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Large-Scale Shell Model for Nuclear Structure and Nuclear Astrophysics Studies

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Abstract: The study of neutron-rich nuclei near ^{132}Sn is interesting and important for both nuclear structure and nuclear astrophysics. For a considerably large model space allowing cross-shell excitations, a new effective Hamiltonian is determined by employing the extended pairing-plus-quadrupole model with monopole corrections. Calculations for two mass regions, for the north-east quadrant of ^{132}Sn with $Z > 50$ and $N > 82$ and for the south-west quadrant with $Z < 50$ and $N < 82$, have been performed recently. The structure of these nuclei is analyzed in detail, and the role of the monopole corrections can be clearly seen.

Key words: large-scale shell model; monopole correction; single-particle state; core-excitation; exotic nuclei

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1 Introduction

The nuclear shell model is the most fundamental method for nuclear structure analysis, which has been successful in describing many properties of the low-lying levels in light and medium nuclei, as well as some heavy nuclei in the vicinity of shell closures. Nuclei with a few valence particles outside a doubly-closed shell have played an essential role in testing nuclear shell models. Apart from its intrinsic importance for nuclear structure, the region around ^{132}Sn is also of astrophysical interest for understanding the formation of the $A \approx 130$ peak of the solar r-process (*i.e.*, the rapid neutron-capture process) abundance distribution. It has been believed that the origin of nearly half of the solar abundances of elements heavier than the Fe group is the astrophysical r-process[1]. The early identification of the classical $N = 82$ r-process waiting-point isotope ^{130}Cd established such a connection to the nuclear structure problem[2]. Although the basic recipe for generating r-process elements is known, many of such capture and β rates are beyond the present limit of experimental access, one has to rely on reliable theoretical calculations.

The relatively simple structure of near doubly closed-shell nuclei is recognized in their observed spectra which are usually understood as consisting of two types of excitations: excitations of valence single particles and excited states formed by couplings of the valence nucleons to core excitations. There have been successful calculations for the nuclei beyond ^{132}Sn by different groups. These calculations may be divided into two classes, treating, respectively, the two types of excitations. The low-energy states were studied microscopically by using the shell-model method with a chosen effective interaction. On the other hand, the high-energy (and often high-spin) states of core excitations were simply interpreted with empirical nucleon-nucleon interactions. These two classes of calculations work for their own applicable states and have contributed greatly to the structure analysis in the mass region. Nevertheless, to study the interplay between them and understand the structure problem as a whole, it is desired to have a unified treatment for the two types of excited states in a manageable shell-model calculation. The challenging question is to find out

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suitable effective shell-model interactions that work for the description of both types of excitation.

The key question is the Hamiltonian in the respective model space[3–4]. A shell model Hamiltonian is usually composed by one-body and two-body terms. In general, the Hamiltonian can be separated into the monopole and multipole parts[5–6]. The monopole part is responsible for the bulk properties of binding energies, shell gaps and so on, while the multipole part, which is dominated by the pairing and quadrupole forces, describes spectroscopy. In fact, the application of the pairing and quadrupole interaction, which simply considers two most important excitation modes in nuclei, have been widely applied in the nuclear structure study for a long time (See Refs. [7–10] and also Ref. [11] for a recent review).

In recent years, a workable Hamiltonian has been proposed for the neutron-rich nuclei near ^{132}Sn[12–13]. It described well and clearly explained the level spectra, up to about 5 MeV of excitation. For the south-west quadrant, for example, the monopole corrections have been determined by using the experimental energy of the core-excited $21/2^+$ level in ^{131}In as a benchmark[13]. It has been shown that the model can also be used to study the chain of $N=82$ isotopes that describes well the properties of the experimentally observed 8^+ isomeric state and the other low-lying levels in ^{126}Pd, ^{128}Pd, and ^{130}Cd, and further predict energy levels and $E2$ transitions for ^{126}Ru and ^{124}Mo[14]. It also can be used to study the quenching of the neutron $N=82$ shell gap near ^{120}Sr with monopole-driving core excitations[15].

