Monte-Carlo Shell Model calculations of Xe and Ba isotopes

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Abstract. The nuclear structure of the quadrupole collective states of even-even Te, Xe, and Ba isotopes is discussed using the nuclear shell model. It shows various phenomena, including the transition of spherical, axially symmetric deformed and triaxially deformed shapes. We show these phenomena are reproduced by our microscopic calculation, and the analysis of the anomalously small $B(E2)$ value of $^{136}\text{Te}$. We also discuss the $g$-factors of Xe isotopes, which exhibit the transition between the spherical and the triaxially deformed shapes.

1. Introduction

In the region of the nuclear chart around $^{132}\text{Sn}$, the structure of even-even nuclei shows various phenomena including the transition between some typical quadrupole collective states. This transition can be interpreted as the “shape” phase transition, but it occurs not rapidly but gradually, because a nucleus consists of a finite number of particles [1]. Several microscopic studies of such transition based on the nuclear shell model have been achieved (ex. see Ref.[2]), but its systematic study has been still lacked since a large amount of computation is required for the description of the transitional states. In this paper, we discuss systematic studies of low-lying collective states of these nuclei in terms of the nuclear shell model microscopically utilizing the Monte Carlo Shell Model (MCSM) [3] and discuss the transitional region precisely.

2. Systematic study of the E2 transition probabilities

In the study of medium-heavy nuclei using the nuclear shell model, the huge dimensions of the Hilbert space of the Hamiltonian matrix often prevents us from diagonalizing the matrix exactly. In order to overcome such difficulty, we have introduced the MCSM, which enables us to obtain the wave functions of ground states and low-lying excited states directly [3]. The validity of the MCSM was demonstrated in the studies of the shape phase transition from a spherical vibrator to axially symmetric rotor [4]. Moreover, we have studied the structure of $^{134}\text{Ba}$, which is known as a good example of the realization of a critical point symmetry $E(5)$ [5, 6], using the MCSM [7]. In this work, we carried out an MCSM calculation for the nuclear structure of the anomalously
small $E2$ transition probability of $^{136}$Te and the $g$-factors of even-even Xe isotopes, which show gradual transition from spherical to triaxially deformed shape.

The model space of the MCSM calculation is taken as one major shell including the intruder orbit. The single-particle energies are taken from experimental excitation energies of $^{131}$Sn, $^{133}$Sn and $^{133}$Sb. The two-body interaction is assumed to consist of the monopole pairing, quadrupole pairing, and quadrupole-quadrupole interactions for identical particles and the quadrupole-quadrupole interaction for a proton-neutron interaction. The strengths of the interaction are determined for reproducing the $2^+_1$, $4^+_1$ excitation energies of semi-magic nuclei [8]. This phenomenological interaction is sufficiently complex for the description of the quadrupole collective states, and simple enough to perform the numerical calculation. We use the same effective charges as in the calculation for Ba isotopes: effective charges are $e_p = 1.6e$ and $e_n = 0.6e$ for proton and neutron, respectively [4]. In the MCSM calculation, we adopt a pair-condensed state

$$|\Phi\rangle = \left(\frac{1}{2} \sum_{ij} \lambda_{ij} c_i^\dagger c_j^\dagger\right)^{N/2} |\!\rangle^\rangle \quad (1)$$

as a many-body MCSM basis [3], where $\lambda_{ij}$, $c_i^\dagger$, $N$ and $\!angle$ are the amplitudes, the creation operator of a valence nucleon in a single-particle orbit $i$, the valence nucleon number, and the inert core, respectively. In the MCSM, the wave functions of the ground state and some low-lying states are provided as the linear combination of the pair-condensed states, which are stochastically selected in terms of the variational principal.

We performed the MCSM around $^{132}$Sn and Figure 1 shows the $B(E2)$ transition probabilities obtained by experiments and the MCSM calculations. The filled symbols show the $E2$ transition probabilities of Sn, Te, Xe, Ba and Ce isotopes obtained experimentally [9]. The isotones with $N = 82$, which are semi-magic nuclei, show the feature of spherical vibrator and their collectivities are small. With increasing neutron number, the collectivity, and the $B(E2)$ on the same time, are increased and shows the feature of an axially symmetric rotor. On the other hand, with decreasing neutron number, the collectivity and $B(E2)$ are increased and show the feature of triaxial deformation.

![Figure 1. $B(E2 : 0^+_1 \rightarrow 2^+_1)$ of Sn (triangle), Te (diamond), Xe (square), Ba (circle), Ce (reverse triangle) isotopes. The filled symbols with dotted lines show the experimental values [9], and the open ones with solid lines show the MCSM results. Taken from Ref.[10].](image)

The MCSM results, which are shown by the open symbols in Fig.1, well reproduce the experimental values consistently in the whole region, where the nuclear structure shows the
transition of various quadrupole collective motions. We focus on the $^{136}\text{Te}$, whose $B(E2)$ is anomalously small, and Xe isotopes in the transitional region between spherical and triaxially deformed shapes in the following sections, individually.

