The structure of the spherical tensor forces in the USD and GXPF1A shell model Hamiltonians^{*}

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Abstract: The realistic shell model Hamiltonians, USD and GXPF1A, have been transformed from the particle-particle (normal) representation to the particle-hole representation (multipole-multipole) by using the known formulation in Ref. [1]. The obtained multipole-multipole terms were compared with the known spherical tensor forces, including the coupled ones. It is the first time the contributions of the coupled tensor forces to the shell model Hamiltonian have been investigated. It has been shown that some coupled-tensor forces, such as $[r^2Y_2 \otimes \sigma]^1$, also give important contributions to the shell model Hamiltonian.

Key words: shell model Hamiltonian, USD, GXPF1A, coupled-tensor force

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1 Introduction

The Shell Model (SM) has been one of the most fundamental theories in nuclear physics. It has been very successful in describing various properties of the low-lying states in light and medium nuclei, such as the binding energies, the spectroscopy and other observables based on the shell model wavefunctions. The key to the success of the SM is the selection of a reliable Hamiltonian. The realistic shell model Hamiltonians, such as the USD [2, 3] in the sd shell, the KB3 [4], FPD6 [5] and GXPF1A [6] in the pf shell, have provided a very good base to study nuclear structure problems microscopically. It is interesting and necessary to investigate the structures of those known Hamiltonians in terms of the spherical tensor forces that are important and thus useful in the construction of new types of shell model Hamiltonians.

A shell model Hamiltonian usually includes a onebody term and a two-body force. Sometimes, if necessary, a three-body force may also be considered [7]. In the present study, we focus on the two body forces which are most widely used. The Hamiltonian can be separated into the monopole part $H_{\rm m}$ and the multipole part $H_{\rm M}$. $H_{\rm m}$ is responsible for the bulk properties, such as binding energies and shell gaps, while $H_{\rm M}$ may provide good spectroscopy.

It is well known that $H_{\rm M}$ is dominated by pairing and quadrupole interactions [1]. Therefore, the modelling with pairing plus quadrupole forces has been very successful in describing various properties of nuclei, especially, for the deformed ones. A typical example is the Projected Shell Model (PSM) [8], which provides a good description of the rotational bands. Other types of tensor forces such as the Gamow-Teller force ($\sigma \tau \cdot \sigma \tau$), octupole and hexadecapole forces are also important parts of the shell model Hamiltonian [1].

However, the importance of the coupled tensor forces, e.g., $[r^l Y_l \otimes \sigma]^{\lambda}$ and $[l \otimes \sigma]^{\lambda}$ (λ is the rank of the coupled tensor), in the shell model Hamiltonian have not yet been analysed. Such analyses are necessary because some coupled-tensor forces have already been found to play important roles, for example, the coupled-tensor forces may lead to dramatic changes in the strength functions of SD and SQ transitions

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[9].

In this paper, we decompose the shell model Hamiltonians into the multipole-multipole form and then investigate various spherical tensor forces associated with those multipole-multipole interactions. The results for the USD and the GXPF1A shell model Hamiltonians are compared.

2 Representations of the Hamiltonian

The shell model Hamiltonian with spin and isospin symmetries can be expressed in the particleparticle representation,

$$H = \sum_{r} \varepsilon_r \hat{n}_r$$

+
$$\sum_{\substack{r \leq s, t \leq u, \\ JT}} V_{rstu}^{JT} \sum_{M, T_z} Z_{MT_z}^{\dagger JT}(rs) Z_{MT_z}^{JT}(tu), \quad (1)$$

where \hat{n}_r is the number operator for the spherical orbit r with quantum numbers (n_r, l_r, j_r) and

$$Z^{\dagger JT}_{MT_{z}}(rs) = (1 + \delta_{rs})^{-1/2} [a^{\dagger}_{r} \otimes a^{\dagger}_{s}]^{JT}_{MT_{z}}$$
(2)

 $[a_r^{\dagger} \otimes a_s^{\dagger}]_{MT_z}^{JT}$ is the creation operator for nucleon pairs in orbits r and s coupled to spin quantum numbers JM and isospin quantum numbers TTz. $Z_{MT_z}^{JT}(tu)$ is the Hermitian conjugate of $Z_{MT_z}^{\dagger JT}(tu)$. A set of the numbers ε_r and V_{rstu}^{JT} determines the Hamiltonian.