2 The EPQQM model

If protons and neutrons in question occupy different shells, which is the case for the ^{132}Sn region, the Hamiltonian can be written by the following proton-neutron representation:

$$
\begin{aligned}
H &= H_{\rm sp}+H_{P_0}+H_{P_2}+H_{\rm QQ}+H_{\rm OO}+H_{\rm HH}+H_{\rm mc}\\
&=\sum_{\alpha,i}\varepsilon_a^i c_{\alpha,i}^\dagger c_{\alpha,i}-\frac{1}{2}\sum_{J=0,2}\sum_{ii'}g_{J,ii'}\sum_M P_{JM,ii'}^\dagger P_{JM,ii'}-\\
&\frac{1}{2}\sum_{ii'}\frac{\chi_{2,ii'}}{b^4}\sum_M :Q_{2M,ii'}^\dagger Q_{2M,ii'}:-\\
&\frac{1}{2}\sum_{ii'}\frac{\chi_{3,ii'}}{b^6}\sum_M :O_{3M,ii'}^\dagger O_{3M,ii'}:-\\
&\frac{1}{2}\sum_{ii'}\frac{\chi_{4,ii'}}{b^8}\sum_M :H_{4M,ii'}^\dagger H_{4M,ii'}:+\\
&\sum_{a\leqslant b,ii'}k_{\rm mc}(ia,i'b)\sum_{JM}A_{JM}^\dagger(ia,i'b)+A_{JM}(ia,i'b)\ .
\end{aligned}
\tag{1}
$$

The above equation includes the single-particle Hamiltonian ($H_{\rm sp}$), the $J=0$ and $J=2$ pairing ($P_0^\dagger P_0$ and $P_2^\dagger P_2$), quadrupole-quadrupole ($Q^\dagger Q$), octupole-octupole ($O^\dagger O$), hexadecupole-hexadecupole ($H^\dagger H$) terms, and the monopole corrections ($H_{\rm mc}$). $P_{JM,ii'}^\dagger$ and $A_{JM}^\dagger(ia,i'b)$ are the pair operators in the *pn* representation, and $Q_{2M,ii'}^\dagger$, $O_{3M,ii'}^\dagger$, and $H_{4M,ii'}^\dagger$ are respectively the quadrupole, octupole, and hexadecupole operators with i (i') for protons (neutrons). The corresponding force strengths are given by the constants $g_{J,ii'}$, $\chi_{2,ii'}$, $\chi_{3,ii'}$, $\chi_{4,ii'}$, and $k_{\rm mc}(ia,i'b)$, and the constant b means the harmonic-oscillator range parameter. We term this Hamiltonian the extended paring-plus-quadrupole model with monopole corrections (EPQQM).

For a given mass region, a proper model space and single particle energies should be determined firstly. For example, for the neutron-rich hole-nuclei south-west to ^{132}Sn, the model space is selected as six proton orbits ($0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2}$, $0g_{7/2}, 1d_{5/2}$) and seven neutron orbits ($0g_{7/2}, 1d_{5/2}, 2s_{1/2}, 0h_{11/2}, 1d_{3/2}$, $1f_{7/2}, 2p_{3/2}$). The single particle energies in Eq. (1) are based on the binding energy and low-lying levels taken from experiment. These proton and neutron single-particle energies used in Refs. [14-15] were taken from literature, with the values of $\varepsilon^\pi_{p3/2}=-17.043$ MeV and $\varepsilon^\pi_{p1/2}=-16.055$ MeV updated according to the latest experiment[16]. The neutron and proton single-particle states of ^{131}Sn and ^{131}In are displayed in Fig. 1.

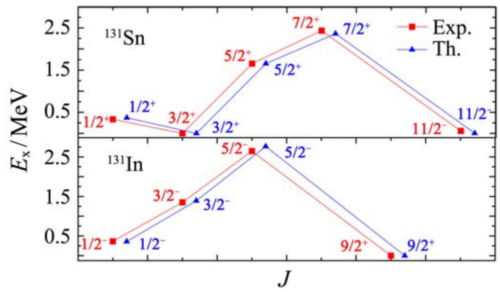

Fig. 1 (color online) The single particle states of ^{131}Sn and ^{131}In compared with experimental data[17].

As the shell-model spaces are different for different mass regions, the force strengths should be adjusted accordingly. The parameters of force strengths listed in Table 1 are those for the south-west quadrant with $Z<50$ and $N<82$[13]. These parameters were obtained from fitting known experimental data of hole-nuclei with $A\approx130$, especially the single-particle states and and other important isomeric states. For example, the single particle states of ^{131}Sn and ^{131}In, and the the core-excited $21/2^+$ level in ^{131}In[18]. Representative results presented in the following are calculated using these force strengths.