3. Anomalously small E2 value of $^{136}\text{Te}$

Figure 1 shows that the experimental $B(E2)$ value of $^{136}\text{Te}$, the neutron number of which is 84, is apparently small in comparison with the tendency of the other nuclei. Moreover, it is smaller than the value predicted by the modified Grodzins’ rule, which is an empirical relation between the excitation energy of the $2^+_1$ state and the $B(E2)$ value [9, 11]. In Fig. 1, the microscopic MCSM calculation well reproduces this anomalously small $E2$ transition probability.

We show the structures of the $0^+_1$ and $2^+_1$ wave functions of $^{136}\text{Te}$ in order to discuss the origin of this anomaly. Figure 2 shows the $2^+_1$ level of $^{136}\text{Te}$, together with those of $^{134}\text{Te}$ and $^{134}\text{Sn}$. The nucleus $^{136}\text{Te}$ has two valence protons and two neutrons, while the neighboring nuclei, $^{134}\text{Te}$ and $^{134}\text{Sn}$, have two valence protons or two valence neutrons, respectively.

![Figure 2. Excitation energy of $2^+_1$ and $B(E2)$ of $^{134,136}\text{Te}$ and $^{134}\text{Sn}$](image)

The ground state wave function of $^{134}\text{Sn}$ is written as

$$|S_\nu\rangle = S^\dagger_\nu |\rangle,$$

(2)

where $|\rangle$ denotes the $^{132}\text{Sn}$ inert core. The $S^\dagger_\nu$ operator is defined as

$$S^\dagger_\nu \equiv \sum_j \alpha_j \left[c^\dagger_j \times c^\dagger_j\right]^{(0)},$$

(3)

where $c^\dagger_j$ denotes the creation operator of a neutron in a single-particle orbit $j$, and $\alpha_j$ indicates an amplitude giving the proper normalization of the state $|S_\nu\rangle$. The values of $\alpha_j$’s are determined by the diagonalization of the Hamiltonian matrix. The ground state wave function of $^{134}\text{Te}$ is written similarly as

$$|S_\pi\rangle = S^\dagger_\pi |\rangle,$$

(4)

with $S^\dagger_\pi$ defined as the corresponding creation operator of a pair of valence protons.
Similarly, the $2^+_1$ state of $^{134}$Sn is provided by a $2^+$ state of two neutrons, called $D_\nu$ pair, on the $^{132}$Sn core. The $2^+_1$ state of $^{134}$Te is given by the $D_\pi$ pair. These D pairs are created by the operators,

$$D_M^\dagger ≡ \sum_{j,j'} D_{M} \beta_{jj'} \left[ c_{j}^\dagger \times c_{j'}^\dagger \right]^{(2)},$$

where the subscript $\pi$ or $\nu$ is omitted for brevity, $M$ means the $z$-component of angular momentum, and $\beta_{jj'}$ stands for amplitude. The values of $\beta_{jj'}$ are determined by the diagonalization of the Hamiltonian matrix for the state $|D\rangle_M ≡ |D_M\rangle$, so that it is properly normalized. We shall omit $M$ hereafter because it is not essential. These S- and D-pairs are usually called collective pairs, because they are comprised of coherent superposition of various nucleon pairs, although the coherence can be modest in the following cases.

Figure 2 shows that the first $2^+$ level is quite well reproduced by the present Hamiltonian. The $B(E2; 0^+_1 \rightarrow 2^+_1)$ value is 0.096 $[e^2b^2]$ and 0.027 $[e^2b^2]$ for $^{134}$Te and $^{134}$Sn, respectively. Experimentally, only the former is known as 0.096(12) $[e^2b^2]$ [13], in a reasonable agreement with the present calculation and also with the results in [13, 14]. For $^{134}$Sn, the $B(E2; 0^+_1 \rightarrow 2^+_1)$ value becomes 0.035 $[e^2b^2]$ in the shell-model calculation by Coraggio et al. [15], whereas the QRPA result by Terasaki et al. [14] gives a considerably smaller value. The present value is in between and closer to the former one. The Nilsson result in [14] seems to resemble the two shell-model values.

The shell-model wave functions of the $0^+_1$, $2^+_1$, and $2^+_2$ states of $^{136}$Te can be written as,

$$|0^+_1\rangle = 0.91 \times |S_\nu \times S_\pi\rangle + \cdots,$$

$$|2^+_1\rangle = 0.82 \times |D_\nu \times S_\pi\rangle + 0.45 \times |S_\nu \times D_\pi\rangle + \cdots,$$

$$|2^+_2\rangle = 0.38 \times |D_\nu \times S_\pi\rangle - 0.76 \times |S_\nu \times D_\pi\rangle + \cdots,$$

where “...” means other minor components and $|S_\nu \times S_\pi\rangle ≡ |S_\nu S_\pi\rangle$, etc. Equation (6) implies that the $0^+_1$ state is accounted for by the state $|S_\nu \times S_\pi\rangle$ up to 83% in probability.

