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Article

Nucleon-Pair Shell Model with Symmetry Broken Basis

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Abstract: The nucleon-pair shell model (NPSM) with broken symmetry basis is studied. The results demonstrate the validity of NPSM with symmetry broken basis, which leads to a significant reduction in the dimensionality of the multi-pair configuration space. We have observed that the axial-deformed basis provides a satisfactory description of the low-lying spectrum, even without the need for the projection procedure. In the case of the triaxial-deformed basis, we have investigated the variation after angular momentum projection, indicating the potential for NPSM to find exact solutions in the half-closed system.

Keywords: shell model; nucleon pair; broken symmetry

1. Introduction

Atomic nuclei are self-bounded quantum many-body systems. Modeling many-body problem is one of the crucial challenging problems in theoretical nuclear physics. There has been much progress in this topic: the Green's function Monte Carlo Method [1,2], the full configuration interaction (FCI) approaches, so-called no-core shell model (NCSM) [3], and the symmetry-adapted no-core shell model [4], etc. The methods mentioned above are limited to the cases for light nuclei. The coupled-cluster method (CC) [5] has been applied to both light nuclei and medium mass nuclei around closed shell. The mean-field theory can be applied to the whole nuclear chat [6], but the mean-field approximation may have lost the key many-body correlation between nucleons. The valence space shell model (SM) play an important role in describing and understanding nuclear structure [7–13]. However, the full-fledged SM studies are still out of reach for the heavy mass nuclei because of the huge number of configurations [14]. There are many models worked on rotational symmetry broken basis, and the angular momenta are restored by projection technique, such as the projected Hartree-Fock [15,16] including variation after projection [15,17], the Hartree Fock-Bogoliubov [15,18–20] and projected relativistic mean-field calculations [21], the Monte Carlo shell model [22,23], the projected shell model [24–26], the projected configuration interaction [27] and projected generator coordinate methods [28,29].

In 1993, a new technique, known as generalized wick theory, has been proposed to calculate the commutators for coupled operators and fermion clusters by Chen et al.[30,31]. Based on this new technique, a nucleon pair shell model (NPSM) has been constructed [32], in which the building blocks of the configuration space are nucleon-pairs. Due to the success of the interacting boson model (IBM)[33], model space of NPSM was truncated to the SD pair subspace, then the model is developed into the so-called SD-pair shell model (SDPSM). It was shown that the collectivity of the low-lying states can be described very well in the SD pair subspace [34–37]. It is also found that within the framework of M-schemed NPSM, the CPU time required in calculating the matrix elements can be reduced a lot [38,39].

At a more fundamental level, the truncation of the NPSM should be studied carefully. Up to now, no one has proved the convergency of the truncation. To compensate for such problem, the basis

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should be constructed by more kinds of collective pairs, and the pair structure coefficients should also be determined by a variation procedure [40–43]. But the dimensionality of the many-pair model space increases rapidly with the number of collective pairs, and hindering its further study. In the NPSM, the nucleon-pairs always have good angular momentum J and the third component M, and the many-body basis keeps the rotational invariance. Therefore, both the total and intermediate angular momentum J or third component M, depending on J-scheme or M-scheme is adopted, should be good quantum numbers. To work with a complete subspace, a group of multi-pair basis should be considered, so we introduce the symmetry broken pairs in the NPSM in this paper, and some preliminary results of half-closed nucleus are given.

The paper is organized as follows: In Section 2, a brief review of the NPSM and the angular momentum projection process are presented. The symmetry broken basis are discussed in Section 3. In Section 4, a summary and discussion is given.

2. The Model

In this paper, as a preliminary report, we discuss the half-closed nuclei only. The general form of the shell model Hamiltonian is adopted as

$$\begin{aligned} H &= \sum_{j_1,j_2,m_1,m_2} \epsilon_{j_1 j_2} c^\dagger_{j_1 m_1} c_{j_2 m_2} + \sum_{j_1\le j_2, j_3\le j_4, J, M} \langle j_1 j_2 | V | j_3 j_4 \rangle_J A^\dagger(j_1 j_2 J M) A(j_3 j_4 J M) \\ A^\dagger(j_1 j_2 J M) &= \frac{1}{\sqrt{1+\delta_{j_1 j_2}}} \left(c^\dagger_{j_1} \times c^\dagger_{j_2} \right)^J_M \\ A(j_3 j_4 J M) &= -\frac{1}{\sqrt{1+\delta_{j_3 j_4}}} \left(c_{j_3,m_3} \times c_{j_4,m_4} \right)^J_M \end{aligned} \tag{1}$$

