

APPLICATION OF THE PFAFFIAN ALGORITHM IN
THE NUCLEAR STRUCTURE STUDY AT HIGH SPINS*

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To expand the multi-quasiparticle (qp) configuration space of the projected shell model, the Pfaffian algorithm is applied to facilitate calculations of the matrix elements. With inclusion of 6-qp states in the projected basis, the yrast band of ^{166}Hf at very high spins is studied, where the observed three anomalies in moment of inertia are well reproduced and explained by the contributions of the 2-qp, 4-qp, and 6-qp states, respectively.

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Nuclei provide us with a natural laboratory to study the interplay between collective and single-particle motions. The ground state of nuclei is a superfluid state with all nucleons coupled pairwise. It has been observed that nuclear rotation can cause a rapid increase in moment of inertia of the nuclei at certain rotational frequency. This phenomenon was explained successfully by pair breaking and alignment of nucleons in orbitals with the highest angular momentum j [1]. As nuclei rotate faster and faster, subsequent pair breakings can occur for the pairs from the next highest j orbitals, forming 4-quasiparticle (qp) states. When approaching the extremes of angular momentum, complex band crossings are expected to occur. In fact, recent experimental measurements have indicated the crucial roles played by 6-qp bands at high spins in $^{166,168}\text{Hf}$ [2, 3].

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It is a challenge to describe this phenomenon in a shell-model framework. The problem lies in the procedure of computing the overlap matrix elements between multi-qp states, which are traditionally calculated with the generalized Wick's theorem [4] that may involve combinatorial complexity when more than 4-qp states are considered. Quite recently, base on the projected shell model (PSM) [5], we have applied an efficient algorithm [6] to calculate the multi-qp matrix elements, which allows us, for the first time, to push the PSM study of the pair-breaking phenomenon to very high spins [7]. As an example, the rotationally induced structural changes of ^{166}Hf are studied.

The PSM begins with a deformed Nilsson+BCS qp basis from which the model space is constructed [5]. For rare-earth nuclei, three major harmonic-oscillator shells are taken in the calculation with $N = 4, 5, 6$ ($N = 3, 4, 5$) for neutrons (protons). The multi-qp configurations up to 6-qp states for even-even nuclei are given as [7]

$$\left\{ |\Phi\rangle, a_{\nu_i}^\dagger a_{\nu_j}^\dagger |\Phi\rangle, a_{\pi_i}^\dagger a_{\pi_j}^\dagger |\Phi\rangle, a_{\nu_i}^\dagger a_{\nu_j}^\dagger a_{\pi_k}^\dagger a_{\pi_l}^\dagger |\Phi\rangle, a_{\nu_i}^\dagger a_{\nu_j}^\dagger a_{\nu_k}^\dagger a_{\nu_l}^\dagger |\Phi\rangle, a_{\pi_i}^\dagger a_{\pi_j}^\dagger a_{\pi_k}^\dagger a_{\pi_l}^\dagger |\Phi\rangle, a_{\nu_i}^\dagger a_{\nu_j}^\dagger a_{\nu_k}^\dagger a_{\nu_l}^\dagger a_{\nu_m}^\dagger a_{\nu_n}^\dagger |\Phi\rangle, a_{\pi_i}^\dagger a_{\pi_j}^\dagger a_{\pi_k}^\dagger a_{\pi_l}^\dagger a_{\pi_m}^\dagger a_{\pi_n}^\dagger |\Phi\rangle, a_{\pi_i}^\dagger a_{\pi_j}^\dagger a_{\nu_k}^\dagger a_{\nu_l}^\dagger a_{\nu_m}^\dagger a_{\nu_n}^\dagger |\Phi\rangle, a_{\nu_i}^\dagger a_{\nu_j}^\dagger a_{\pi_k}^\dagger a_{\pi_l}^\dagger a_{\pi_m}^\dagger a_{\pi_n}^\dagger |\Phi\rangle \right\}, \quad (1)$$

where $a_\nu^\dagger$ ($a_\pi^\dagger$) denote neutron (proton) qp creation operators associated with the qp vacuum $|\Phi\rangle$. The PSM wave function is a linear combination of projected states

$$|\Psi_{IM}^\sigma\rangle = \sum_{K\kappa} f_{IK\kappa}^\sigma \hat{P}_{MK}^I |\Phi_\kappa\rangle, \quad (2)$$

where $|\Phi_\kappa\rangle$ are the qp-states in (1). $\hat{P}_{MK}^I$ is the angular momentum projection operator [5]. The energies and wave functions are obtained by solving the eigenvalue equation

$$\sum_{K'\kappa'} \left(H_{K\kappa, K'\kappa'}^I - E_I^\sigma N_{K\kappa, K'\kappa'}^I \right) f_{IK'\kappa'}^\sigma = 0, \quad (3)$$

with the projected matrix elements of the Hamiltonian and the norm

$$H_{K\kappa, K'\kappa'}^I = \langle \Phi_\kappa | \hat{H} \hat{P}_{KK'}^I | \Phi_{\kappa'} \rangle, \quad N_{K\kappa, K'\kappa'}^I = \langle \Phi_\kappa | \hat{P}_{KK'}^I | \Phi_{\kappa'} \rangle. \quad (4)$$

