Fission of SHN & its hindrance: odd nuclei & isomers.*

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After shortly analyzing data relevant to fission hindrance of odd-A nuclei and high-$K$ isomers in superheavy (SH) region we point out the inconsistency of current fission theory and propose an approach based on the instanton formalism. A few results of this method, simplified by replacing selfconsistency by elements of the macro-micro model, are given to illustrate its features.

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1. Introduction

Occurrence of isomers - relatively long-lived excited states - is well established in many nuclei, including SH region, see e.g. [1]. It is believed that the approximate conservation of the high-$K$ quantum number (related to the axial symmetry of a nucleus) combined with the low excitation result in the hindrance of their electromagnetic decay. The macro-micro model based on the deformed Woods-Saxon (W-S) potential predicts [2, 3, 4] high-$j$ orbitals lying close to the Fermi level in $Z = 102 - 110$ nuclei. This explains presence of known isomers and suggests both new ones and high-$K$ ground- or low-lying states in odd and odd-odd nuclei. Such states could live longer than the ground states (g.s.) which makes the study of their stability, and in particular, of their spontaneous fission (SF), very interesting.

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Table 1. Fission half-lives and hindrance factors for the K-isomers and ground states in the first well.

| Nucleus | $K^*$ | $T_{sf}(g.s.)$  | $T_{sf}(izo)$  | HF = $T_{sf}(izo)/T_{sf}(g.s.)$ |
|---------|-------|------------------|------------------|-------------------------------|
| $^{250}\text{No}$ | 9     | 3.7 $\mu$s       | > 45 $\mu$s      | > 10                          |
| $^{254}\text{No}$ | 10    | $3\times10^4$ s  | 1400 s           | $\approx 10^3$                |
| $^{254}\text{Rf}$ | 11    | 23 $\mu$s        | > 50 $\mu$s      | > 2                           |

2. SF hindrance in odd nuclei & isomers

It is known that fission half-lives of odd nuclei are 3-5 orders of magnitude longer than those of their even-even neighbours - see e.g. the recent review [5]; slightly smaller odd-even hindrance is observed for fission isomers in actinides [6]. This phenomenon is usually attributed to the specialization energy - increase in fission barrier due to configuration ($K$-number) constraint. Notice, however, that such increase should depend on the $\Omega$ (projection of the angular momentum on the symmetry axis) of the odd orbital, because of smaller level densities for larger $\Omega$, while the data contradict this. [5].

The data on fission hindrance of high-$K$ isomers in heaviest nuclei are given in Table B and Fig. 13 in [7]. After eliminating likely erroneous point for $^{262}\text{Rf}$ - see [5], the one for $^{256}\text{Fm}$, based on only two observed fission events [8], and not much informative lower bounds on $T_{sf}(izo)$ (i.e. much smaller than $T_{sf}(g.s.)$), only data for $^{250}\text{No}$ [9] and $^{254}\text{No}$ [10] are left. The recent measurement [11] added new data on $^{254}\text{Rf}$. All three are given in Tab. 1, and may be prudently summarized by saying that hindrance factors HF = $T_{sf}(izo)/T_{sf}(g.s.) > 10$ are possible. Data on multiple fission isomers in even-even actinides [6], when interpreting higher-lying ones as high-$K$ configurations in the second well, suggest HF = 1-10 for Pu isotopes and $10^3$-$10^4$ in Cm isotopes.

Within the present theory, the fission hindrance is related to the blocking mechanism: one blocked orbital corresponds to a configuration of an odd nucleus, two blocked orbitals give rise to a 2 quasi-particle isomer in an even-even nucleus, etc. One expects an increase in energy of the isomeric configuration $E_{conf}$, which involves a specialization energy for blocked orbitals, relative to the adiabatic one over a whole region of deformation. In general, this modifies both the shape and height of the isomer fission barrier in comparison to that of the g.s., as it follows from energy landscape $E_{conf} - E_{exc}$, with $E_{exc}$ - the excitation energy of the isomer above the g.s. Specialization energy must depend both on the symmetry of the barrier configuration and the dynamics. While the data suggest that specialization energy increases the barrier in some cases, very large isomeric vs. g.s. fission barrier
increase is obtained in calculations for many configurations with blocked high-Ω orbitals. In Fig. 1 we show energy landscapes around and beyond the second minimum in $^{242}$Cm: the adiabatic one and for a fixed $K = 10$ state (no intrinsic parity is indicated as the reflection symmetry is broken), corresponding to the $K^\pi = 10^-$, dominantly $\nu 11/2^+ [615], \nu 9/2^- [734]$ configuration in the II-nd well, a unique candidate for a high-$K$ isomer there.
Huge rise of the fission barrier height and width for the isomer relative to the adiabatic one can be seen in Fig. 1. In view of this, the experimental relative HF [6] for two shape isomers in $^{242}$Cm might be understood as coming solely from the hindrance of the EM decay to the g.s. in the II-nd well, with the subsequent fission of the latter. Another calculated large rise in barrier due to blocking the high-$\Omega$ orbitals may be seen in Fig. 3 in [4], this time for the predicted $K^\pi = 12^-$ g.s. of the SH odd-odd nucleus $^{272}$Mt.