where j_i stands for a oscillator single particle orbit (nlj), $c^\dagger_{j_1 m_1}$ is the single-particle creation operator, $c_{j_2 m_2}$ is the single-particle annihilation operator, $\epsilon_{j_1 j_2}$ is the single-particle energy, the symbol $\times$ represent angular momentum coupling, which is given

$$\left(c^\dagger_{j_1} \times c^\dagger_{j_2} \right)^J_M = \sum_{m_1,m_2} \langle j_1 m_1, j_2 m_2 \mid J M \rangle \, c^\dagger_{j_1,m_1} c^\dagger_{j_2,m_2} \tag{2}$$

where $\langle j_1 m_1, j_2 m_2 \mid J M \rangle$ is Clebsch-Gordan (CG) coefficient.

2.1. NPSM Framework

The building blocks of the NPSM are collective pairs with good angular momentum J and third component M, designated as $A^{J\dagger}_M$, which is built from many non-collective pairs $A^{J\dagger}_M(j_a j_b)$,

$$\begin{aligned} A^{J\dagger}_M &= \sum_{j_a j_b} y(j_a j_b J) A^{J\dagger}_M(j_a j_b) \\ &= \sum_{j_a j_b} y(j_a j_b J) \left(c^\dagger_{j_a} \times c^\dagger_{j_b} \right)^J_M \end{aligned} \tag{3}$$

Then the multi-pair basis can be constructed in both M-scheme [38,39] and J-scheme [32,36], respectively,

$$A^\dagger(J_1 M_0, \ldots, J_N M_N)_M = A^{J_1\dagger}_{M_1} \ldots A^{J_N\dagger}_{M_N}, \;\; M = \sum_{i=1}^N M_i \tag{4}$$

and

$$A^\dagger(J_1, \ldots, J_N, J M)_M = (\ldots((A^{J_1\dagger} \times A^{J_2\dagger})^{L_2} \times A^{J_3\dagger})^{L_3} \times \cdots \times A^{J_N\dagger})^J_M \tag{5}$$

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When certain collective pairs are considered, a set of multi-pair basis are constructed, and those bases are dependent on each pair structure coefficients. The matrix elements of Hamiltonian can be carried out by using the commutators between collective pairs [32,36,38,39]. Then the Hamiltonian can be diagonalized in such subspace, and the sum of few lowest energies E can be minimized

$$E = \sum_i E_i(J_i) \tag{6}$$

Taking into consideration of the broken rotational symmetry of pairs, the collective pairs with good angular momentum are mixed. First, we would like to introduce the axial-deformed pairs, which are given by summing the pairs with the same quantum number M and different angular momentum J,

$$P^\dagger_M = \sum_J A^{J\dagger}_M \tag{7}$$

where the axial-deformed pairs P_M keep the third component of angular momentum as a good quantum number. A set of multi-pair basis with fixed total third component M are constructed, after the collective pairs are introduced,

$$|\phi_M\rangle = P^\dagger_{M_1} \dots P^\dagger_{M_N}|0\rangle, \quad M = \sum_{i=1}^{N} M_i \tag{8}$$

The Hamiltonian can be diagonalized in a subspace with fixed total third component M.

One can also introduce the triaxial-deformed pairs,

$$P^\dagger = \sum_{JM} A^{J\dagger}_M \tag{9}$$

where both the angular momentum J and third component M are mixed to break the rotational invariance. The multi-pair basis is given,

$$|\phi\rangle = P^\dagger_1 \dots P^\dagger_N|0\rangle \tag{10}$$

Since all rotational symmetry are broken, only one basis exists. In current work, the triaxial-deformed pairs $P^\dagger_i$ are chosen to be different, where the pair structure coefficients are independent for the different triaxial-deformed pairs.

