Theoretical Description of K-Isomers

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Abstract. A proper treatment of $K$-mixing is the key to understanding $K$-isomers. Here, we present a method based on the projected shell model. This method differs from the usual description of multi-quasiparticle states by introducing a transformation to the laboratory frame and a subsequent configuration mixing in that frame. It allows a quantitative study on the degree of $K$-violation through direct calculations of electromagnetic transitions.

Keywords: K-isomers, K-mixing, projected shell model

PACS: 21.60.Cs, 21.20.-k

INTRODUCTION

Many long-lived, highly-excited isomers in deformed nuclei owe their existence to the approximate conservation of the $K$ quantum number \[1, 2\]. The selection rule for an electromagnetic transition would require that the multipolarity of the decay radiation, $\lambda$, be at least as large as the change in the $K$-value ($\lambda \geq \Delta K$). However, symmetry-breaking processes make possible transitions that violate the $K$-selection rule; such ‘$K$-forbidden’ transitions are hindered, rather than strictly forbidden. Much depending on the degree of the $K$-violation, decays from a high $K$ state to low-lying low $K$ states can have half-lives that range from nanoseconds to years.

It is thus clear that a proper description of $K$-violation in terms of $K$-mixing is at the heart of understanding $K$-isomers. A theoretical model that can treat $K$-mixing has preferably the basis states that are eigenstates of angular momentum $I$. Diagonalization of two-body interactions mixes these states and the resulting wavefunctions contain the information on the degree of $K$-mixing. In this kind of approach, the mixing and its consequences are discussed in the laboratory frame rather than in a body-fixed frame in which $K$ is originally defined.

THE PROJECTED SHELL MODEL

The projected shell model (PSM) \[3, 4\] is a shell model that starts from a deformed basis. In the standard version of the PSM, the shell-model basis is constructed by considering a few quasiparticle (qp) orbitals near the Fermi surfaces and performing angular momentum projection (if necessary, also particle-number projection) on the chosen configurations. With projected multi-qp states as the basis states of the model, the PSM is designed to describe the rotational bands built upon qp excitations \[3, 5\]. The PSM has been rather successful in calculating the high-spin states of normally-deformed and superdeformed nuclei (see, for example, Refs. \[3, 7\]).
In many of the existing calculations, the PSM begins with deformed Nilsson single-particle states, with pairing correlations incorporated into these states by a BCS calculation. This defines a set of deformed qp states (with \( a_\nu^\dagger \) and \( a_\pi^\dagger \) being the creation operator for neutrons and protons, respectively) with respect to the qp vacuum \( |0\rangle \). The PSM basis construction is then implemented in the multi-qp states with the following forms

- e-e nucleus: \( \{ |0\rangle, a_\nu^\dagger a_\nu^\dagger |0\rangle, a_\nu^\dagger a_\nu^\dagger a_\pi^\dagger |0\rangle, a_\nu^\dagger a_\nu^\dagger a_\pi^\dagger a_\pi^\dagger |0\rangle, \ldots \} \)
- o-o nucleus: \( \{ a_\nu a_\pi^\dagger |0\rangle, a_\nu^\dagger a_\nu^\dagger a_\pi^\dagger a_\pi^\dagger |0\rangle, a_\nu^\dagger a_\nu^\dagger a_\pi^\dagger a_\pi^\dagger a_\pi^\dagger |0\rangle, \ldots \} \)
- odd-\( \nu \) nucleus: \( \{ a_\nu |0\rangle, a_\nu a_\nu a_\nu^\dagger |0\rangle, a_\nu a_\pi a_\pi^\dagger a_\pi^\dagger |0\rangle, a_\nu a_\pi a_\pi^\dagger a_\pi^\dagger a_\pi^\dagger |0\rangle, \ldots \} \)
- odd-\( \pi \) nucleus: \( \{ a_\pi |0\rangle, a_\nu a_\nu a_\nu^\dagger |0\rangle, a_\nu a_\pi a_\pi^\dagger a_\pi^\dagger |0\rangle, a_\nu a_\pi a_\pi^\dagger a_\pi^\dagger a_\pi^\dagger |0\rangle, \ldots \} \)

The omitted index for each creation operator contains information on the Nilsson orbitals. In fact, this is the standard way of building multi-qp states. However, the present model goes a step beyond by transforming these states from the body-fixed frame to the laboratory frame and mixing them in the laboratory frame through two-body residual interactions.

