We discuss the effect of kinetic energy of the relative motion becoming spurious for separate fragments on the selfconsistent mean-field fission barriers. The treatment of the relative motion in the cluster model is contrasted with the necessity of a simpler and approximate approach in the mean-field theory. A scheme of the energy correction to the Hartree-Fock is proposed. The results obtained with the effective Skyrme interaction SLy6 show that the correction, previously estimated as $\sim 8 \text{ MeV}$ in $A = 70 - 100$ nuclei, amounts to 4 MeV in the medium heavy nucleus $^{198}\text{Hg}$ and to null in $^{238}\text{U}$. However, the corrected barrier implies a shorter fission half-life of the latter nucleus. The same effect is expected to lower barriers for multipartition (i.e. ternary fission, etc) and make hyperdeformed minima less stable.

1. Introduction

It seems that the existing calculations of fission barriers overestimate energies of nuclear configurations close to scission by including a spurious contribution of kinetic energy of the fragments' relative motion. This may be seen as follows: The binding of two separated selfbound systems is equal to $E_{\text{sep}} = B_1 + B_2 + V_{\text{int}}$, with $B_i$ fragment binding energies and $V_{\text{int}}$ Coulomb energy. For a compound system, energy $E(1+2)$, should tend to $E_{\text{sep}}$ for separate entities, hence it should not contain fragment center of mass (c.m.) energies $E_{\text{c.m.}}(i)$. However, in a standard Hartree-Fock (HF), energy of a two-piece configuration still contains the term $E_{\text{c.m.}}(\text{rel}) = E_{\text{c.m.}}(1) + E_{\text{c.m.}}(2) - E_{\text{c.m.}}(1+2)$, corresponding to the relative motion of two fragments.

Within the mean-field theory, this overestimate arises from the c.m. kinetic energy correction that has to be subtracted from the expectation value of the Hamiltonian (energy functional) to obtain the binding. The expectation value of the operator $(\sum_k p_k^2)/(2AM)$ on the Slater state reads:

$$E_{\text{c.m.}}(A) = \frac{1}{2AM} \left( \sum_{k=1}^{A} \langle k | p^2 | k \rangle - \sum_{k \neq l}^{A} \langle k | p | l \rangle \langle l | p | k \rangle \right), \tag{1}$$
with \( k, l \) labelling occupied single particle states, and \( M \) nucleon mass. One should include one \( E_{c.m.} \) correction for a compound system, two corrections for two separate fragments, three corrections for three fragments, etc. For two distant fragments, \( A_1 + A_2 = A \), if one could distinguish particles belonging to each, which would imply the vanishing expectation value \( \langle (\sum_{k \in \bar{1}} p_k) \cdot (\sum_{l \in \bar{2}} p_l) \rangle \),

\[
E_{c.m.}(A_1) + E_{c.m.}(A_2) = E_{c.m.}(A) + \frac{A_2 E_{c.m.}(A_1) + A_1 E_{c.m.}(A_2)}{A}.
\] (2)

The second term on the right-hand side is just the asymptotic (for the distance \( R \to \infty \)) value of kinetic energy of the fragments’ relative motion, \( E_{c.m.}(rel) = \langle P^2_{rel} \rangle / (2\mu) \), with \( P_{rel} = (A_2/A) \sum_{k \in \bar{1}} p_k - (A_1/A) \sum_{k \in \bar{2}} p_k \), and \( \mu = MA_1A_2/A \). This quantity becomes spurious for a two-piece system as it does not contribute to the binding. As noted by Berger and Gogny, this asymptotic term should be subtracted from the HF energy to obtain proper fusion barriers.

In practical HF calculations the \( E_{c.m.} \) correction is included in various forms (see 3). Here we confine the discussion to effective interactions which use the natural definition (1). With such interactions one obtains \( E_{c.m.} = 5.5 - 8 \) MeV for \( A = 40 - 250 \), decreasing with \( A \). This quantity should be subtracted from \( E(1 + 2) \) in a consistent theory: partially - for shapes with constriction, totally - for two-piece systems. This subtraction is usually included in calculations of fusion barriers (otherwise the barriers are too high 4,5,6), but omitted in fission studies. However, even for fusion barriers, a gradual dependence of the correction on the compactness of the system is missing.

As found in Ref. 2, the subtraction of the asymptotic value of \( E_{c.m.}(rel) \) brings the calculated HF fission barriers closer to the experimental values in medium-size \( A = 70 - 100 \) nuclei. In the present work we estimate the effect of the shape-dependent correction \( E_{c.m.}(rel, \text{shape}) \) on fission barriers in heavier nuclei, using the Skyrme effective interaction SLy6 7 (section 3). The correction is discussed and defined in section 2, where we also consider a different treatment of the relative kinetic energy in the cluster model and in the mean-field theory. Conclusions are given in section 4.

