hamiltonian from the SCMF calculation is outlined. Sec. 3 presents results for spectroscopic calculations of the odd-mass Eu isotopes as a proof of the method. Sec. 4 highlights recent applications mentioned above, followed by a short summary and concluding remarks in Sec. 5.

2 Theoretical framework

The IBFM Hamiltonian for an odd-mass nucleus contains the even-even (boson) core Hamiltonian $\hat{H}_{\rm B}$, a single-particle Hamiltonian that describes the unpaired nucleon $\hat{H}_{\rm F}$, and a term that describes the interaction between bosons and fermions $\hat{H}_{\rm BF}$:

$$\hat{H}_{\rm IBFM}=\hat{H}_{\rm B}+\hat{H}_{\rm F}+\hat{H}_{\rm BF}. \tag{1}$$

For low-energy states, the dominant components in the boson space are the s (spin 0^+) and d (spin 2^+) bosons, which correspond to the correlated pairs of $J=0^+$ and 2^+ pairs of valence nucleons, respectively[19]. The number of bosons equals the number of valence (spherical open-shell) proton and neutron pairs (particle or hole pairs). For the boson Hamiltonian $\hat{H}_{\rm B}$ we employ the standard form[3]: $\hat{H}_{\rm B}=\epsilon_d\hat{n}_d+\kappa\hat{Q}\cdot\hat{Q}+\kappa'\hat{L}\cdot\hat{L}$, with the d-boson number operator $\hat{n}_d=d^\dagger\cdot\tilde{d}$, the quadrupole operator $\hat{Q}=s^\dagger\tilde{d}+d^\dagger\tilde{s}+\chi[d^\dagger\times\tilde{d}]^{(2)}$, and the angular momentum operator $\hat{L}=\sqrt{10}[d^\dagger\times\tilde{d}]^{(1)}$. ϵ_d, κ, κ' and χ are parameters that are to be determined by the SCMF calculation. The fermion Hamiltonian for a single nucleon reads $\hat{H}_{\rm F}=\sum_j\epsilon_j[a_j^\dagger\times\tilde{a}_j]^{(0)}$, with ϵ_j the single-particle energy of the spherical orbital j. For the particle-core coupling $\hat{H}_{\rm BF}$ we use the simplest form[11]:

$$\begin{aligned}\hat{H}_{\rm BF}=&\sum_{jj'}\Gamma_{jj'}\hat{Q}\cdot[a_j^\dagger\times\tilde{a}_{j'}]^{(2)}+\\&\sum_{jj'j''}\Lambda_{jj'}^{j''}:[[d^\dagger\times\tilde{a}_j]^{(j'')}\times[a_{j'}^\dagger\times\tilde{d}]^{(j'')}]^{(0)}:+\\&\sum_j A_j[a_j^\dagger\times\tilde{a}_j]^{(0)}\hat{n}_d,\end{aligned} \tag{2}$$

where the first, second, and third terms are referred to as the quadrupole, exchange, and monopole interactions, respectively. The physical meaning of each term is discussed in Ref. [10]. For the strength parameters $\Gamma_{jj'}$, $\Lambda_{jj'}^{j''}$, and A_j the following expressions[21] are employed:

$$\Gamma_{jj'}=\Gamma_0\gamma_{jj'}, \tag{3}$$

$$\Lambda_{jj'}^{j''}=-2\Lambda_0\sqrt{\frac{5}{2j''+1}}\beta_{jj''}\beta_{j'j''}, \tag{4}$$

$$A_j=-\sqrt{2j+1}A_0, \tag{5}$$

where $\gamma_{jj'}=(u_ju_{j'}-v_jv_{j'})Q_{jj'}$ and $\beta_{jj'}=(u_jv_{j'}+v_ju_{j'})Q_{jj'}$, and the matrix element of the quadrupole operator in the single-particle basis $Q_{jj'}=\langle j||Y^{(2)}||j'\rangle$. The factors u_j and v_j denote the occupation probabilities of the orbit j.

