Nuclear structure of $^{178}$Hf related to the spin-16, 31-year isomer
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ABSTRACT: The projected shell model is used to study the multi-quasiparticle and collective excitations of $^{178}$Hf. With an axially symmetric basis, the spin-16 isomer at 2.4 MeV appears to be well separated in energy/spin space from other configurations. However, projected energy surface calculations suggest that $^{178}$Hf has significant softness to axially asymmetric shapes, which can strongly modify the level distribution. The implications for photodeexcitation of the isomer are discussed.

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Long-lived isomers – excited nuclear states with inhibited electromagnetic decay – may be considered to offer a form of energy storage [12]. The possibility to trigger the decay by the application of external electromagnetic radiation has attracted much interest and potentially could lead to the controlled release of nuclear energy. First reports of the triggering of the spin-16, 2.4 MeV isomer in $^{178}$Hf with low-energy ($< 100$ keV) photons [3, 4, 5] have, however, been refuted [6, 7]. Meanwhile, the threshold photon energy for triggering the isomer remains unknown. This situation contrasts with the recent determination of a threshold triggering energy of 1.01 MeV for the spin-9, 75 keV isomer in $^{180}$Ta [8], and subsequently the discrete intermediate states involved in the excitation/deexcitation pathway have been identified [9]. The significantly higher energy of the $^{178}$Hf isomer leads to the expectation of a lower triggering threshold, on account of the higher level density, even allowing for the pairing difference between the even-even and odd-odd nucleon numbers in $^{178}$Hf and $^{180}$Ta, respectively. The higher isomer energy in $^{178}$Hf also leads to greater potential with regard to the utility of triggered energy release.
The two-step process of triggered gamma-ray emission is depicted schematically in Fig. 1. A nucleus in an isomeric state is first excited to an intermediate state by absorption of an incident photon. An intermediate state may serve as a "gateway" that connects the isomer to the ground state (g.s.). If the selection rules for transitions between the gateway and the g.s. are fulfilled, then enhanced gamma-decay, usually a multi-step gamma-cascade, is expected to occur. In determining the favourable conditions for triggering gamma-ray emission from the isomer, it is necessary to have information on the structure of possible gateway states, as well as possible paths of electromagnetic transitions to and from these states. Experimentally, only a few states close to the $^{178}$Hf isomer have been observed and documented in the literature [10,11]. The purpose of the present letter is twofold: to demonstrate that the projected shell model (PSM) [12] is an appropriate theory for studying high-spin isomers and associated excitations, including potential gateway states; and to show that in the $^{178}$Hf case, in order to trigger emission from the $^{16+}$ isomer with low-energy photons, a series of external excitations via gateway states may be necessary. In addition, the gateway states should be sufficiently mixed with low-$K$ components.

The long half-life (31 years) of the 2.4 MeV isomer in $^{178}$Hf is to a large extent dependent on the approximate conservation of the $K$ quantum number, where $K$ is the projection of the angular momentum on the body-fixed symmetry axis. The isomer has $K^\pi = 16^+$. Spontaneous electromagnetic transitions from a high-$K$ state to a lower-energy, low-$K$ state are strongly hindered by the $K$ selection rule [13], $|\Delta K| \leq \lambda$, with $\lambda$ being the transition multipolarity. The spontaneous decay of the $^{178}$Hf isomer involves inhibition factors of close to 100 per degree of $K$ forbiddenness, $\nu = \Delta K - \lambda$, with total inhibition $\approx 100^\nu$ [14]. This strong inhibition supports the view that $^{178}$Hf has an axially symmetric intrinsic shape.

In a deformed, axially symmetric nucleus, a high-$K$ state is made by summing the contributions from several unpaired quasiparticles. An $n$-quasiparticle ($n$-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. Among the $2^{n-1}$ states, the state with the highest $K$ value, $K = \sum_i |K_i|$, is usually energetically favoured.
and the most likely to form an yrast state (lowest energy state for a given angular momentum). Deformed nuclei with \( A \approx 180 \) have several high-\( K \) single-particle (both neutron and proton) orbitals close to the Fermi surface, and several multi-qp high-\( K \) states in this mass region are found to be yrast \([15,16]\).

The physics of multi-qp states is well incorporated in the PSM framework. The PSM follows closely the shell-model philosophy, and in fact is a shell model constructed in a deformed 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 \([17]\) to form a rotational-invariant basis in the laboratory frame; finally a two-body Hamiltonian is diagonalised in the projected basis. In contrast to mean-field methods \([18]\) employed in the study of multi-qp states, the PSM can produce fully correlated shell-model states, and can generate well-defined wave functions, allowing us to compute, without further approximations, the quantities such as transition probabilities.