Equation (7) implies that the first excited state of $^{136}$Te is shown to be mainly contributed by the proton excitation up to 67% in probability, while the second excited state is mainly by the neutron excitation, which can be seen in Eq.(8). This decoupling of the proton-neutron excitation decreases the collectivity and $B(E2; 2^+_1 \rightarrow 0^+_1)$, because the effective charge of neutrons is far smaller than that of protons. In Fig. 2(b), the $B(E2; 2^+_1 \rightarrow 0^+_1)$ of $^{134}$Sn is very small, because the $2^+_1$ state is excited from $0^+_1$ state by neutron excitation.

Figure 2 shows that this decoupled excitation is caused by the large difference between the $2^+_1$ excitation energies of $^{134}$Sn and $^{134}$Te, which are interpreted as the difference of the pairing gaps of neutrons and protons. Because the difference of the pairing gaps is caused mainly by the imbalance between the neutron number and proton number, this decoupling excitation seems to be one of the peculiar characteristics of neutron-rich medium-heavy nuclei, except for semi-magic nuclei.

4. g-Factors of Xe Isotopes

We move on the transitional region of Xe isotopes between triaxially deformed and spherical shapes. In our shell-model calculation, $^{4}$Xe is considered to comprise $^{132}$Sn, 4 valence protons, and 136—$A$ neutron holes, where $A$ denotes a mass number. The $B(E2)$ values of Xe isotopes can be seen in Fig.1. and the MCSM calculation well reproduces the gradual increase of the collectivity with decreasing neutrons, or adding neutron holes to the $^{132}$Sn inert core. The effective interaction and the model space of the MCSM calculation are the same as those used in Fig.1.

Figure 3 shows the nuclear magnetic moments of the first excited states of Xe isotopes in the region of the gradual transition from spherical ($A \simeq 136$) to triaxially deformed states.
The structure of the semi-magic nucleus, $^{136}$Xe, is suitably described by the picture of single-particle motion, which means that the valence protons occupy the lowest valence orbit $\pi 1g_{7/2}$. Therefore, the $^{136}$Xe has small collectivity and rather large $g$-factor, which is close to that of the $\pi 1g_{7/2}$ orbit, or $g = 0.80$. On the other hand, the $g$-factors of $^{134}$Xe and lighter Xe isotopes are shown to be close to the results of the proton-neutron interacting boson model (IBA-II) [16] and these isotopes are well described by the triaxially deformed nuclei. The IBA-II predicts slower transition than that of the experiment, and fails in describing the small $g$-factors of transitional nuclei. The prediction of the collective model, $Z/N$, is also shown by the dotted line for comparison.

B. A. Brown and his collaborators performed the fully microscopic shell-model calculation with the exact diagonalization of the Hamiltonian matrix based on the $G$-matrix effective interaction [17]. They provided the $g$-factors of $^{136,134}$Xe, which are shown by the open triangles in Fig.3. They show remarkable agreement with the experimental values. However, it might have been difficult to perform such microscopic calculation of the lighter nuclei, because the dimension of their Hamiltonian matrix grows exponentially depending on the number of valence nucleons. (Note again that the valence neutrons are considered as the hole states on the $^{132}$Sn inert core.)

Because the MCSM calculation does not have such difficulty, our calculation reaches $^{130}$Xe. The MCSM calculation reproduces the experimental values well in the whole region including $^{136}$Xe and $^{134}$Xe, whose $g$-factors show the sudden change. The $g$-factors of $^{132}$Xe and $^{130}$Xe are close to the results of the IBA-II, and the calculation of $^{124-128}$Xe is in progress.

The MCSM calculation and the work by B.A.Brown et al. suggest that the nuclear shell model calculation with full configuration mixing is essential to describe both the structures interpreted as the single particle motion and the collective motion, and sudden decrease of $g$ factor from $^{136}$Xe to $^{134}$Xe in the transitional region. Only the MCSM calculation can obtain the $^{130-136}$Xe isotopes consistently.

5. Summary
The transition probabilities and magnetic moments provided by the MCSM show apparent characteristics of the quadrupole collective motion and agree well with the experimental values. The usefulness of the MCSM calculation has been verified by examining the $B(E2)$ values in the region around $^{132}$Sn. We preformed the MCSM calculation on the $^{136}$Te and Xe isotopes, which are good examples of the transitional structure of the quadrupole collective states.

The unusually small value of $B(E2; 0_1^+ \rightarrow 2_1^+)$ of $^{136}$Te has been explained without any adjustment. By the analysis of the wave function of the excited states, we see that the first
excited state is mainly constructed by the neutron excitation, while the second excited state is mainly by the neutron excitation. This anomaly is caused by this proton-neutron decoupled excitation, which is one of the interesting phenomena of neutron-rich nuclei.

The g-factors of Xe isotopes are also well reproduced by the MCSM calculation in the region of the gradual transition of different types of quadrupole collective states with varying the neutron number.

Acknowledgments

The present work was supported by the Grant-in-Aid for Specially Promoted Research (13002001) from the Ministry of Education, Science, Sport, Culture and Technology. Some of the conventional calculations were made by the code OXBASH [18].

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