Table 1 The two-body force strengths (in MeV).

ii'	$g_{0,ii'}$	$g_{2,ii'}$	$\chi_{2,ii'}$	$\chi_{3,ii'}$	$\chi_{4,ii'}$
pp	0.250	0.158	0.102	0.032	0.001 4
nn	0.129	0.047	0.140	0.004	0.000 8
pn	0	0	0.082	0	0.000 9

3 Results and discussion

The nucleus ^{131}In has one proton-hole as compared to ^{132}Sn. Its low-lying states are single-particle ones and highly-excited states may be cross-shell excitations. It has $9/2^+$ as the ground state and has three lowest negative-parity states $1/2^-$, $3/2^-$ and $5/2^-$. To describe the cross-shell excitations, it is important to take properly experimental information to describe the size of the energy gap. In this aspect, the experimentally-determined isomer levels[18], $17/2^+$ and $21/2^+$ in ^{131}In at 3.782 and 3.764 MeV, respectively, provided a direct measure of the size of the $N=82$ shell gap that was considered as an important piece of structure information for this mass region. Our calculated two levels are 3.792 and 3.759 MeV for $17/2^+$ and $21/2^+$ respectively, and their configurations are obtained to be $\pi g_{9/2}^{-1}\nu h_{11/2^-}^{-1} f_{7/2}$.

Note that in order to obtain the above results, two monopole correction terms, $M1 \equiv k_{\rm mc}(\nu h_{11/2}, \nu f_{7/2}) = 0.52$ MeV and $M2 \equiv k_{\rm mc}(\pi g_{9/2}, \nu h_{11/2}) = -0.40$ MeV, were added to the Hamiltonian. The monopole correction $M1$ leads to a correct neutron $N=82$ shell gap that strongly affects core-excited states from the neutron orbit $h_{11/2}$ to $f_{7/2}$ across the $N=82$ shell gap. The monopole correction $M2$ is attractive between the proton orbit $g_{9/2}$ and the neutron orbit $h_{11/2}$. As shown in Fig. 2, the two monopole correction terms shift the levels of $17/2^+$ and $21/2^+$ significantly down so that they compare well with the experimental data. The so-determined Hamiltonian can be furthermore used to study the hole structure of many $A \approx 130$ nuclei, for example, the experimental levels of odd-odd nuclei ^{130}In, the 2^+, 4^+, 6^+ and 8^+ levels of even-even nuclei ^{130}Cd, and the low-lying and high excited states of ^{130}Sn[13].

In Fig. 3, we show the calculated three groups of core-excitation in ^{131}In, with the configurations $\pi g_{9/2}^{-1}\nu h_{11/2^-}^{-1} f_{7/2}$, $\pi p_{1/2}^{-1}\nu h_{11/2^-}^{-1} f_{7/2}$, and $\pi g_{9/2}^{-1} \nu d_{3/2^-}^{-1} f_{7/2}$. As for the members of $\pi g_{9/2}^{-1}\nu h_{11/2^-}^{-1} f_{7/2}$, the levels $17/2^+$, $21/2^+$, as mentioned before, are the two experimentally-known core-excited states. Two other states with $23/2^+$ and $25/2^+$ are predicted to be nearly degenerate with the $21/2^+$ state, and the $19/2^+$ state is also very close to $17/2^+$. These are

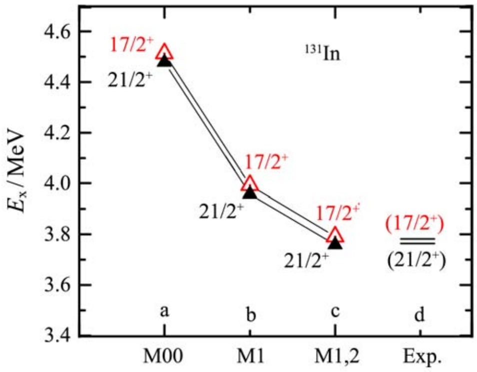

Fig. 2 (color online) The effects of monopole correction of $M1 \equiv k_{\rm mc}(\nu h_{11/2}, \nu f_{7/2})$ and $M2 \equiv k_{\rm mc}(\pi g_{9/2}, \nu h_{11/2})$ for core-excited levels of $17/2^+$ and $21/2^+$ at ^{131}In. Part "a" marked with M00 means calculations without these two monopole corrections, part "b" marked with $M1$ means with $M1$ only, and part "c" marked with $M1,2$ means with both $M1$ and $M2$, and part "d" marked with Exp. means the experimental data.

