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Fission Barriers of Two Odd-Neutron Heavy Nuclei

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Abstract. The fission barriers of two odd-neutron heavy odd nuclei,namely the ^{235}U and ^{239}Pu isotopes have been calculated within a self-consistent Hartree–Fock-plus-BCS approach with blocking. A Skyrme nucleon-nucleon effective interaction has been used together with a seniority force to describe pairing correlations. A full account of the genuine time-reversal symmetry breaking due to the presence of an unpaired nucleon has been incorporated at the mean field level. The SIII and SkM* parametrizations of the Skyrme interaction have been retained as well as for a part a newer parametrization, SLy5*. The seniority force parameters have been fitted to reproduce experimental odd-even mass differences in the actinide region. To assess the relevance of our calculated fission barrier distribution (as a function of the quantum numbers), we have studied the quality of our results with respect to the spectroscopy of band heads (for configurations deemed to be a pure single particle character) in the ground and fission isomeric states. Fission barriers of the considered odd nuclei have been compared with what is obtained for their even-even neighbouring isotopes (namely ^{234}U and ^{236}U, ^{238}Pu and ^{240}Pu respectively) to determine the so-called specialization energies. Various corrections and associated uncertainties have been discussed in order to compare our results with available data.

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1 Introduction

The deformation properties of two odd-neutron heavy odd nuclei, namely the ^{235}U and ^{239}Pu isotopes have been calculated within a self-consistent Hartree–Fock-plus-BCS approach with blocking. This includes the spectroscopic properties at both the ground and fission isomeric states as well as the fission barrier heights. A Skyrme nucleon-nucleon effective interaction has been used together with a seniority force to describe pairing correlations.

Two Skyrme parametrizations have been mainly considered, namely the SIII [1] and SkM* [2] parameter sets. They have been shown to yield reasonable spins and parities in a systematic study of more than 300 odd-neutron and odd-proton nuclei [3], with an agreement at least comparable with the results of the more phenomenological approach (Folded-Yukawa plus Finite range Droplet Model) of P. Möller [4]. Moreover, it has been shown recently [5] that the SIII interaction yields rather good magnetic moments for deformed nuclei over the whole chart of nuclides. On the other hand the SkM* interaction has been explicitely built to yield good fission barrier heights [2]. This is why we have chosen these interactions, which are rather old, to study the fission barrier distribution of odd fissioning nuclei. Nevertheless, to initiate a study of the effect of terms in the Skyrme Energy Density Functional which are not included in these parametrisations (as the square of the spin-current tensor for instance) we have also performed some calculations with the SLy5* force [6].

To determine the value of the seniority force parameters, we have computed microscopically for a sample of odd-neutron and odd-proton nuclei in the actinide region, the three-point mass differences $\Delta_q^{(3)}(N_q)$ defined for instance for the neutrons by

$$\Delta_n^{(3)}(N) = \frac{(-1)^N}{2}\big[S_n(N,Z) - S_n(N+1,Z)\big], \tag{1}$$

where $S_n(N,Z)$ represent the neutron separation energy of a nucleus with N neutrons and Z protons. As noted in Refs. [7, 8], such differences for odd N (resp. Z) and even Z (resp. N) values are essentially reflecting neutron (resp. proton) pairing properties. The nuclei which have been included in the sample satisfy the following a priori conditions: i) be rigidly deformed so that quantum fluctuations of the vibrational type might be reasonably ignored; ii) correspond to a strong regime of BCS pairing correlations (as measured by the product of the single-particle level density at the Fermi surface by a typical BCS pairing matrix element in comparison with 1) to avoid low pairing regimes where the BCS approximation is known to be strongly incorrect. The results obtained with the retained seniority force parametrizations and for the two Skyrme forces under consideration, are displayed in Table 1.

Table 1. Calculated values of the odd-even mass difference $\Delta_q^{(3)}$ (in keV) within two Skyrme parametrizations in comparison with experimental data (exp). The charge state q is the one of the unpaired nucleon in the corresponding nucleus.