As an illustrative application of the method, we consider the case of a single nucleon coupled to an axially-deformed nuclei, *i.e.*, the low-energy spectra of the isotopes $^{147-155}$Eu. These nuclei were extensively investigated in the earlier IBFM calculation[20] and, therefore, one can directly compare the present results with those obtained in a purely phenomenological approach. The corresponding even-even core nuclei $^{148-154}$Sm present excellent examples of the shape transition from the nearly-spherical and axially-deformed shapes[3].

The first step is to determine the parameters for the even-even core Hamiltonian $\hat{H}_{\rm B}$. To this aim we employ the procedure developed in Ref. [22]: the constrained self-consistent mean-field (SCMF) calculation based on a given EDF determines the microscopic deformation energy surface as function of the polar deformation parameters β and γ[1]; This energy surface is mapped onto the corresponding expectation value of the boson Hamiltonian in the intrinsic (coherent) state[23] of the interacting-boson system, and this mapping completely determines the parameters of $\hat{H}_{\rm B}$. Only the strength parameter κ' for the $\hat{L}\cdot\hat{L}$ term is determined separately so that the cranking moment of inertia in the IBM intrinsic state becomes equal to the one obtained from the self-consistent cranking calculation at the mean-field minimum[24].

For the fermion valence space we include all the spherical single-particle orbits in the proton major shell $Z = 50 \sim 82$: $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$ and $3s_{1/2}$ for positive-parity, and $1h_{11/2}$ for negative-parity, with single-particle energies and occupation probabilities determined by the SCMF calculation constrained at zero deformation. The three strength parameters of $\hat{H}_{\rm BF}$ ($\varGamma_0$, $\varLambda_0$ and A_0) are the only parameters that are fitted to data, separately for positive- and negative-parity states for each nucleus.

Having determined all the parameters, the Hamiltonian $\hat{H}_{\rm IBFM}$ is numerically diagonalised to yield excitation spectra and electromagnetic transition rates of a given odd-mass nucleus.

3 Odd-mass Eu isotopes

In Fig. 1 we display triaxial quadrupole binding energy maps of the even-even $^{148-154}$Sm nuclei in the $\beta-\gamma$ plane ($0 \leqslant \gamma \leqslant 60°$), obtained from the constrained self-consistent relativistic Hartree-Bogoliubov (RHB) calculation[7] based on the DD-PC1 EDF[25] and a separable pairing force of finite range[26]. The energy surfaces clearly exhibit a gradual increase of deformation of the prolate minimum with increasing neutron number, from nearly spherical ^{148}Sm to well-deformed prolate shapes at ^{154}Sm, and the evolution of the γ-dependence of the potentials. The shape evolution corresponds to the transition from the $U(5)$ to the $SU(3)$ limits of the IBM[3]. The energy surfaces of ^{150,152}Sm indicate that these are transitional nuclei, characterised by a softer potential around the equilibrium minimum both in the β and γ directions, typical of the quantum shape phase transition[28].

In Fig. 2 we show the calculated excitation energies for the low-lying positive- ($\pi = +1$) and negative-parity ($\pi = -1$) yrast states in $^{147-155}$Eu isotopes as functions of neutron number, in comparison with available experimental data[27]. The present calculation reproduces the experimental systematics reasonably well. The structural evolution is characterized by the