Starting from the deformed Nilsson scheme \([19]\) plus a subsequent BCS calculation, one builds the shell model space (for even-even systems) through multi-qp states:

\[
|\phi_\kappa\rangle = \{ |0\rangle, \alpha_{n_i}^\dagger \alpha_{n_j}^\dagger |0\rangle, \alpha_{p_k}^\dagger \alpha_{p_l}^\dagger |0\rangle, \alpha_{n_i}^\dagger \alpha_{n_j}^\dagger \alpha_{p_k}^\dagger \alpha_{p_l}^\dagger |0\rangle, \ldots \},
\]

where \( \alpha^\dagger \) is the creation operator for a qp and the index \( n \) (or \( p \)) denotes neutron (or proton) Nilsson quantum numbers which run over the low-lying orbitals. The qp states are defined in a space with three major shells (\( N = 4, 5, 6 \) for neutrons and \( N = 3, 4, 5 \) for protons). The corresponding qp vacuum is \(|0\rangle\).

In the case that the nuclear potential is axially symmetric, the basis states in (1) are labelled by \( K \). Thus, the projected multi-qp \( K \)-states are the building blocks in our shell-model wave function

\[
|\Psi_M^{I\sigma}\rangle = \sum_\kappa f_\kappa^{I\sigma} \hat{P}_M^{I\sigma} |\phi_\kappa\rangle.
\]

In Eq. (2), \( \kappa \) labels the basis states and \( \sigma \) the states with the same angular momentum. \( \hat{P}_M^{I\sigma} \) is the angular momentum projector \([17]\). The coefficients \( f_\kappa^{I\sigma} \) in Eq. (2) are determined by diagonalisation of the Hamiltonian. Diagonalisation is the process of configuration mixing (here, \( K \)-mixing). Thus, the required physics, \( i.e. \) constructing multi-qp states with good angular momentum and parity and mixing these states through residual interactions, is properly incorporated in the model. Electromagnetic transition probabilities can be directly computed by using the resulting wave functions.

The Hamiltonian employed in the PSM \([12]\) is

\[
\hat{H} = \hat{H}_0 - \frac{1}{2} \chi \sum_\mu \hat{Q}_\mu^\dagger \hat{Q}_\mu - G_M \hat{P}_M^\dagger \hat{P} - G_Q \sum_\mu \hat{P}_\mu^\dagger \hat{P}_\mu,
\]
where $\hat{H}_0$ is the spherical single-particle Hamiltonian, which contains a proper spin–orbit force [19]. The other terms in Eq. (3) are quadrupole-quadrupole, and monopole- and quadrupole-pairing interactions, respectively. 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

$$G_M = \left[20.12 \mp 13.13 \frac{N-Z}{A}\right] A^{-1},$$

with “−” for neutrons and “+” for protons, which reproduces the observed odd–even mass differences in the mass region. Finally, the strength parameter $G_Q$ for quadrupole pairing was simply assumed to be proportional to $G_M$, with a proportionality constant 0.16, as commonly used in PSM calculations [12].

For $^{178}\text{Hf}$, the model basis is built with the deformation parameters $\varepsilon_2 = 0.251$ and $\varepsilon_4 = 0.056$. These values are taken from the literature [20]. Fig. 2 shows the calculated energy levels in $^{178}\text{Hf}$, compared with the known data [10]. 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. The dominant structure of each band can be read from the wave functions. We found that the $6^+$ band has a 2-qp structure $\{\nu[512]_{\frac{5}{2}^-} \oplus \nu[514]_{\frac{7}{2}^-}\}$.
the 16$^+$ band has a 4-qp structure $\{\nu[514]_{5/2}^- \oplus \nu[624]_{9/2}^+ \oplus \pi[404]_{7/2}^+ \oplus \pi[514]_{9/2}^-\}$, the first (lower) 8$^-$ band has a 2-qp structure $\{\nu[514]_{5/2}^- \oplus \nu[624]_{9/2}^+\}$, the second (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. 2) obtained from the same diagonalisation process, form a complete spectrum including the high-$K$ isomeric states and candidate gateway states.

In order to study the possible gateway states through which triggered isomeric emissions might occur, in Fig. 3 we plot the high-$K$ bands lying close in energy to the 16$^+$ isomer. We plot also the calculated lower 8$^-$ band via which the gamma-cascade could reach the g.s. The 16$^+$ isomeric band is found to be yrast, above which there are many other 4-qp high-$K$ bands with either positive or negative parity. It can be seen from Fig. 3 that the 16$^+$ isomeric band is well separated from the other bands, leaving an energy gap of nearly 500 keV. However, the bandhead energies of the other high-$K$ bands are not much higher than the 16$^+$ isomer, and an external energy of $<100$ keV may be able to excite the 16$^+$ isomer.