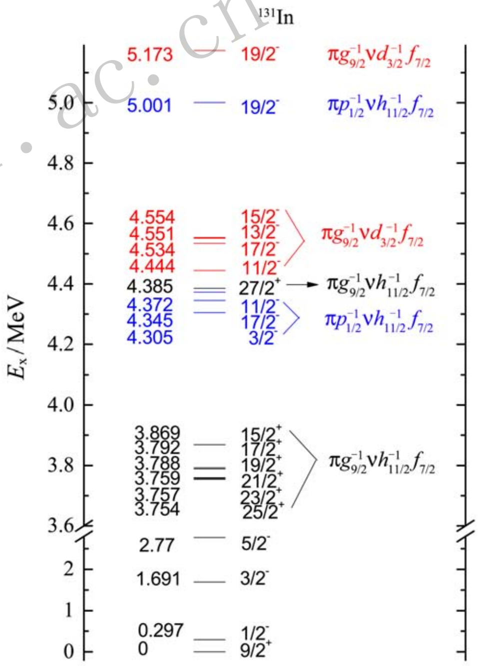

Fig. 3 (color online) Obtained low-lying and core-excited states of ^{131}In from the present shell-model calculation employing the EPQQM Hamiltonian.

consequences of cross-shell excitations, in which an $h_{11/2}$ neutron below the $N=82$ shell gap is excited to occupy the upper levels above the gap. Furthermore, other core-excited states can be predicted, for example, the members of the negative-parity configuration $\pi p_{1/2}^{-1}\nu h_{11/2^-}^{-1} f_{7/2}$. This is due to the coupling of the lowest-excited proton-hole $\pi p_{1/2}$ state to the neutron $\nu h_{11/2^-}^{-1} f_{7/2}$ particle-hole excitation. The high energy levels of negative-parity configuration $\pi g_{9/2}^{-1}\nu d_{3/2^-}^{-1} f_{7/2}$ is also one of the predictions from the present calculation, which lie in the energy region from 4.76 to 5.35

MeV.

In our calculation, the configuration of $15/2^+$ to $21/2^+$ levels in ^{131}Sn is given as $\nu h_{11/2}^{-1} d_{3/2}^{-1} f_{7/2}$ that agrees with the results in Ref. [20]. As shown in the left part of Fig. 4, the $21/2^+$ level with 4.859 MeV in theory fits very nice to the experimental one at 4.99 MeV, and the $17/2^+$ level also fits well to the experimental one at 4.273 MeV, which also agree with the previous results[20–21]. The configuration of the multiplet levels from $15/2^-$ to $23/2^-$ is $\nu h_{11/2}^{-2} f_{7/2}$, and their energies are given well in our results. As shown in the right part of Fig. 4, the energy of $15/2^-$ level at 3.933 MeV fits well to the experimental one at 4.102 MeV. The theoretical level $23/2^-$ with 4.478 MeV nears the experimental one at 4.605 MeV. The above discussions are the strong support to our treatment for the neutron core excitation configuration of $\nu h_{11/2}^{-1} f_{7/2}$ in Hamiltonian.

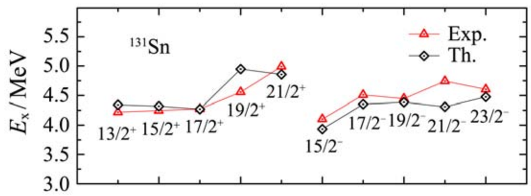

Fig. 4 (color online) Comparison of the high-spin part of the calculated energy levels (black quadrangle) with experimental data (red triangle) in ^{131}Sn[13].

Very recently we have also studied the level spectra of ^{129}Sn, ^{129}In, ^{129}Cd, and ^{129}Ag, which includes low-lying levels and high core-excitation[19]. In our future research, we will perform large-scale shell-model calculations on the hole-particle nuclei situated in the quadrant south-east of the doubly-magic ^{132}Sn. The low-lying levels of ^{133}In, ^{134}In, ^{131}Cd and ^{132}Cd will be studied.

4 Conclusion

In this short contribution, we presented a new Hamiltonian suitable for the nuclei near the doubly-magic ^{132}Sn. It consists of the two-body $J=0$ and $J=2$ pairing ($P_0^\dagger P_0$ and $P_2^\dagger P_2$), quadrupole-quadrupole ($Q^\dagger Q$), octupole-octupole ($O^\dagger O$), hexadecupole-hexadecupole ($H^\dagger H$) terms, as well as the monopole corrections ($H_{\rm mc}$). A useful EPQQM model was established after fitting to known experimental data, which includes five parameters for the proton-proton interactions, five parameters for the neutron-neutron interactions, two parameters for the proton-neutron interactions, and two monopole corrections. The model has been tested, for example for the $Z<50$ and $N<82$ nuclei, by describing the level spectra, up to 5 MeV of excitation for ^{131}In, ^{131}Sn, ^{130}In, ^{130}Cd, and ^{130}Sn. In the future, we will apply the model for the exotic south-east mass region with $Z<50$ and $N>82$ and calculate the β-decay and election capture rates that the nuclear astrophysics study are interested in.

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