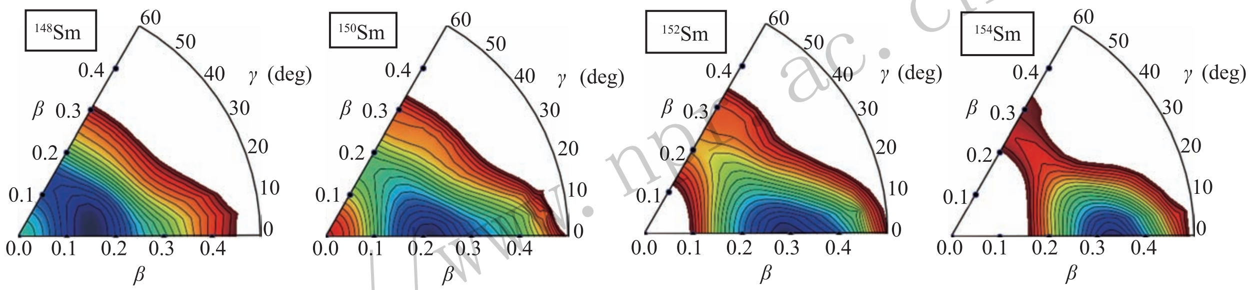

Fig. 1 (color online) Self-consistent RHB triaxial quadrupole binding energy maps of the even-even $^{148-154}$Sm isotopes in the β–γ plane ($0 \leqslant \gamma \leqslant 60°$). The energy difference between the neighbouring contours is 250 keV.

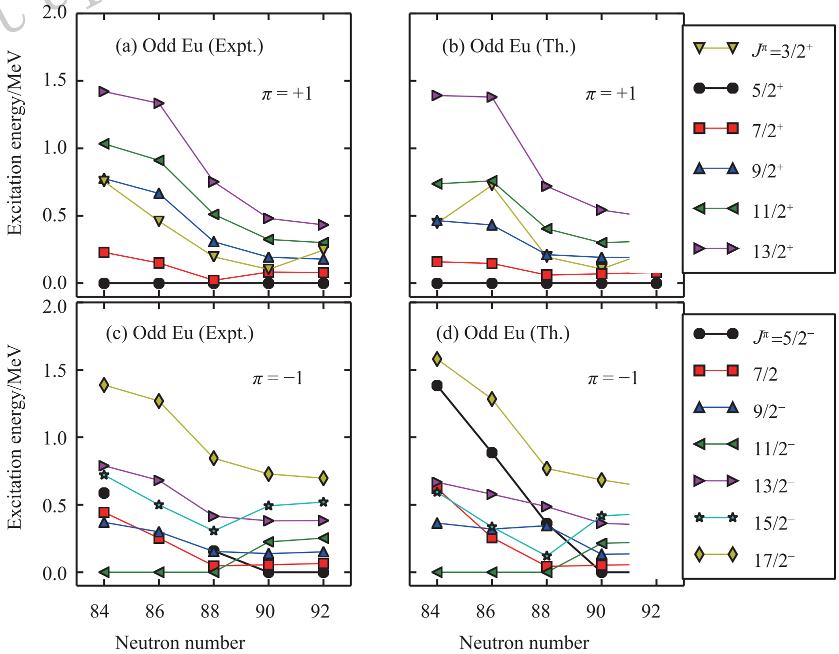

Fig. 2 (color online) Evolution of excitation energies of low-lying (a,b) positive- ($\pi = +1$) and (c,d) negative-parity ($\pi = -1$) yrast states as functions of neutron number in the $^{147-155}$Eu isotopes.

change in the spin of the ground state at a particular nucleus[29]. Indeed one sees from the figure that the ground-state spin changes at $N=90$ in odd-mass Eu isotopes for negative parity. For the positive-parity states, the change does not occur, but still the $5/2^+$ level becomes minimal in energy at $N=88$.

The model can also describe details of excitation spectra and decay patterns in individual nuclei. Figure 3 displays the low-energy level scheme of the nucleus ^{153}Eu. The theoretical results are in a very good agreement with experiment. The present results reproduce data on the same level of accuracy as the fully phenomenological approach[20]. From Fig. 3 the two positive-parity bands built on the states $J^\pi=5/2^+$ and $3/2^+$ are assigned to the $K^\pi=5/2^+$ and $K^\pi=3/2^+$ rotational bands, respectively. The level energies of these $J(J+1)$ rotational bands exhibit the strong-coupling $\Delta J=1$ systematics. The positive-parity bands based on $5/2^+_1$ and $3/2^+_1$ predominantly correspond to the $1g_{7/2}$ and $2d_{5/2}$ proton configurations, respectively, with significant mixing of the two