Triaxiality of the fission saddle could decrease specialization energy as well as odd-even and isomeric HFs. Another mechanism acting in this direction would be a non-selfconsistent variation of pairing gaps, minimizing the action $\int \sqrt{2B(q)(V(q) - E)dq}$, proposed in [12] ($q$ -deformation, $B(q)$ - mass parameter, $V(q)$ - deformation energy and $E$ - g.s. energy). Based on an earlier idea of [13] and calculations [14], this interesting result is, however, doubtful since: 1) the cranking formula for inertia was used as a general one, 2) an analog of the velocity - momentum constraint, crucial for the condition of minimal action, was ignored. As we show below, the lack of a proper inertia parameter is the main obstacle in the treatment of fission of a system with blocked levels.

3. Failure of the standard SF rate evaluation with blocked states

In even-even nuclei, pairing provides an energy gap of at least $2\Delta$ between the g.s. and the lowest 2 q.p. excitation; this amounts to more than 1 MeV in heavy nuclei. One can thus assume that there are no sharp level crossings of a many-body system and that the adiabatic approximation can be applied. This leads to the well-known cranking formula for the inertia parameter, which can be used to compose action integral and minimize it over various fission trajectories.

The situation changes drastically for odd and odd-odd nuclei. In such a case, the neutron or proton contribution to the cranking mass parameter $B_{q,q_j}$, derived as if the adiabatic approximation were legitimate, reads:

$$B_{q,q_j} = 2\hbar^2 \left[ \sum_{\mu,\nu \neq \nu_0} \frac{\langle \mu | \frac{\partial \hat{H}}{\partial q_i} | \nu \rangle \langle \nu | \frac{\partial \hat{H}}{\partial q_j} | \mu \rangle}{(E_\mu + E_\nu)^3} (u_\mu v_\nu + u_\nu v_\mu)^2 \right]$$

$$+ \frac{1}{8} \sum_{\nu \neq \nu_0} \left( \frac{\varepsilon_\mu \partial \Delta}{\partial q_i} - \Delta \frac{\partial \varepsilon_\mu}{\partial q_i} \right) \left( \frac{\varepsilon_\nu \partial \Delta}{\partial q_j} - \Delta \frac{\partial \varepsilon_\nu}{\partial q_j} \right) \frac{E_\mu^5}{E_\nu^5}$$

$$+ 2\hbar^2 \sum_{\nu \neq \nu_0} \frac{\langle \nu | \frac{\partial \hat{H}}{\partial q_i} | \nu_0 \rangle \langle \nu_0 | \frac{\partial \hat{H}}{\partial q_j} | \nu \rangle}{(E_\nu - E_{\nu_0})^3} (u_\nu u_{\nu_0} - v_\nu v_{\nu_0})^2.$$
Here, the ground state corresponds to the odd nucleon occupying the orbital $\nu_0$. It is assumed that the one pairing gap $\Delta$ and one Fermi energy $\lambda$ describe simultaneously the g.s. and its two-quasiparticle excitations: those with the odd particle in the state $\nu_0$ (which give contribution in the square bracket) and those with the odd particle in the state $\nu \neq \nu_0$ and the orbital $\nu_0$ paired (whose contribution is in the third line of the formula). The quantity $\tilde{\varepsilon}_\nu$ is defined by $\tilde{\varepsilon}_\nu = \varepsilon_\nu - \lambda$, $u$ and $v$ are the usual BCS occupation amplitudes. It is clear that this expression is invalid whenever a close avoided crossing is encountered, as the contribution proportional to $(E_{\nu_0} - E_{\nu_0})^{-3}$ is nearly singular there. Moreover, due to a partial occupation of levels, the singularity may come about from a degeneracy of the quasiparticle energies of orbitals at the opposite sides of the Fermi level. Already these two reasons make the cranking formula unusable. But there is still another deficiency: a departure from the symmetry preserved on a part of the fission trajectory produces a negative contribution to the inertia parameter whose magnitude would depend on the proximity of the relevant level crossing and could dominate the whole expression. Therefore a more suitable method which goes beyond the adiabatic approximation is needed.