The central task in numerical calculations is to evaluate rotated matrix elements in the Hamiltonian and the norm

$$\mathcal{H}_{\kappa\kappa'} = \langle \Phi_\kappa | \hat{H}[\Omega] | \Phi_{\kappa'} \rangle, \quad \mathcal{N}_{\kappa\kappa'} = \langle \Phi_\kappa | [\Omega] | \Phi_{\kappa'} \rangle, \quad (5)$$

with the operator $[\Omega] = \hat{R}(\Omega)/\langle\Phi|\hat{R}(\Omega)|\Phi\rangle$ [5]. Since $\mathcal{H}_{\kappa\kappa'}$ can be decomposed into terms expressed by the “linked” contraction and $\mathcal{N}_{\kappa\kappa'}$ [5], the main task then concentrates on treating efficiently $\mathcal{N}_{\kappa\kappa'}$, which can be rewritten as the following explicit form

$$\mathcal{N}_{\kappa\kappa'} = \langle\Phi|a_1 \cdots a_n[\Omega]a_1^\dagger \cdots a_{n'}^\dagger|\Phi\rangle. \quad (6)$$

It was pointed out [6] that in applying the generalized Wick’s theorem, a matrix element of Eq. (6) involving n and n' qps, respectively in the left-hand and right-hand side of $[\Omega]$, contains $(n + n' - 1)!!$ terms. In practice, the number of terms becomes so large that it is nearly impossible to write down expressions explicitly for more than 4-qp states.

By using the Fermion coherent state and Grassmann integral, a general expression for (6) in terms of the Pfaffian can be derived [6]

$$\langle\Phi|a_1 \cdots a_n[\Omega]a_1^\dagger \cdots a_{n'}^\dagger|\Phi\rangle = \text{Pf}(X) = \text{Pf} \begin{pmatrix} B & C \\ -C^T & A \end{pmatrix}, \quad (7)$$

where X is a skew-symmetric matrix with dimension $(n + n') \times (n + n')$. The indices of rows and columns for B run from 1 to n ($1, \dots, n$) and the ones for A run from $1'$ to n' ($1', \dots, n'$). For matrix C in Eq. (7), the indices of rows run from 1 to n and those of columns run from $1'$ to n' . The Pfaffian is defined as

$$\text{Pf}(\mathcal{A}) \equiv \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i=1}^n a_{\sigma(2i-1)\sigma(2i)} \quad (8)$$

for a skew-symmetric matrix $\mathcal{A}$ with dimension $2n \times 2n$, of which matrix elements are a_{ij} . The symbol σ is a permutation of $\{1, 2, 3, \dots, 2n\}$, $\text{sgn}(\sigma)$ is its sign, and S_{2n} represents a symmetry group. This makes it possible and efficient to work with the expanded PSM configuration in (1).

For the calculation, we employ the Hamiltonian with separable forces

$$\hat{H} = \hat{H}_0 - \frac{1}{2}\chi_{QQ} \sum_{\mu} \hat{Q}_{2\mu}^\dagger \hat{Q}_{2\mu} - G_M \hat{P}^\dagger \hat{P} - G_Q \sum_{\mu} \hat{P}_{2\mu}^\dagger \hat{P}_{2\mu}, \quad (9)$$

where $\hat{H}_0$ is the spherical single-particle term including the spin-orbit force, and the rest is the quadrupole+pairing type of interactions, with inclusion of the quadrupole-pairing term.

Figure 1 shows the so-called back-bending plot for ^{166}Hf , where twice the moment of inertia, 2Θ , is plotted as a function of square of rotational frequency ω^2 . In the calculation, the deformation parameters are fixed as $\varepsilon_2 = 0.208$ and $\varepsilon_4 = 0.013$ taken from Ref. [8]. Anomalies in 2Θ can be

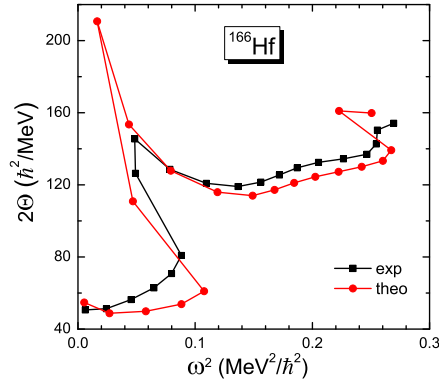


Fig. 1. (Color online) Back-bending plot for ^{166}Hf . The calculated results are compared with the data taken from Ref. [2]. This figure is taken from Fig. 1 of Ref. [7].

clearly seen as ω increases, roughly at $\omega^2 \approx 0.10, 0.15$ and 0.25 , corresponding to spin $I \approx 12, 24$ and 34 , respectively. The first anomaly exhibits the largest effect, causing a sharp increase in 2Θ . This is known as the first back-bending, corresponding to breaking and alignment of a neutron $i_{13/2}$ pair. The second anomaly in Fig. 1 corresponds to the small increase in 2Θ at $\omega^2 \approx 0.15$, which is nicely reproduced by the PSM. At this rotational frequency, an additional $h_{11/2}$ proton pair is broken and their spins are aligned along the axis of rotation. The third anomaly belongs to the few known cases that have ever been observed: 2Θ jumps suddenly again at $\omega^2 \approx 0.25$. The observation is correctly described by the present calculation, and is understood as a simultaneous breaking of two neutron $i_{13/2}$ pairs and one $h_{11/2}$ proton pair.

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