The Hamiltonian in Eq. (1), ready for use in a shell model calculation, can be rigorously separated into the monopole part $H_{\rm m}$,

$$H_{\rm m} = \sum_{r} \varepsilon_r \hat{n}_r$$

+
$$\sum_{r \leqslant s, T} V_{rs}^T \sum_{JM, T_z} Z^{\dagger JT}_{MT_z}(rs) Z_{MT_z}^{JT}(rs), \quad (3)$$

where

$$V_{rs}^{T} = \frac{\sum_{J} (2J+1) V_{rsrs}^{JT}}{\sum_{J} (2J+1)},$$
(4)

and the multipole part $H_{\rm M}$,

$$H_{\mathrm{M}} = \sum_{\substack{r \leqslant s, t \leqslant u, \\ JT}} W_{rstu}^{JT} \sum_{M, T_z} Z_{MT_z}^{\dagger JT}(rs) Z_{MT_z}^{JT}(tu), \quad (5)$$

with

$$W_{rstu}^{JT} = \begin{cases} V_{rstu}^{JT} - V_{rs}^{T} \text{ (for } r = t \text{ and } s = u) \\ V_{rstu}^{JT} \text{ (for } r \neq t \text{ or } s \neq u) \end{cases}.$$
(6)

According to the prescription of Ref. [1], $H_{\rm M}$ can be transformed into the particle-hole representation,

$$H_{\rm M} = \sum_{rstu\lambda\tau} (\lambda\tau) f_{rtsu}^{\lambda\tau} [S^{\lambda\tau}(rt) \otimes S^{\lambda\tau}(su)]^{00}, \quad (7)$$

where

$$(\lambda\tau) \equiv \sqrt{(2\lambda+1)(2\tau+1)},\tag{8}$$

$$f_{rtsu}^{\lambda\tau} = \omega_{rtsu}^{\lambda\tau} \sqrt{(1+\delta_{rs})(1+\delta_{tu})}/4, \qquad (9)$$

$$S^{\lambda\tau}_{\mu\tau_z}(rt) = [a^{\dagger}_r \otimes \tilde{a}_t]^{\lambda\tau}_{\mu\tau_z}.$$
 (10)

Here $\tilde{a}_{jm,\tau_z} = (-1)^{j+m+1/2+\tau_z} a_{j-m,-\tau_z}$. Notice that \tilde{a}_t is a good tensor but a_t is not. W_{rstu}^{JT} and $\omega_{rtsu}^{\lambda\tau}$ can be related through equations in Ref. [1].

Replacing pairs by single indices rt = a and su = b, we bring the matrix $f_{ab}^{\lambda\tau} = f_{rtsu}^{\lambda\tau}$ to diagonal form through unitary transformation $u_{ak}^{\lambda\tau}$,

$$f_{ab}^{\lambda\tau} = \sum_{k} u_{ak}^{\lambda\tau} u_{bk}^{\lambda\tau} e_{k}^{\lambda\tau}, \qquad (11)$$

then

$$H_{\rm M} = \sum_{\lambda\tau,k} (\lambda\tau) e_k^{\lambda\tau} [M_k^{\lambda\tau} \otimes M_k^{\lambda\tau}]^{00}, \qquad (12)$$

$$M_{k,\mu\tau_z}^{\lambda\tau} = \sum_{a} u_{ak}^{\lambda\tau} S_{\mu\tau_z}^{\lambda\tau}(a).$$
(13)

On the other hand, let's denote $T^{\lambda\tau}_{\mu\tau_z} = T^{\lambda}_{\mu}(R)T^{\tau}_{\tau_z}(\tau)$ as a product of irreducible spherical tensors in coordinate + spin space (*R*) and the isospin space (τ). Then the tensor force can be constructed as the scalar product of $T^{\lambda\tau}$,

$$T^{\lambda\tau} \cdot T^{\lambda\tau} = (-1)^{\lambda+\tau} (\lambda\tau) [T^{\lambda\tau} \otimes T^{\lambda\tau}]^{00}, \qquad (14)$$

$$T^{\lambda\tau}_{\mu\tau_z} = (\lambda\tau)^{-1} \sum_{rt} \langle r \| T^{\lambda\tau} \| t \rangle S^{\lambda\tau}_{\mu\tau_z}(rt), \quad (15)$$

where $\langle r \| T^{\lambda \tau} \| t \rangle$ is the reduced matrix element of $T^{\lambda \tau}$. Actually, one has

$$\langle r \| T^{\lambda\tau} \| t \rangle = \langle j_r \| T^{\lambda}(R) \| j_t \rangle \langle 1/2 \| T^{\tau}(\tau) \| 1/2 \rangle.$$
 (16)