2.2. Restore Rotational Symmetry

The rotational symmetry can be restored by the standard projection process via quadrature over orthogonal functions. The advantage of the rotation of a state with good total angular momentum J and third component does not mix total angular momentum J, but does mix the third component [15].

$$\hat{R}(\alpha,\beta,\gamma)|JK\rangle = \sum_M D^{(J)}_{M,K}(\alpha,\beta,\gamma)|JM\rangle \tag{11}$$

where $D^{(J)}_{M,K}(\alpha,\beta,\gamma)$ is a Wigner D matrix, $\hat{R}(\alpha,\beta,\gamma)$ is the rotation operator over the Euler angles $\Omega = (\alpha,\beta,\gamma)$

$$\hat{R}(\Omega) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z} \tag{12}$$

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where $\hat{J}_z$ and $\hat{J}_y$ are the generators of rotations about the z and y axes, respectively. The Wigner D functions are the matrix elements of the rotation operator in a basis with good angular momentum quantum numbers, and the Wigner D functions compose of a complete orthogonal set,

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma D^{J'}_{k'm'}(\alpha,\beta,\gamma)^* D^{J}_{km}(\alpha,\beta,\gamma) = \frac{8\pi^2}{2j+1}\delta_{m'm}\delta_{k'k}\delta_{J'J} \tag{13}$$

To carry out angular momentum projection, the collective pairs should be rotated. For the collective pairs with definite angular momentum J and M, the rotation is

$$\hat{R}(\Omega)A^{J\dagger}_M\hat{R}^{-1}(\Omega) = \sum_{M'} D^{J}_{MM'}(\Omega)A^{J\dagger}_M \tag{14}$$

For triaxial-deformed pairs case, the rotation of pairs are given as

$$\hat{R}(\Omega)P^{\dagger}\hat{R}^{-1}(\Omega) = \sum_{JMM'} D^{J}_{MM'}(\Omega)A^{J\dagger}_M \tag{15}$$

Any rotational symmetry broken basis $|\phi\rangle$ is a mixture of states with good angular momenta

$$|\phi\rangle = \sum_{J,i} |\phi; JM_i\rangle \tag{16}$$

where index i are used to distinguish components with same quantum number J but different third component M_i. Applying the rotation operator to the basis,

$$\hat{R}(\Omega)|\phi\rangle = \sum_{J,i}\sum_{M'} D^{J}_{M',M_i}(\Omega)|\phi; JM_i\rangle \tag{17}$$

where M_i indicate the quantum number in initial state, and M' denote the third component in rotated state. The norm matrix elements are projected out by the standard equation,

$$N^{J}_{MK} = \frac{8\pi^2}{2J+1}\int d\Omega \mathcal{D}^{(J)*}_{M,K}(\Omega)\langle\Psi|\hat{R}(\Omega)|\Psi\rangle \tag{18}$$

The Hamiltonian matrix elements are given

$$H^{J}_{MK} = \frac{8\pi^2}{2J+1}\int d\Omega \mathcal{D}^{(J)*}_{M,K}(\Omega)\langle\Psi|\hat{H}\hat{R}(\Omega)|\Psi\rangle \tag{19}$$

Then the generalized eigenvalue problems for every J are solved, where the solutions are labeled by r,

$$\sum_K H^{J}_{MK}g^{(J)}_{K,r} = E_r \sum_K N^{J}_{M,K}g^{(J)}_{K,r}, \tag{20}$$

In this work, we only perform variation after projection on triaxial-deformed basis.

3. Numerical Results

3.1. Axial-Deformed Basis

Usually the collective pairs with lowest angular momenta J, such as S (J = 0), D (J =2) and G (J = 4), are considered. For the low-lying states, these collective pairs should be dominant. The dimension of multi-pair basis increases dramatically when more types of collective pairs are included. Originally those many-pair basis are non-normal and non-orthogonal, the Hamiltonian matrix elements should be transformed to normal orthogonal basis. To this end, one have to diagonalize the norm matrix,

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which are very painful for large configuration space. On the contrary, the dimension of configuration space will be reduced when the rotation symmetry is broken. As shown in Figure 1, the dimension increases slowly for the case with axial-deformed basis, where the angular momentum J of collective pairs are mixed but third component M does not.