The angular-momentum-projected multi-qp states are thus the building blocks in the PSM wavefunction, which can be generally written as

\[
|\psi_M^{I\sigma}\rangle = \sum_\kappa \sum_{I\leq K} f_{IK}^{I\sigma} \hat{P}_K^I |\phi_\kappa\rangle = \sum_\kappa \sum_{I\leq K} f_{IK}^{I\sigma} \hat{P}_K^I |\phi_\kappa\rangle.
\] (1)

The index \( \sigma \) labels states with same angular momentum and \( \kappa \) the basis states. \( \hat{P}_K^I \) is the angular-momentum-projection operator and the coefficients \( f_{IK}^{I\sigma} \) are weights of the basis states.

The weights \( f_{IK}^{I\sigma} \) are determined by diagonalization of the Hamiltonian in the spaces spanned for various nuclear systems as listed above, which leads to the eigenvalue equation (for a given \( I \))

\[
\sum_{\kappa'} (H_{\kappa\kappa'} - E_{\sigma} N_{\kappa\kappa'}) f_{\kappa'}^{I\sigma} = 0.
\] (2)

The Hamiltonian and the norm matrix elements in Eq. (2) are given as

\[
H_{\kappa\kappa'} = \langle \phi_\kappa | \hat{H} \hat{P}_K^I | \phi_{\kappa'} \rangle, \quad N_{\kappa\kappa'} = \langle \phi_\kappa | \hat{P}_K^I | \phi_{\kappa'} \rangle.
\] (3)

Angular-momentum-projection on a multi-qp state \( |\phi_\kappa\rangle \) with a sequence of \( I \) generates a band. One may define the rotational energy of a band (band energy) using the expectation values of the Hamiltonian with respect to the projected \( |\phi_\kappa\rangle \)

\[
E_{\kappa}^I = \frac{H_{\kappa\kappa}}{N_{\kappa\kappa}} = \frac{\langle \phi_\kappa | \hat{H} \hat{P}_K^I | \phi_\kappa \rangle}{\langle \phi_\kappa | \hat{P}_K^I | \phi_\kappa \rangle}.
\] (4)

In a usual approximation with independent quasiparticle motion, the energy for a multi-qp state is simply taken as the sum of those of single quasiparticles. This is the dominant term. The present theory modifies this quantity in the following two steps. First, the band energy defined in Eq. (4) introduces the correction brought by angular
momentum projection and the two-body interactions, which accounts for the couplings between the rotating body and the quasiparticles in a quantum-mechanical way. Second, the corresponding rotational states are mixed in the subsequent procedure of solving the eigenvalue equation (2). The energies are thus further modified by the configuration mixing.

If the deformed states are axially symmetric, each of the basis states in (1), the projected $|\phi_k\rangle$, is a $K$-state. For example, an $n$-qp configuration gives rise to a multiplet of $2^{n-1}$ states, with the total $K$ expressed by $K = |K_1 \pm K_2 \pm \cdots \pm K_n|$, where $K_i$ is for an individual neutron or proton. In this case, shell model diagonalization, i.e. solving the eigenvalue equation (2), is completely equivalent to $K$-mixing. The amount of the mixing can be obtained from the resulting wavefunctions.

The above discussion is independent of the choice of the two-body interactions in the Hamiltonian. In practical calculations, the PSM uses the pairing plus quadrupole-quadrupole Hamiltonian (that has been known to be essential in nuclear structure calculations [12]) with inclusion of the quadrupole-pairing term

$$\hat{H} = \hat{H}_0 - \frac{1}{2} \chi \sum_{\mu} \hat{Q}_\mu^\dagger \hat{Q}_\mu - G_M \hat{P}_\mu^\dagger \hat{P}_\mu - G_Q \sum_{\mu} \hat{P}_\mu^\dagger \hat{P}_\mu.$$ (5)

The strength of the quadrupole-quadrupole force $\chi$ is determined in such a way that it has a self-consistent relation with the quadrupole deformation $\varepsilon_2$. The monopole-pairing force constants $G_M$ are

$$G_M = \left[ G_1 \mp G_2 \frac{N - Z}{A} \right] A^{-1},$$ (6)

with “−” for neutrons and “+” for protons, which reproduces the observed odd–even mass differences in a given mass region if $G_1$ and $G_2$ are properly chosen. Finally, the strength $G_Q$ for quadrupole pairing was simply assumed to be proportional to $G_M$, with a proportionality constant 0.16, as commonly used in the PSM calculations [3].