A close look at Fig. 3 suggests, however, that in order to excite the 16$^+$ isomer to the states of the 8$^-$ band, a series of external excitations may be necessary, otherwise the deexcitation would return to the original isomer. The excitation may proceed stepwise among the gateway states, until it arrives in a low-$K$ state (a possible state is a member of the 8$^-$ band) from which spontaneous decay to the g.s. is possible. Of course, if such a multi-step excitation is required, then the probability would be very low. In addition, in order to link to the 8$^-$ band, the gateway states should contain sufficient $K \approx 8$ components. The latter requirement is usually difficult to fulfill in an axially symmetric nucleus; however, the discussion below may open a possibility, through non-axial distortions.

The picture shown in Fig. 3 has been obtained by assuming an axial basis, and it could be modified if the nucleus exhibits significant deviation from the axial shape. The amount of triaxial deformation is given by an additional deformation parameter, $\gamma$. To see if the $\gamma$ degree of freedom plays a role in $^{178}$Hf, we have newly extended the capability of the PSM to study energy surfaces as a function of the two quadrupole deformation parameters, $\varepsilon_2$ and $\gamma$, based on exact projection calculations in three-dimensional Euler space [21][22]. Here, we calculate the angular-momentum-projected energies having the form

$$E^I(\varepsilon_2, \gamma) = \frac{\langle \phi(\varepsilon_2, \gamma) | \hat{H} \hat{P}^I | \phi(\varepsilon_2, \gamma) \rangle}{\langle \phi(\varepsilon_2, \gamma) | \hat{P}^I | \phi(\varepsilon_2, \gamma) \rangle}. \quad (5)$$

For comparison, the unprojected energy surfaces are also calculated. The unprojected energy contains a mixture of states with good angular momenta.

Energy surfaces for states with angular momentum $I = 0, 2, \cdots, 10$ are plotted in Fig. 4. The left part of Fig. 4 shows the energies as a function of $\varepsilon_2$ with $\gamma = 0$. A minimum at $\varepsilon_2 = 0.25$ is seen, which is consistent with the use of $\varepsilon_2 = 0.251$ in the calculations of Figs. 2 and 3. The unprojected energy surface has a similar form, but the minimum has a slightly smaller $\varepsilon_2$ value. In the right part of Fig. 4, energies are calculated as a function of $\gamma$, with the minimum value of $\varepsilon_2 = 0.25$. It is interesting to observe that the unprojected surface has a minimum at $\gamma = 0$, suggesting that this nucleus is axially

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symmetric. However, the projected surfaces exhibit a qualitatively different pattern: For all the spin states with $I = 0, 2, \cdots, 10$, the energies with small $\gamma$ are almost constant, and they start to rise only for $\gamma > 15^\circ$. This suggests a softness to axially asymmetric shapes. Note that such qualitative differences between projected and unprojected calculations have been discussed before in another context [23].

Nuclei having flat energy surfaces in the $\gamma$ direction have recently been suggested [24] to be critical point nuclei sitting in the transitional region between the axially deformed and triaxially deformed phases. The energy surfaces in Fig. 4 indicate that $^{178}$Hf has a character close to that of critical point nuclei with considerable $\gamma$ softness. Therefore, the $\gamma$ degree of freedom may play a significant role in this nucleus. Xu et al. [25] studied the importance of $\gamma$ deformation for high-$K$ bandheads in $^{178}$W and $^{182}$Os, and for some hafnium isotopes [26]. While axial symmetry was predicted for the hafnium cases, the calculations for multi-qp states were restricted to bandhead shapes and energies, and not the associated rotational excitations. Our calculations now suggest that $^{178}$Hf exhibits a significant $\gamma$ softness already near its ground state. The $\gamma$ softness may strongly enhance excitation of the gateway states. However, an extension of the PSM for the description of multi-qp states, with the $\gamma$ degree of freedom explicitly included, does not yet exist.

To summarise, in the PSM the multi-qp states with good angular momentum serve as the building blocks, and mixing of these states is incorporated through two-body residual interactions. Our calculations for $^{178}$Hf show that the $16^+$ isomer lies well separated in energy from other states, suggesting that a series of external excitations may be necessary to trigger isomeric emission. However, axially asymmetric energy-surface calculations show that in $^{178}$Hf there is considerable $\gamma$ softness. This fact, in the context of recent discussions of critical point nuclei [24], indicates that not only this particular example,
Figure 4. Energy surfaces for states with angular momentum $I = 0, 2, \ldots, 10$. The energies are calculated as function of (a) quadrupole deformation $\varepsilon_2$ with $\gamma = 0$, and (b) $\gamma$ deformation with $\varepsilon_2 = 0.25$. Full (dashed) curves correspond to projected (unprojected) calculations.

but also other nuclei in this mass region, may be significantly influenced by the $\gamma$ degree of freedom. The $\gamma$-softness may strongly enhance excitation of the gateway states, in favour of triggering isomer decay. To describe multi-qp states properly, and to further guide experiments in finding candidate nuclei for triggered gamma-ray emission, an advanced theory following the projected shell model concept, with the $\gamma$ degree of freedom included, is very much desired. Work along these lines is in progress.

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