It is remarkable that a correction of similar property and magnitude, although based on completely different grounds, 8 has been introduced in macroscopic-microscopic calculations 9,10 in order to obtain a better agreement with the experimental fission barriers in the same regions of nuclei.

2. General discussion

The difficulty in the determination of the fission or fusion barrier discussed here is pertinent to nuclear models in which the binding energy of the far separated nuclei 1 and 2 treated as a one system is different from \( B_1 + B_2 \), with \( B_i \) determined separately. Since the standard HF belongs to this category, it needs a correction which would ensure that \( E(1 + 2) \to B_1 + B_2 \) in fission (with \( E(1 + 2) \) understood
as adiabatic energy). The smoothness of such correction with the evolving nuclear shape is a natural requirement.

At the heart of the difficulty lies the identity of particles that impedes a definition of the relative coordinate and motion of two interacting subsystems. This problem is crucial in studies of light nuclei, where it is treated within the resonant group method (RGM) that is basically a version of the generator coordinate method (GCM). A cluster configuration $A_1 + A_2$ is represented as an expansion $\Phi_A = \int d\varphi(r)\Phi_r$ onto an overcomplete basis formed by states $\Phi_r = A_{A_1A_2}[\delta(r - r_{rel})\Phi_{A_1}\Phi_{A_2}]$ with $\Phi_A$, the cluster states depending on intrinsic coordinates, $\varphi$ the amplitude of the relative motion and $A_{A_1A_2}$ the antisymmetrizer containing permutations mixing the coordinates of the first $A_1$ with those of the last $A_2$ nucleons. Thus, the label $r$ of the basis states assumes the role of the intercluster coordinate.

From the Schrödinger equation for $\Phi_A$ one obtains the Hill-Wheeler equation for the amplitude of the relative motion in coordinate $r$, with a well defined Hamiltonian. However, a decomposition of this Hamiltonian into kinetic and potential parts, $T + U$, is arbitrary: The relative kinetic energy operator is assumed as $T = -\frac{\hbar^2}{2\mu}(\nabla_r)^2$ with the reduced mass $\mu$, and this fixes the potential $U$. So obtained potentials are much deeper in the compound nucleus region than those implied by the mean field; in this way the Pauli exclusion influences the relative motion of the overlapping clusters.

It follows that while the RGM (or GCM) provides a solution to the relative motion problem, its ingredients, like the potential $U$, do not seem to be of much use for the mean-field theory. As an application of the full RGM (GCM) method for heavy nuclei would be prohibitively difficult, one would rather include a kinetic energy correction in the relatively simple HF method to improve energy asymptotics for separated clusters. However, this cannot be just the expectation value of $[A/(2MA_1A_2)]P_{rel}^2$ in the Slater state: Owing to the incompatibility of the $P_{rel}$ variable with the antisymmetry of the Slater determinant, its value, $\langle p^2 \rangle + \sum_{k\neq l}^A | \langle k | p | l \rangle |^2 / [A(A-1)]/(2M)$, is by $\sim 10$ MeV larger than the proper value of $E_{c.m.}(rel)$. This is why obtaining the correct value of Eq. requires an extension that goes beyond HF. Some guidance might be provided by realistic internuclear potentials used in fusion studies, e.g.

One possibility to proceed is to introduce a measure of the fragment separation $\xi$ which would replace the relative distance $r$ and define the subtracted portion of the relative kinetic energy, $E_{c.m.}(rel, \text{shape}) = \xi E_{c.m.}(rel)$. To this aim, consider dispersion of the number of particles in the $k$-th HF orbital, residing in the volume $V_k$ of the first fragment with $A_1$ nucleons. This reads $p_k(1-p_k)$, with $p_k = \int_{V_k}^1 | \psi_k |^2$ (with many-particle correlations ignored). For completely divided fragments the $k$-th wave function is localized, so $p_k = 0$ or 1 and dispersion vanishes. We define $\xi$ by
means of dispersion averaged over the occupied orbitals:

\[ \xi = 1 - \left( \frac{2}{A} \right) \frac{\sum_{k-occ} p_k (1 - p_k)}{\bar{p}(1 - \bar{p})} = \left( \frac{2}{A} \right) \frac{\sum_{k-occ} (p_k - \bar{p})^2}{\bar{p}(1 - \bar{p})}, \quad (3) \]

with \( \bar{p} = 2 \sum_{k-occ} p_k / A = A_1 / A \) (with obvious modifications for pairing included).

So defined \( \xi \) is positive, reaches the maximal value 1 for separated fragments and falls to zero for wave functions uniformly smeared over two fragments. It has thus necessary properties to show main effects of a gradual inclusion of \( E_{c.m.}(rel) \) in HF energy.