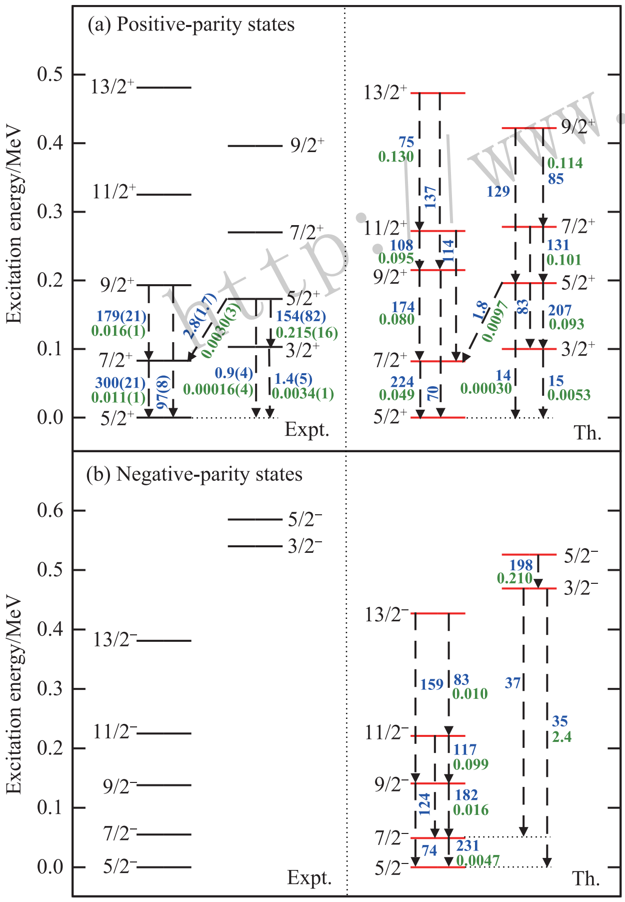

Fig. 3 (color online) Low-energy level scheme the isotope ^{153}Eu. Numbers along arrows are B(E2) (thick, in color blue) and B(M1) (slanted, in color green) values in W.u., respectively. Experimental data are from Ref. [27].

configurations. The model also reasonably describes the electromagnetic transition rates.

4 Applications

4.1 Signatures of shape phase transitions

We have already seen in Fig. 2 several signatures of the shape phase transitions in odd-mass Eu nuclei, *e.g.*, change of the ground-state spin. Nuclear shape phase transition is characterised by a discrete change of order parameters as functions of the control parameter (nucleon number). To show such a phase transitional behaviour of observables in a more vivid manner, we consider the differential of a given quantity $\mathcal{O}$ for a nucleus with mass A as its absolute value averaged over the lowest bands i, that is,

$$\delta\mathcal{O}=\frac{1}{n}\sum_{i=1}^{n}|\mathcal{O}_{i,A}-\mathcal{O}_{i,(A-2)}|. \qquad (6)$$

For $\mathcal{O}$, in this contribution we consider: $\overline{B(\mathrm{E2})}$, an average B(E2) for transitions between the band-head of a given band with spin J_0 and the lowest n states with spin $J_0+\Delta J$ with $\Delta J=1$ and 2; the energy difference $E(J_1,J_0)=E(J_1)-E(J_0)$ with $E(J_0)$ and $E(J_1)$ ($J_1=J_0+\Delta J$ with $\Delta J=1,2$) being the energies of the band-head and the first excited state in a band, respectively; the energy ratio between the lowest two excited states (with spin $J_1=J_0+\Delta J$ and $J_2=J_0+2\Delta J$) in a given band $R(J_2,J_1,J_0)=[E(J_2)-E(J_0)]/[E(J_1)-E(J_0)]$.