EXAMPLES

The nucleus $^{178}$Hf has become a center of recent discussion on $K$-isomers. The possibility to trigger the 2.45MeV, 31-year isomer decay by the application of external electromagnetic radiation has attracted much interest and potentially could lead to the controlled release of nuclear energy [13, 14]. Information on the detailed structure and transition of the isomeric and the surrounding states thus becomes a crucial issue. In the PSM calculation for $^{178}$Hf [15], the model basis was built with the deformation parameters $\varepsilon_2 = 0.251$ and $\varepsilon_4 = 0.056$ (values taken from Ref. [16]). Fig. 1 shows the calculated energy levels in $^{178}$Hf, compared with the known data [17]. Satisfactory agreement is achieved for most of the states, except that for the bandhead of the first $8^−$ band and the $14^−$ band, the theoretical values are too low.

It was found that the obtained states are generally $K$-mixed. One may still talk about the dominant structure of each band by studying the wavefunctions. We found that the $6^+$ band has mainly a 2-qp structure $\{v[512]5/2^- \oplus v[514]7/2^-\}$, the $16^+$ band has a 4-qp structure $\{v[514]7/2^- \oplus v[624]9/2^+ \oplus \pi[404]7/2^+ \oplus \pi[514]9/2^-\}$, the first (lower) $8^−$ band has a 2-qp structure $\{v[514]7/2^- \oplus v[624]9/2^+\}$, the second
FIGURE 1. Comparison of the PSM calculation for the rotational bands in $^{178}$Hf with data. This figure is adopted from Ref. [15].

(higher) $8^-$ band has a 2-qp structure $\{ \pi [404]7/2^+ \oplus \pi [514]9/2^- \}$, and the $14^-$ band has a 4-qp structure $\{ \nu [512]5/2^- \oplus \nu [514]7/2^- \oplus \pi [404]7/2^+ \oplus \pi [514]9/2^- \}$. These states, together with many other states (not shown in Fig. 1) obtained from the same diagonalisation process, form a complete spectrum including the high-$K$ isomeric states. Electromagnetic transitions between any two of these states can be directly calculated by using the wavefunctions, as done in the previous publications (see, for example, Refs. [18, 19]). Results will be reported elsewhere.

FURTHER DEVELOPMENTS

The preceding discussions suggest that the projected shell model can be a useful tool for understanding $K$-isomers. So far, not much has been done along these lines except for a few selected applications [15, 20, 21]. Therefore, there is a large room for exploring the usefulness of the model. In addition, three straightforward extensions may be necessary in order to explain some of the current $K$-isomer data.

- **Enlargement of the configuration space** – There have been impressive high-$K$ isomer data suggesting configurations with up to 10-quasiparticles. The current model space of the PSM does not have these configurations and must be enlarged.
- **High-order multipole transitions** – In some examples, violation of the $K$-quantum number can only be understood through electromagnetic transitions with high-order multipolarity. The current PSM code includes only the $B(M1)$ and $B(E2)$ parts. The
high-order transition rates must be considered.

- **The effective forces** – The pairing plus quadrupole Hamiltonian has been proven successful for many of the structure calculations. However, other effects such as the octupole correlation have also been considered important in some cases. Additional terms, such as the monopole-monopole and octupole-octupole interactions, can be included into the model if these are important for certain discussions.

**SUMMARY**

We have shown that the physics of $K$-mixing in multi-qp states is well-incorporated in framework of the projected shell model. The model follows the shell-model philosophy closely and may be viewed as a shell model constructed in a projected multi-qp basis. More precisely, the basis is first built in the qp basis with respect to the deformed-BCS vacuum; then rotational symmetry, violated in the deformed basis, is restored by angular-momentum-projection to form a basis in the laboratory frame; finally a two-body Hamiltonian is diagonalized in the projected multi-qp basis. The model can thus produce fully-correlated shell-model states and can generate well-defined wavefunctions, allowing one to compute, without any approximations, electromagnetic transition probabilities.

**ACKNOWLEDGMENTS**

This work is partly supported by NSF under contract PHY-0140324.

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