4. Instanton motivated approach to SF of odd nuclei & isomers

Our idea is based on the instanton formalism applied to the SF process, which was formulated for the mean-field setting in [15], [16] and further investigated in [17]. The instanton equations given there read:

\[ \hbar \frac{\partial \phi_i(\tau)}{\partial \tau} = (\zeta_i - \hat{h}(\tau))\phi_i(\tau), \]

which are basically the time dependent Hartree-Fock equations transformed to the imaginary time $t \to -i\tau$ with a periodicity fixing term $\epsilon_k \phi_k$ (since the bounce solutions should fulfill the periodicity condition $\phi_k(-T/2) = \phi_k(T/2)$). In these equations, $\phi_i$, $i = 1, ..., N$ are the single-particle (s.p.) states composing the $N$-body Slater state and $\zeta_i$ are the Floquet exponents which for the selfconsistent instanton would be equal to the s.p. energies at the metastable minimum, $\zeta_i = \epsilon_i(q_{min})$. However, for a finite imaginary-time interval $[-T/2, T/2]$, $\zeta_i \neq \epsilon_i(q_{min})$, although they tend to this limit when $T \to \infty$. The Eq. (2) conserve the overlaps $\langle \phi_i(-\tau) | \phi_j(\tau) \rangle = \delta_{ij}$. The instanton action is given by:

\[ S = \hbar \int_{-T/2}^{T/2} d\tau \sum_{i=1}^{N} \langle \phi_i(-\tau) | \partial_\tau \phi_i(\tau) \rangle = \int_{-T/2}^{T/2} d\tau \sum_{i=1}^{N} \langle \phi_i(-\tau) | \zeta_i - \hat{h}(\tau) | \phi_i(\tau) \rangle. \]
The Eq. (2) are more difficult to handle than their real-time counterparts since the selfconsistent Hamiltonian $\hat{h}[\phi^*(-\tau), \phi(\tau)]$ is now nonlocal in $\tau$.

Here we replace the selfconsistent mean field in (2) by the phenomenological Hamiltonian with a deformed W-S potential. This can be viewed as a simplification of a selfconsistent theory to a macro-micro version. In this approach the collective velocity $\dot{q}$ must be provided as an external information. We take it from:

$$B_{even}(q)\dot{q}^2 = 2(V(q) - E), \quad (4)$$

where $q$ is a collective coordinate (e.g. the quadrupole moment) along a chosen path through the barrier, $E$ is the g.s. energy, $V(q)$ - potential energy, and $B_{even}(q)$ - inertia parameter for the neighbouring even-even nucleus.

In solving the equations with the W-S potential we restrict to the subspace of the $N$ adiabatic orbitals $\psi_\mu(q)$. In this subspace, there are $N$ bounce solutions $\phi_i(\tau)$, each of which tends to the s.p. orbital $\psi_i(q_{\text{min}})$ at the metastable minimum as $T \to \pm \infty$. By expanding the solutions onto adiabatic orbitals,

$$\phi_i(\tau) = \sum_\mu C_{\mu i}(\tau) \psi_\mu(q(\tau)), \quad (5)$$

we obtain the following set of equations for the square matrix of the coefficients $C_{\mu i}(\tau)$:

$$\hbar \frac{\partial C_{\mu i}}{\partial \tau} + \dot{q} \sum_\nu \langle \psi_\mu(q(\tau)) | \frac{\partial \psi_\nu(q(\tau))}{\partial q} \rangle C_{\nu i} = [\zeta_i - \epsilon_\mu(q(\tau))] C_{\mu i}. \quad (6)$$

The conservation of overlaps leads to the condition on $C_{\mu i}(\tau)$:

$$\sum_{\mu=1}^N C_{\mu i}^*(-\tau) C_{\mu j}(\tau) = \delta_{ij}. \quad (7)$$

Thus, the quantity $p_{\mu i}(\tau) = C_{\mu i}^*(-\tau) C_{\mu i}(\tau)$ may be considered as a quasi-occupation (it can be negative or even complex in general case) of the adiabatic level $\mu$ in the bounce solution $i$, with $\sum_{\mu} p_{\mu i}(\tau) = 1$, $\sum_i p_{\mu i} = 1$. The action coming from one occupied s.p. bounce state $\phi_i(\tau)$ is:

$$S_i = \hbar \int_{-T/2}^{T/2} d\tau \sum_{\mu=1}^N [\zeta_i - \epsilon_\mu(q(\tau))] p_{\mu i}(\tau), \quad (8)$$

and the total action is a sum of the contributions from the occupied s.p. bounce states: $S_{\text{tot}} = \sum_{i,\text{occ}} S_i$. 