Nucleus	$\Delta_q^{(3)}$		exp
	SkM*	SIII	
^{231}Th	510	739	661
^{235}U	567	562	624
^{239}Pu	525	490	444
^{241}Pu	452	541	534
^{245}Cm	678	641	469
^{249}Cf	550	496	520
^{229}Ac	681	582	794
^{237}Np	573	541	568
^{241}Am	502	860	470
^{249}Bk	806	575	568

2 Some Theoretical Aspects

In a fermionic system having an odd number of particles there is a genuine breaking of the time-reversal symmetry. The many-body Hamiltonian possesses this symmetry, but this is not the case within the mean field approximation. It is nevertheless assumed that the couplings between the nucleonic spin and orbital degrees of freedom with vector parts of the mean field so obtained, represent reasonably well the actual polarization of a core of paired particles when a single particle is added to (or removed from) it. These couplings involve time-odd densities like currents and spin-vector density functions among others, see Ref. [9]. We have considered here a minimal version of the corresponding time-odd mean field parts for the SIII and SkM* calculations (see Ref. [5] for details), whereas more time-odd terms (so-called full version) have been considered in calculations with the SLy5* interaction.

It has been explicitely shown that the inclusion of an unpaired nucleon in such heavy nuclei yields time-reversal breaking parts in the solution which are merely perturbative. This has allowed us to define unambiguously quasi-pairs of states (equivalent to Cooper pairs of Kramers dengenerate single particle states) from which one may build the equivalent of the restricted so-called Bogoliubov-Valatin transformation. The vacuum for such quasiparticles has the same formal definition than the usual BCS wavefunction.

Axial symmetry has been imposed. This constitutes a genuine limitation for the description of the inner barrier region (and may be also near the second barrier). Intrinsic parity symmetry has been allowed to be broken. This is a necessary condition to correctly reproduce the properties of the outer barrier.

We have broken only one quasi-pair. The limitation to such seniority-one states limits ourselves to low excitation regimes (typically up to a typical pairing delta energy value).

To describe the full nuclear dynamics of such well-deformed nuclei we resort to the unified model redundant description of Bohr and Mottelson where the nuclear wave function is written in the laboratory frame as (with usual notation)

$$|IM\alpha K\pi\rangle = \sqrt{\frac{2I+1}{16\pi^2}}\Big(D^I_{MK}|\Psi^\alpha_{K\pi}\rangle + (-)^{I+K}D^I_{M-K}\hat{T}|\Psi^\alpha_{K\pi}\rangle\Big), \quad (2)$$

where $|\Psi^\alpha_{K\pi}\rangle$ is the many-body HF + BCS solution, incorporating polarization effects due to the unpaired particle, $\hat{T}$ is the time reversal operator and where, by convention, K will be considered here as being positive. In the following, we shall denote this many-body state by $|\Psi_K\rangle$ for brevity.

The corresponding Hamiltonian involving collective (Euler angles) and many-body degrees of freedom is written as

$$\hat{H}^{\rm BM} = \hat{H}^{\rm int} + \frac{(\hat{\mathbf{I}} - \hat{\mathbf{J}})^2}{2\mathcal{J}_C} \,, \quad (3)$$

where $\hat{H}^{\rm int}$ represents the Hamiltonian of the many-body (intrinsic) degrees of freedom from which we substract a spurious rotational component according to the simple Lipkin ansatz [10], $\hat{\mathbf{I}}$ is the total angular momentum for both collective and many-body degrees of freedom and $\hat{\mathbf{J}}$ is a priori the angular momentum associated to the many-body degrees of freedom. Due to the redundancy of the model however, i.e. to avoid a double counting of the core contribution to the rotational energy one replaces in the collective rotational energy, the many-body angular momentum $\hat{\mathbf{J}}$ by its restriction $\hat{\mathbf{j}}$ to the mere space of the unpaired particle (whose wave function will be later noted $|\alpha K\pi\rangle$).

We will neglect here any interband Coriolis coupling allowing only internal coupling for K=1/2 solutions. We have just to evaluate diagonal matrix elements of $\hat{H}^{\rm BM}$. One readily finds for the intrinsic energy part $E^{\rm int}_{\alpha K\pi}$:

$$E^{\rm int}_{\alpha K\pi} = \langle\Psi_K|\hat{H}|\Psi_K\rangle - \frac{1}{2\mathcal{J}_L}\langle\Psi_K|\hat{\mathbf{J}}^2|\Psi_K\rangle + \frac{\hbar^2}{2\mathcal{J}_L}K(K+1) \,, \quad (4)$$