For convenience, the reduced matrix elements are normalized as

$$v_a^{\lambda\tau} = v_{rt}^{\lambda\tau} = \frac{\langle r \| T^{\lambda\tau} \| t \rangle}{\sqrt{\sum_{r't'} \langle r' \| T^{\lambda\tau} \| t' \rangle^2}}.$$
 (17)

To associate $M_k^{\lambda\tau}$ with the certain irreducible spherical tensor operator $T^{\lambda\tau}$, one can calculate the following quantity,

$$A(M_k^{\lambda\tau}, T^{\lambda\tau}) = \left(\sum_a u_{ak}^{\lambda\tau} v_a^{\lambda\tau}\right)^2.$$
 (18)

The value of $A(M_k^{\lambda\tau}, T^{\lambda\tau})$, ranging from 0 to 1, measures the contribution of the $T^{\lambda\tau}$ force in Eq. (14) to the multipole term $e_k^{\lambda\tau}[M_k^{\lambda\tau} \otimes M_k^{\lambda\tau}]^{00}$. If $A(M_k^{\lambda\tau}, T^{\lambda\tau}) = 1$, $M_k^{\lambda\tau}$ is exactly the same as $T^{\lambda\tau}$. If $A(M_k^{\lambda\tau}, T^{\lambda\tau}) = 0$, there is no relation between $M_k^{\lambda\tau}$ and $T^{\lambda\tau}$. Notice that $u_k^{\lambda\tau}$ vectors form a complete set and we have

$$\sum_{k} A(M_k^{\lambda\tau}, T^{\lambda\tau}) = 1.$$
(19)

3 Calculations and discussions

Among the known shell model Hamiltonians, the USD and the GXPF1A Hamiltonians have been very successful in describing various properties in sd shell nuclei and fp shell nuclei. Their structures in terms of the spherical tensor forces may provide a guidance to construct new types of shell model Hamiltonians useful in new nuclear regions.

In the present calculations, for each $\lambda \tau$, we diagonalize the matrix $f^{\lambda \tau}$ and obtain the eigenvalues $e_k^{\lambda \tau}$ and the corresponding eigenvectors $u_k^{\lambda \tau}$. The value of $e_k^{\lambda \tau}$ measures the strength of the multipole-multipole interaction of $M_k^{\lambda \tau}$. The important terms in Eq. (12) should be those with relatively large $|e^{\lambda\tau}|$. In Fig. 1 and Fig. 2, the locations of $e_k^{\lambda\tau}$ are marked with open stars and the values of $A(M_k^{\lambda\tau}, T^{\lambda\tau})$ have been shown as the columns at the positions of $e_k^{\lambda\tau}$.

The results for USD and GXPF1A Hamiltonians are shown in Fig. 1 and Fig. 2, respectively. The irreducible spherical tensor operators include not only the simple ones, i.e., $\hat{\sigma}$, \hat{l} and $r^{\lambda}Y_{\lambda}$, but also the coupled ones, $[r^{l}Y_{l}\otimes\hat{\sigma}]^{\lambda}$ and $[\hat{l}\otimes\hat{\sigma}]^{\lambda}$, whose contributions to the realistic shell model Hamiltonian have not yet been studied. Just like the vectors of $u_{k}^{\lambda\tau}$ which are orthogonal, we have numerically checked that the $v^{\lambda\tau}$ vectors of the considered tensors are also orthogonal to each other. For simplicity, only those tensors with ranks up to 4 are considered. The operators with negative parity are not considered in the present study since they couple orbits from different main shells and thus vanish in the studied Hamiltonians.

Fig. 1. The structure of the tensor forces in the USD Hamiltonian. The star symbols show the locations of $e^{\lambda \tau}$ in Eq. (12) and the values of $A(M_k^{\lambda \tau}, T^{\lambda \tau})$ have been shown as the columns at the positions of $e_k^{\lambda \tau}$.





Fig. 2. The same as Fig. 1, but for the GXPF1A interaction.

From Fig. 1 and Fig. 2 we can see some common points:

(1) In both Hamiltonians, the most important term is the quadrupole-quadrupole interaction whose $|e^{\lambda\tau}|$ is the largest. The Gamow-Teller interaction $\sigma\tau\cdot\sigma\tau$ and the hexadecapole-hexadecapole interaction are also very important, as has already been turned out in Ref.[1].