Table 2. Instanton action values compared with the adiabatic ones in the 2-level system for different maximal velocities $\dot{q}_{\text{max}}$ and two values of interaction strength $V_{\text{int}}$. Here $(E_2 - E_1)_{\text{min}} = 2V_{\text{int}}$ and the ratio $\hbar\dot{q}_{\text{max}}/(E_2 - E_1)_{\text{min}}$ should be sufficiently small for the adiabatic approximation to hold.

| $V_{\text{int}}$ [MeV] | $S_{\text{inst}}/\hbar$ | $S_{\text{adiab}}/\hbar$ |
|-------------------------|-------------------------|-------------------------|
| 0.5                     | 1.183 0.770 0.569       | 2.015 1.007 0.672       |
| 1.0                     | 0.398 0.218 0.149       | 0.459 0.229 0.152       |

One can ask whether the instanton action tends to the adiabatic one in the limit of small $\dot{q}$. The comparison of action values for various $\dot{q}$ for a two level system is shown in Tab. 2. The adiabatic action is generally higher than the one obtained from the instanton, but with decreasing $\dot{q}$ both values converge to each other, as one would expect. For stronger interaction between levels (implying smaller nonadiabatic coupling) the convergence is even faster.

We present the behaviour of solutions to Eq. (6) and resulting action values for four $\Omega^\ast = 1/2^+$ neutron levels taken from the deformed W-S potential for $^{272}$Mt isotope along the axial (close to static) fission path. The energy levels are depicted in Fig. 2. The continuous path was determined based on the energy landscape calculated for $\beta_{20}, \beta_{40}$ deformation parameters with the minimization over $\beta_{60}, \beta_{80}$. The instanton solution starting

![Energy levels](image-url)
and ending as the last occupied state below the Fermi level at the minimum (the lowest one in Fig. 2) is shown in Fig. 3 in terms of quasi-occupations introduced above. One can see that the particle remains mostly in the initial adiabatic state, except in the vicinity of the avoided crossings where it excites to the second adiabatic level. As long as these crossings are isolated (no other level comes close to them), the excitations to higher states are negligible. This behaviour is in contrast to what we know from the real time dynamics; the closest analogy would be the 2-level Landau-Zener model, where, if the system starts in the lower state at $t = -\infty$ and some nonadiabatic transitions take place during the evolution, then there is a nonzero probability (given by the Landau-Zener formula) that the system will end up in the upper state at $t = +\infty$.

A comparison of the instanton action (for the above solution) with the adiabatic one is presented in Tab. 3 for three different collective velocities $\dot{q}$ - the one from Eq. (4), and two scaled down by a constant factor. As may be seen, the adiabatic formula overestimates the instanton action, giving the

\begin{table}[h]
\centering
\begin{tabular}{c|cc}
$\hbar\dot{q}_{\text{max}}$ [MeV] & $S_{\text{inst}}/\hbar$ & $S_{\text{adiab}}/\hbar$
\hline
0.14 & 2.6818 & 55.048 \\
0.09 & 2.4892 & 36.699 \\
0.06 & 2.3492 & 25.689 \\
\end{tabular}
\caption{Comparison of the action corresponding to the lowest state obtained from the instanton solution ($S_{\text{inst}}$) and in the adiabatic approximation ($S_{\text{adiab}}$) for a few values of maximal collective velocity $\dot{q}_{\text{max}}$.}
\end{table}
values more than order of magnitude larger. This shows how far from the adiabatic limit we actually are in this case of the unpaired level undergoing sharp avoided crossings.

A difference in total action between the odd nucleus and its even-even neighbour comes from: 1) a difference in $\dot{q}$ and 2) the contribution of the last state occupied by the unpaired nucleon. The integrands of the total action for six or seven particles on the lowest four out of $N=8$, $\Omega^* = 3/2^+$ neutron levels in $^{272}$Mt, with the 4-th state empty or singly occupied, are shown in Fig. 4. As one can see, the contribution of the odd nucleon is rather smooth and moderate (in general, it can be negative). Note that contributions to $S$ from other $\Omega$s and parity will still decrease its part in the total.

![Fig. 4. Comparison of the total action integrands for six (black line) and seven (red line) neutrons.](image)

**5. Conclusions**

Experimental data suggest a mechanism for fission hindrance for high-$K$ isomers similar as that for odd-$A$ nuclei in the whole SH region. Pairing plus specialization energy (configuration preserving) mechanism seems to have a too strong effect, as judged from energy landscapes for some odd-$A$ nuclei. However, the current description of fission half-lives, employing adiabatic approximation, is not suitable for odd-$A$ nuclei and isomers. The instanton method adapted to the mean-field formalism may provide a basis for the minimization of action. The preliminary, non-selfconsistent studies indicate that in this method the action is well defined for an arbitrary path and the contribution to action of the odd nucleon is not large. The formalism for paired systems includes dynamic changes of pairing gaps as postulated...
in [13], but such that follow from the Hamiltonian-like dynamics [17]. Their study and work on the inclusion of the selfconsistency are under way.

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