Fig. 4 displays the differentials of the above quantities for the odd-mass Eu nuclei. One notices that apart from only a few exceptions, that is, $\delta E(J_1,J_0)$ for the positive-parity states in odd-mass Eu, the differentials of the considered quantities exhibit a pronounced discontinuity at the transitional nuclei either at $A=151$ or 153, where the potential becomes notably soft in both β and γ directions (see, Fig. 1). We have shown[12] that the differentials of the characteristic quantities in the even-even core Sm nuclei also exhibit abrupt changes between the nuclei with mass number $A=150$ and 152, and that these do occur in the corresponding odd-mass systems.

4.2 Octupole correlations in odd-mass nuclei

Octupole shape is a recurrent theme of interest, as indeed a number of new experiments are either running or being planned to measure it, *e.g.*, in the mass $A\approx 220$ and 144 (for a review, see Ref. [30]). The octupole deformation is also relevant for odd-mass nuclei, which however, have not been so extensively studied theoretically as for the even-even nuclei. We have extended the method to include octupole degrees of freedom in odd-mass systems[16], and analysed the role of octupole correlations in neutron-rich Ba isotopes in the mass $A \approx 144$.

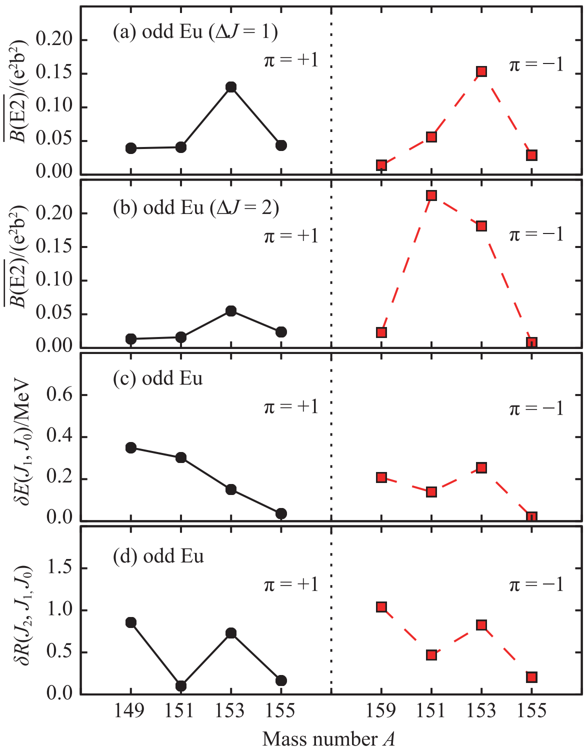

Fig. 4 (color online) Differentials of $\overline{B(E2)}$ with $\Delta J = 1$ (a-1, a-2) and $\Delta J = 2$ (b-1, b-2), excitation energy $\delta E(J_1, J_0)$ (c-1, c-2) and the energy ratio $\delta R(J_2, J_1, J_0)$ (d-1, d-2), for the odd-mass Eu isotopes, as functions of the mass number A.

Fig. 5 depicts the axially-symmetric (β_2, β_3) deformation energy surface for the nucleus ^{144}Ba, calculated with the constrained RHB method. A minimum with non-zero β_3 deformation ($\beta \approx 0.1$) is seen. The $\beta_2 - \beta_3$ RHB energy surface has been mapped onto the *sdf*-IBM Hamiltonian, which has been used to describe both positive- and negative-parity states in the considered even-even Ba nuclei. The *sdf*-IBFM Hamiltonian has been constructed in a similar way to the *sd*-IBFM one, but more free parameters are involved (the procedure to determine the parameters for the *sdf*-IBFM is described in great detail in Ref. [16]).

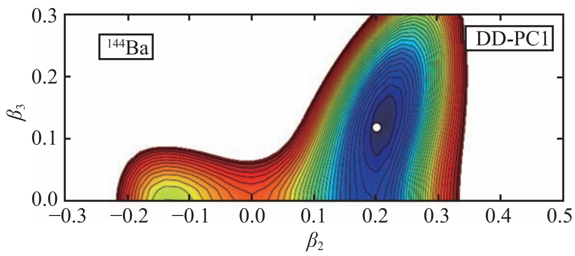

Fig. 5 (color online) The $\beta_2 - \beta_3$ RHB deformation energy surfaces for ^{144}Ba. The energy difference between neighbouring contours is 200 keV. Equilibrium minimum is identified by open circle.