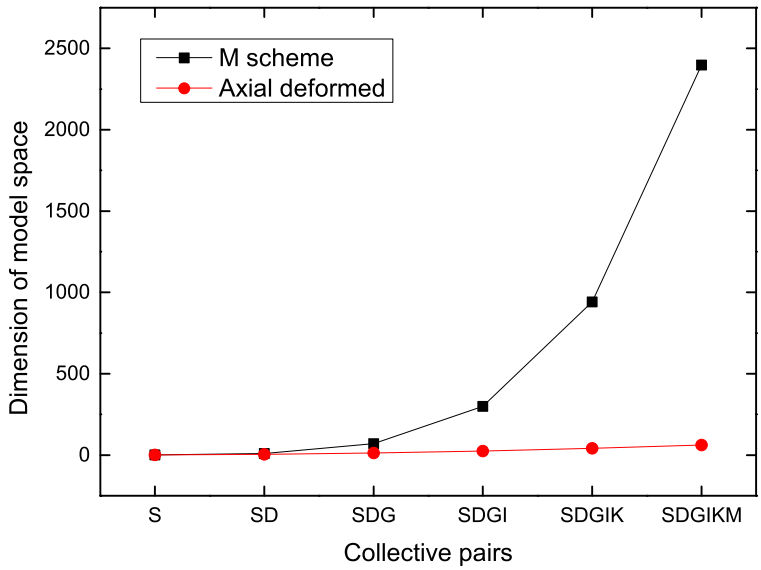

Figure 1. The dimension of configuration space for 3 identical pairs against the types of collective pairs are presented. The spherical basis in M-scheme and the axial-deformed basis are shown. The collective pair S, D, G, I, K and M are the pairs of angular momentum J = 0, 2, 4, 6, 8 and 10, respectively.

As a preliminary report, the low-lying spectrum of ^{138}Sn are studied for axial-deformed basis. We assume that the nucleus ^{132}Sn is a closed core and the 82-126 shell($0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, and $0i_{13/2}$) is chosen as the valence neutrons shell.

The two-body matrix elements of the effective interaction are derived from the CD-Bonn NN potential [44]. The strong short-range repulsion term is renormalized by integrating out the high-momentum components above a certain cutoff momentum Λ [45]. A smooth potential $V_{\mathrm{low}-k}$, keeping the physics of bare nucleon-nucleon interaction up to Λ, is constructed, and can be used in calculations of shell model effective interactions. In this work, Λ is fixed as 2.2 fm^{-1}. Then the shell model effective interaction, with the Coulomb force for protons, is carried out within the framework of $\hat{Q}$-box folded-diagram expansion [46–48]. In this paper, the $\hat{Q}$-box is calculated up to the second order in $V_{\mathrm{low}-k}$.

Our configuration are constructed by SDG collective pairs. Although the angular momentum J of each collective pairs is mixed, the third component M is a good quantum number and the total M of each multi-pair basis is also a good quantum number. The effective Hamiltonian is diagonalized in this subspace and the pair structure coefficients are determined by searching the minimum energy.

The lowest energy levels in each axial-deformed subspace with different third component M in the NPSM are shown in Figure 2, where the shell model calculations are carried out using KSHELL code [49]. It is seen that the results got from the NPSM are close to the SM. The shift of 2^+ level from the NPSM to SM is 0.059 MeV, and the shift of 4^+ is 0.095 MeV. Those results suggest the low-lying levels of ^{138}Sn can be described in the SDG pair subspace. This result suggested that the NPSM can reproduce the spectrum very well with the axial-deformed basis.

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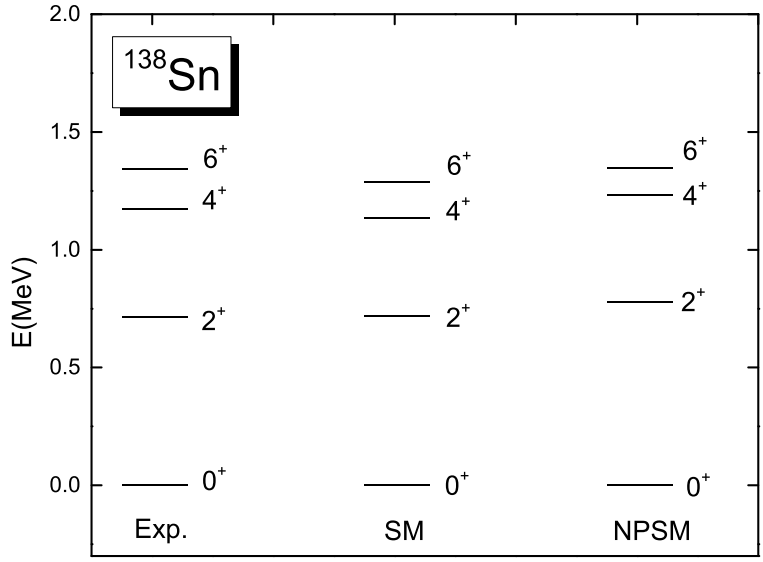

Figure 2. The low-lying spectrum of ^{138}Sn are studied in the shell model and NPSM with axial-deformed basis.