(2) For all $\lambda \tau$, the values of $e^{\lambda \tau}$ are distributed around zero and for each λ , the distribution of $e^{\lambda \tau = 1}$ is more compact than that of $e^{\lambda \tau = 0}$, showing that the tensor forces with $\tau = 1$ may generally be less important than those with $\tau = 0$.

Additionally, some details can be seen by comparing USD with GXPF1A:

(1) In the $\lambda \tau = 10$ channel, the important forces are those with tensor $\hat{\sigma}$, \hat{l} and the coupled-tensor $[r^2 Y_2 \otimes \sigma]^1$. In the USD Hamiltonian, $\hat{\sigma}$ and $[r^2 Y_2 \otimes \sigma]^1$ are mixed in the lowest and the second lowest multipole terms and the lowest term is mainly contributed by $\hat{\sigma}$. In GXPF1A, however, the lowest multipole term in total comes from $[r^2Y_2 \otimes \sigma]^1$ and the second lowest one from $\hat{\sigma}$. This fact implies that $[r^2Y_2 \otimes \sigma]^1$ may be more important than $\hat{\sigma}$ in the fp shell model space. The $\hat{l} \cdot \hat{l}$ interaction always takes the highest $\lambda \tau = 10$ term, but the role of $[\hat{l} \otimes \sigma]^1 \cdot [\hat{l} \otimes \sigma]^1$ is not clear, since it lies at the negative side in USD, but the positive side in GXPF1A.

(2) In the $\lambda \tau = 11$ channel of both USD and GXPF1A, apart from the important Gamow-Teller interaction, other values of e^{11} are very close to zero. The e^{11} terms in GXPF1A can be neatly assigned to the known tensors, however, the situation in USD is somewhat complicated.

(3) In the $\lambda \tau = 20$ channel, the quadrupolequadrupole interaction, whose e^{20} is far below the others, is the most important. The second important multipole term should be those with e^{20} right below 1. Surprisingly, from both Fig. 1 and Fig. 2, neither $[r^2Y_2\otimes\sigma]^2$ nor $[\hat{l}\otimes\sigma]^2$ is assigned to the second lowest multipole term, and this problem remains to be answered.

(4) In the $\lambda \tau = 21$ channel, the GXPF1A has a neatly detached $e^{21} = -0.99$ MeV and the assigned operator is $r^2 Y_2 \tau$. In USD, although the $r^2 Y_2 \tau$ operator is also assigned to the lowest $e^{21} = -0.70$ MeV term, however, there is no apparent gap between the lowest and the second lowest terms.

(5) For the channels with $\lambda \ge 3$, one can see that both USD and GXPF1A have very similar features. It should be mentioned that since the r^3Y_3 is a negative parity operator and absent in the present studied Hamiltonians, only the coupled tensors were considered for the $\lambda = 3$ channel. It is seen that the non-negligible tensors for both USD and GXPF1A are r^4Y_4 , $r^4Y_4\tau$, $[r^2Y_2 \otimes \sigma]^3$ and $[r^2Y_2 \otimes \sigma]^3\tau$. All of them are assigned to the lowest or largest $e^{\lambda\tau}$ in their corresponding channels.

4 Summary

The USD and GXPF1A have been widely used in the studies of the sd shell and fp shell nuclei and believed to be good Hamiltonians. These two realistic Hamiltonians, after subtracting the monopole

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parts, have been transformed from the particleparticle representation (normal form) to the particlehole representation (multipole-multipole form) by using the formulation presented in Ref. The [1].obtained multipole-multipole interactions are compared with the known tensor forces, including some coupled-tensor forces, whose contributions to the shell model Hamiltonian have been studied for the first time. The results show that the dominant terms are still the quadrupole-quadrupole, Gamow-Teller and Hexadecapole-Hexadecapole interactions. However, it is found that the coupled-tensor force $[Q \otimes \sigma]^1 \cdot [Q \otimes \sigma]^1$ is even more important than the usually used $\sigma \cdot \sigma$ in the GXPF1A interaction.

Most of the tensor forces considered here can be assigned to the multipole terms with relatively large $|e^{\lambda\tau}|$ values. This aspect may lead to the possibility that the realistic Hamiltonian could be approximately expressed by the combination of those tensor forces and it would be easy to construct a shell model Hamiltonian by properly adjusting the coupling constant for each of the underlying tensor forces.

It should be mentioned that pairing is also a very important part of the shell model Hamiltonian, as it has been pointed out that the monopole pairing and the quadrupole pairing have already been included in the USD and GXPF1 Hamiltonians. The treatment of the pairing together with other particle-particle type forces in the particle-particle representation will been done in the forthcoming paper.

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