where $\hat{H}$ is the Hamiltonian in use in the HF plus BCS approach and $\mathcal{J}_L$ is the moment of inertia inherent to the Lipkin projection ansatz. Up to a very good approximation, one then finds for the expectation value of $\hat{H}^{\rm BM}$ in the nuclear state $|IM\alpha K\pi\rangle$:

$$E^{\rm BM}_{I\alpha K\pi} = E^{\rm int}_{\alpha K\pi} + \frac{\hbar^2}{2\mathcal{J}_C}\Big[I(I+1) + \langle\alpha K\pi|\frac{\hat{\mathbf{j}}^2}{\hbar^2}|\alpha K\pi\rangle - 2K^2 + \delta_{K,\frac{1}{2}}a(-1)^{I+\frac{1}{2}}(I+\frac{1}{2})\Big], \quad (5)$$

where a is the usual decoupling parameter and $\mathcal{J}_C$ is the moment of inertia of a core polarized by the unpaired nucleon (implying in particular quenched pairing correlations).

Assuming now that $\mathcal{J}_C$ and $\mathcal{J}_L$ are identical and noted as $\mathcal{J}$, one gets for the energy of band head $E^{\rm b.h.}_{\alpha K\pi}$ where $I = K$:

$$E^{\rm b.h.}_{\alpha K\pi} = \langle \Psi_K | \hat{H} | \Psi_K \rangle - \frac{1}{2\mathcal{J}} \langle \Psi_K^{(\rm core)} | \hat{\mathbf{J}}^2 | \Psi_K^{(\rm core)} \rangle + \frac{\hbar^2}{2\mathcal{J}} \Big[2K + \delta_{K,\frac{1}{2}} a (-1)^{K+\frac{1}{2}} (K + \frac{1}{2}) \Big], \quad (6)$$

where $|\Psi_K^{(\rm core)}\rangle$ denotes the core BCS wavefunction which is built from $|\Psi_K\rangle$ by excluding the unpaired nucleon state and its quasi-pair partner.

3 Results

Let us discuss, first of all, some results pertaining to the ground state properties. We note that the calculated ground state quadrupole moments reproduce rather well the corresponding data extracted from B(E2) measurements [11]. For the four U and Pu isotopes bracketing the considered ^{235}U and ^{239}Pu nuclei, they agree within 0.1 - 0.3 barn for the three Skyrme interactions in use. Spectroscopic quadrupole moments for odd nuclei are also very well reproduced (deduced from our calculated intrinsic moments by the Standard Bohr-Mottelson formula). One finds for instance for the 7/2$^-$ ground state in ^{235}U, the values (in nuclear magneton) 4.98, 4.78 and 4.92 (for SIII, SkM* and SLy5* interactions respectively) to be compared with two measured values [12] which are 4.936(6) and 4.55(9).

The rotational band head spectroscopy of the two ^{235}U and ^{239}Pu isotopes are displayed on the Figure 1. The retained band heads correspond to configurations which are analyzed in Ref. [13] as being of a single particle nature and lying experimentally below 0.65 MeV (a typical pairing gap value) to be reasonably deemed as being of a seniority-1 nature. The moments of inertia have been calculated according to the Inglis-Belyaev formula [14] increased uniformly by 32%, as proposed in Ref. [15] to take into account time-odd self-consistent terms dubbed as Thouless-Valatin corrections. The decoupling constant has been calculated as usual from the expectation value of the $\hat{j}_+\hat{T}$ operator for the single particle state $|\alpha K\pi\rangle$ of the unpaired particle (with $K = +1/2$).

The data on band heads in the fission isomeric well are scarce. We know them only for the ^{239}Pu nucleus (and not for ^{235}U). The lowest band is found with SIII and SkM* interactions to be 5/2$^+$ as they should and the excitation energy of the 9/2$^-$ band head found experimentally [16] to be 203 keV is calculated as 127 and 139 keV for the SIII and SkM* interactions respectively. The moments of inertia and hence the relevant combination of deformation and pairing properties