The excitation spectra are shown in Fig. 6. The lowest two negative-parity bands, built on the $5/2_1^-$ and $7/2_1^-$ states, are characterized by the coupling of the unpaired neutron in the $1h_{9/2}$ single-particle orbital to the *sd* boson space. The lowest positive-parity state $9/2_1^+$ is described by the coupling of the $1i_{13/2}$ orbital to *sd*-boson states. The theoretical $\pi = +1$ band built on the $7/2_1^+$ state is constructed by the coupling of the $1h_{9/2}$ single-neutron configuration to states with one *f*-boson. The theoretical $11/2_1^+$ level, calculated at 705 keV, can be compared with the experimental $11/2^+$ state at 670 keV[31], which has been suggested as a candidate for an octupole state. Non-negligible E3 transition strength from the $7/2_1^+$ band to the negative-parity ground-state band is predicted in the present calculation.

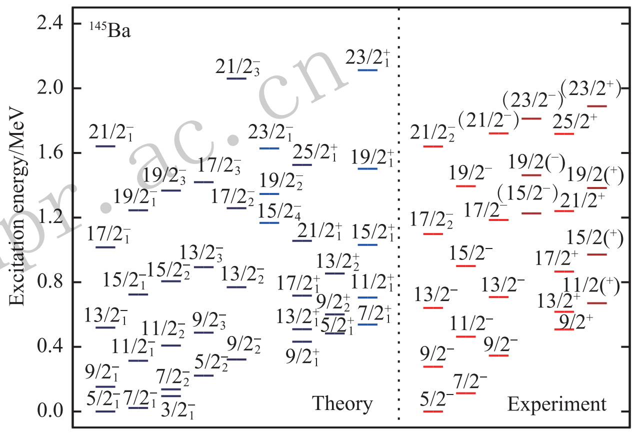

Fig. 6 (color online) Low-lying energy spectra for the nucleus ^{145}Ba. The levels for the theoretically and experimentally proposed octupole states are shown as thick lines.

5 Conclusion

In this contribution, we have reviewed a recently developed method for calculating spectroscopic properties of medium-mass and heavy odd-mass nuclei. Most of the parameters of the IBFM Hamiltonian used to describe the coupled system of the unpaired particle(s) plus boson-core, are uniquely determined based on the microscopic nuclear EDF framework. Only the strength parameters of the particle-boson coupling are specifically adjusted to data for each nucleus. As an illustrative example, the low-energy excitation spectra and transition rates of $^{147-155}$Eu have been analyzed, and a very good agreement with data has been obtained. Other selected results from this method have been discussed. The microscopic approach in which the even-even core is described in terms of bosonic degrees of freedom, and only the fermion degrees of freedom of the unpaired particle(s) are treated explicitly, enables an accurate, computationally feasible, and systematic description of a wealth of new data on isotopes with odd nucleon number(s).

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奇质量核的超越平均场玻色子费米子模型描述

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摘要： 对近年发展起来的一个基于核密度泛函理论和粒子核心耦合方案来计算中重质量奇 A 核谱性质的理论方法进行了评述。该方法首先在平均场层面通过选择合适的能量密度泛函和对力结构来自洽求解偶偶核心的势能曲面、球单粒子能级和奇粒子占有率，进一步将得到的结果作为微观输入来建立相互作用玻色子费米子模型哈密顿量，其中三个与粒子核心耦合强度相关的参数需要通过拟合一些特定奇质量核低激发谱数据来最终确定。通过对轴形变奇质量Eu同位素的低激发能谱和电磁跃迁几率的系统研究来说明该模型方法的有效性。另外，还讨论了该方法在描述轴形变奇质量核形状相变以及描述丰中子奇质量Ba同位素中八极关联方面的应用。

关键词： 核能量密度泛函；相互作用玻色子费米子模型；奇质量核

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