3.2. Triaxial-Deformed Basis

The NPSM was also studied with the triaxial-deformed basis. There are two ways to recover the rotational symmetry: Variation before projection (VBP) and variation after projection (VAP). Here the VAP is used. The low-lying levels of ^{20}O nucleus is studied with the USDA interaction [50]. Only one basis is used for each level in our variation procedure. The results given in Figure 3 show that the NPSM are in consistent with those got in the SM. For example, the first 2^+ level from SM is -21.70088 MeV, the one from NPSM is also -21.70088 MeV, the difference between the SM and NPSM is close to the limit of machine precision.

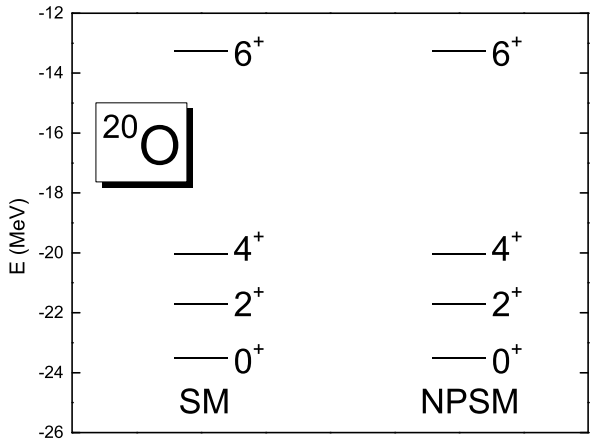

Figure 3. The low-lying spectrum of ^{20}O are studied in the shell model and NPSM with triaxial-deformed basis.

To generate more levels with same angular momenta J, more basis should be used in configuration space. For example, if we want to obtain the second 2^+ states, the first 2^+ level should be calculated first, which can be described by one basis, after determining the parameters for the first basis, the second

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basis are considered in the model space, then the parameters of the second basis are fixed by a variation procedure.

As shown in Figure 4, the lowest 5 levels with J=2 and J=4 are calculated in the SM and NPSM with triaxial-deformed basis. We found that the difference between the NPSM and SM is negligible within the machine precision limit. Those results suggest that if the VAP is adopted, there may be no significant difference between the NPSM and SM.

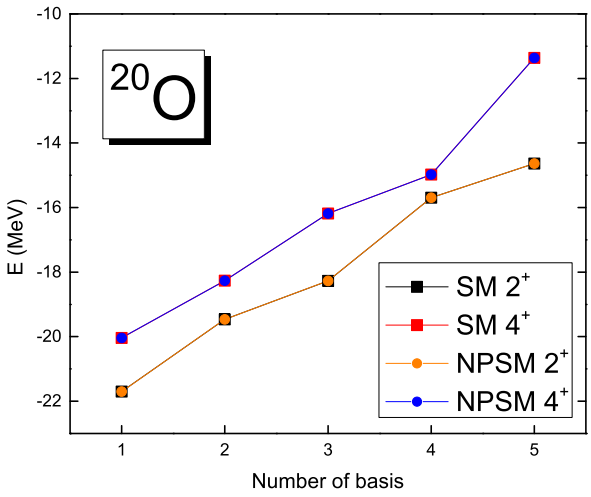

Figure 4. The levels with J=2 and J=4 of ^{20}O are calculated in the SM and NPSM with triaxial-deformed basis.

4. Summary and Discussion

In this paper, the validity of the symmetry broken basis in the NPSM was studied. It was found that the NPSM with axial-deformed basis can reproduce the low-lying spectrum of the half-closed nucleus very well. If the triaxial-deformed basis and variation after projection were used for half-closed nucleus, the difference between the NPSM and SM is negligible. These results may suggest that the axial-deformed basis and triaxial-deformed basis may provide a satisfied description for low-lying spectrum. The case for the proton-neutron coupled open system will be studied in our next work.

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