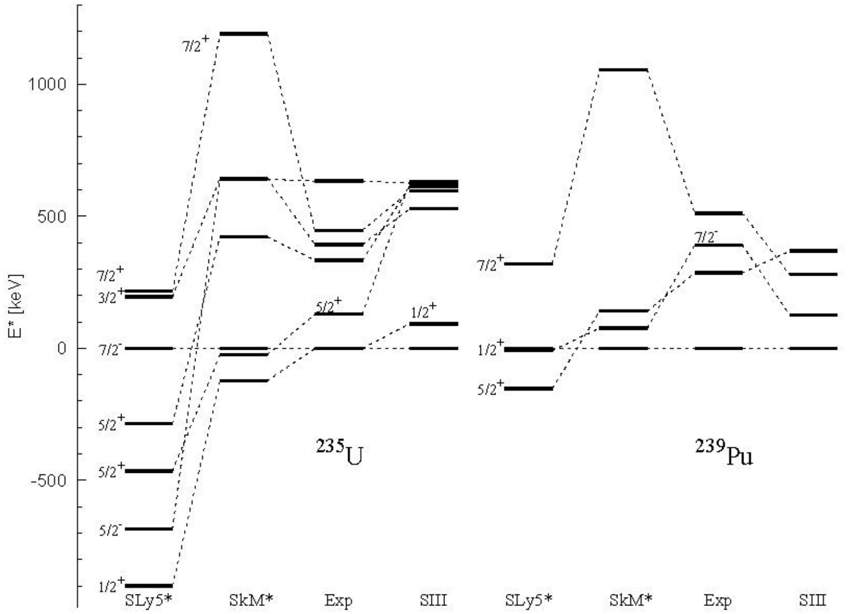

Figure 1. Partial band-heads of ^{235}U and ^{239}Pu calculated with the SkM* and SIII interactions without rotational correction in the *minimal time-odd* scheme and the SLy5* in the *full time-odd* scheme with comparison to the experiments.

are also rather well reproduced since we agree with data for the excitation of the two first excited levels in the 5/2$^+$ band to better than 10 keV with both interactions.

The fission barriers of the three Plutonium isotopes (^{238}Pu, ^{239}Pu, ^{240}Pu) calculated with the SkM* interaction are displayed on Figure 2 as an example of results where the intrinsic parity breaking has not been allowed (in the vicinity of the outer barrier). One notices the rather wide distribution of fission barrier heights or so-called (after Wigner) specialization energies (extending well over a 1 MeV span).

Table 2. Fission barrier heights (in MeV) for the inner (E_A) and the outer (E_B) barriers calculated with the SkM* interaction.

Nucleus (K^π)	$E_A^{\mathrm{eval.}}$	$E_A^{\mathrm{calc.}}$	$E_B^{\mathrm{eval.}}$	$E_B^{\mathrm{calc.}}$
^{234}U	4.80	5.42	5.50	-
^{235}U $(7/2^-)$	5.25	7.18	6.00	5.94
^{236}U	5.00	6.21	5.67	-
^{238}Pu	5.60	6.45	5.10	-
^{239}Pu $(1/2^+)$	6.20	7.71	5.70	4.66
^{240}Pu	6.05	7.25	5.15	-

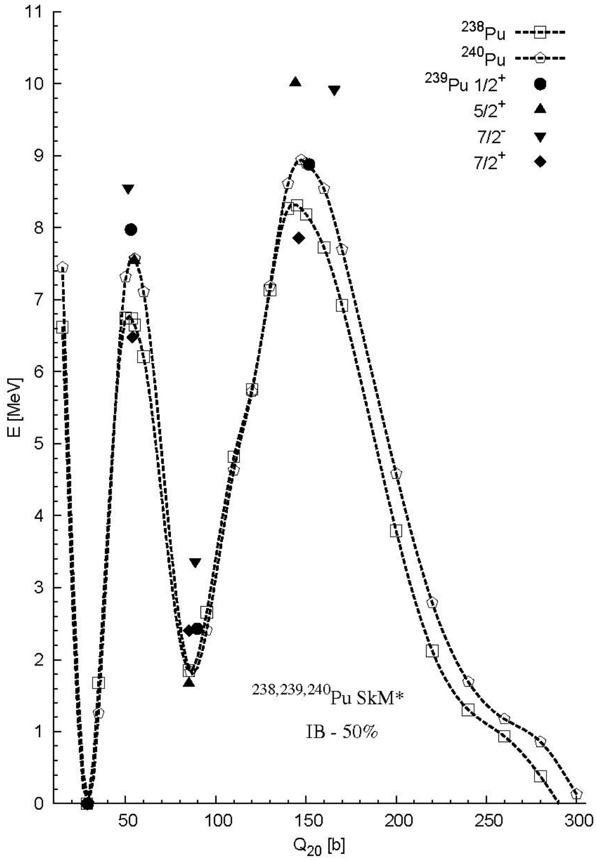

Figure 2. The fission barrier heights of the four considered K^{π} configurations of ^{239}Pu nucleus (with a conserved parity symmetry) are plotted with respect to the deformation energy curves of the ^{238,240}Pu nuclei. The results used for the plot are obtained with SkM* parametrization and including the reduction factor of 50% for the rotational correction calculated using the Belyaev formula.

A sample of results of ^{239}Pu fission barriers (for K=1/2 and K = 5/2) calculated with the SkM* and SLy5* interactions allowing for the breaking of the intrinsic parity, is shown on Figure 3. As well known considering asymmetrical solutions considerably lowers the outer barrier height. It is apparent that while the fission barrier heights obtained with the SkM* interaction lie in the right range, this is not the case of what is obtained with the SLy5* interaction.

Finally we summarize in Table 2 the results obtained for the fission barrier heights of the six following isotopes: ^{234}U, ^{235}U, ^{236}U, ^{238}Pu, ^{239}Pu, ^{240}Pu. Note that a significant part of the two high inner fission barrier heights might be

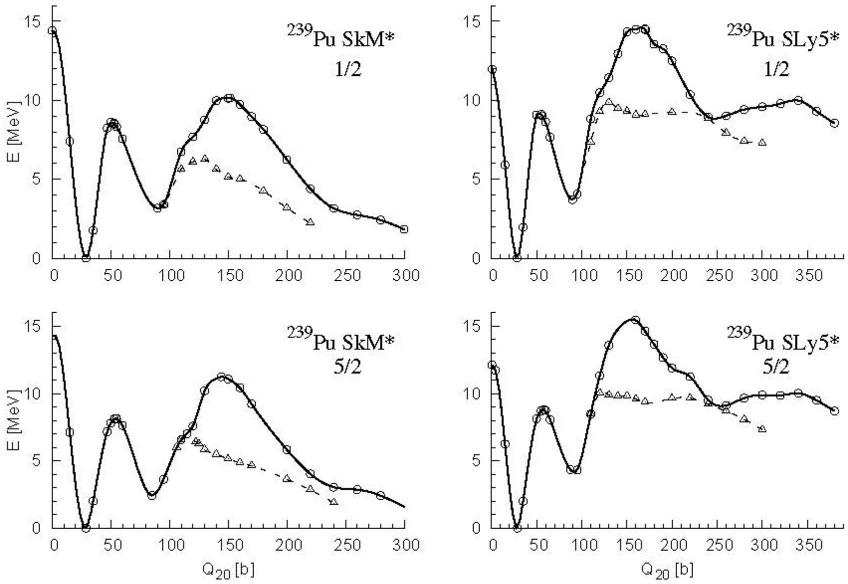

Figure 3. Deformation energy curves of ^{239}Pu as a function of deformation Q_{20} with parity symmetry breaking calculations obtained with the SkM* and the SLy5* parametrizations.

due to the undue imposition of axial symmetry in this deformation region. In this Table, the evaluated data are taken from the RIPL-3 IAEA compilation [17].

4 Conclusion

In such calculations of fission barrier heights, there are many sources of errors which are of two different natures. Some are due to the practical way by which they are obtained and could be somewhat estimated (convergence with respect to the basis size [18], use of the Slater approximation [19], imposition of axial symmetry [18], effect of the projection on good parity states [20], uncertainty related to the spurious rotational energy correction) they can be evaluated to lie within the 0.5 - 1 MeV interval. Some others are related with the physical relevance of the interactions in use, pertaining to the surface tension (in the liquid drop sense) or/and level densities at the Fermi surface (impacting shell effect energies and pairing energies). They could not be quantified and their estimation can only result from actual calculations as ours. If the results fall into the error bars of the calculational process, one may deem that the considered interaction yields reasonably good fission properties. This seems to be almost the case for the SkM* interaction. On the other hand, our results confirm the already noted good spectroscopic properties of the SIII interaction. Finally from what has been studied here, it does not seem that the SLy5* interaction brings any substantial improvement, to say the least, to the reproduction of both fission barrier heights and nuclear spectra of deformed nuclei.

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