Subtraction of a varying portion of \( E_{c.m.}(rel) \) will change energy balance between configurations with and without constriction, lowering the former with respect to the latter. As found in the study of fusion barriers, values of \( \xi \) at the barrier vary between 0.7 and 0.9 and decrease together with the interfragment distance \( R \). The latter is defined as the distance between the centers of mass of two half-spaces, containing \( A_1 \) and \( A_2 \) nucleons. Clearly, fusion barriers calculated using the shape-dependent correction \( \xi E_{c.m.}(rel) \) are higher than those obtained by subtracting the whole asymptotic value \( E_{c.m.}(rel) \). The related increase in the barrier height will depend on the slope \( dV/dR \) (without any correction): a small increase for a large positive slope, a larger increase (and the barrier shift towards smaller \( R \)) for small positive or negative slopes. For example, with the SLy6 force, the inclusion of the \( \xi \)-dependence leads to the increase in fusion barrier by 1.8 MeV for \( ^{48}\text{Ca}+^{48}\text{Ca} \) and by 2.5 MeV for \( ^{48}\text{Ca}+^{208}\text{Pb} \), with the inward shift of the barrier top by 0.6 and 1.5 fm, respectively.

In the present study of fission barriers we use a different prescription for the relative kinetic energy correction. For a system of \( A \) nucleons consider its division \( A_1 + A_2 \) into volumes \( V_1 \) and \( V_2 \). Calculate the quantity \( p_k \) for each wave function and call it localized in \( V_1 \) (\( V_2 \)) if \( p_k > 1 - \epsilon \) (\( p_k < \epsilon \)), with some small \( \epsilon \) (we use \( \epsilon = 0.03 \)). Suppose that for a given nuclear shape (configuration) \( N_1 \) wave functions are localized in \( V_1 \) and \( N_2 \) in \( V_2 \). Then the correction for this shape is defined as

\[ E_{c.m.}(rel, shape) = \frac{N_1}{A_1} E_{c.m.}(N_1) + \frac{N_2}{A_2} E_{c.m.}(N_2) - \frac{N_1 + N_2}{A} E_{c.m.}(N_1 + N_2). \quad (4) \]

This quantity tends to 0 for no localization and to the asymptotic value \( E_{c.m.}(rel) \) for divided fragments (full localization). The correction is more directly related to the localized orbitals than \( \xi E_{c.m.}(rel) \), but still not completely satisfactory. Ultimately, it would be desirable to define the correction for relative kinetic energy as a part of the energy functional and treat it variationally.

3. Shape-dependent correction to barriers

We have calculated the fission barriers with and without the \( E_{c.m.}(rel, shape) \) correction in \( ^{198}\text{Hg} \) and \( ^{238}\text{U} \). Pairing was included as the delta interaction in the BCS scheme, using the cutoff according to the prescription of Ref. \[^{14}\]. The delta interaction strength was fixed at \( V_n = 316 \text{ MeV fm}^3 \) for neutrons and \( V_p = 322 \text{ MeV fm}^3 \) for protons.
Fig. 1. Fission barrier in $^{198}$Hg without (squares) and with (circles) the $E_{c.m.}(\text{rel, shape})$ correction.

The calculated fission barrier in $^{198}$Hg (Fig. 1) is mass-symmetric ($A_1 = A_2$) and the saddle corresponds to a large elongation with the quadrupole moment close to $Q = 300\text{ b}$, cf Fig. 2. To relate Fig. 1 to other studies, we mention that the energy plot for $Q < 20\text{ b}$, calculated with the Gogny interaction, may be found in Fig. 2 of 15, while the whole macroscopic-microscopic fission barrier was given in Fig. 3 of 16. Between the secondary minimum at $Q = 45\text{ b}$ and $Q \approx 100\text{ b}$ the HF minima are soft to mass-asymmetry or even slightly mass-asymmetric. Our calculated barrier of 27.5 MeV is lowered owing to the $E_{c.m.}(\text{rel, shape})$ correction to 23.7 MeV vs. the experimental value of 20.4 MeV 17 and 19.3 MeV calculated in 16. It may be seen that the relative kinetic energy correction of 3.8 MeV at the $^{198}$Hg fission barrier is smaller than those for $A = 70 - 100$ nuclei 2, but still significant.

The calculated barrier in $^{238}$U is shown in Fig. 3. The triaxial first hump of 7.55 MeV at $Q = 60\text{ b}$ and the mass-asymmetric second hump of 8 MeV at $Q = 125\text{ b}$ (that agrees with the result with SLy6 reported in 18) are both larger than the experimental barriers (inner and outer) close to 6 MeV 19,20. At the second barrier, the neck is still not yet developed (cf shapes in Fig. 4) and single-particle orbitals are not well localized in parts of the volume corresponding to $A_1 = 138$ and $A_2 = 100$, the partition chosen close to the maximum of the experimental mass yield 21. Hence the $E_{c.m.}(\text{rel, shape})$ correction vanishes and does not influence the barrier height in this case. For quadrupole moments $Q > 125\text{ b}$ the localization begins and the correction grows slowly with $Q$. At $Q = 200\text{ b}$ (shape in Fig. 4) it amounts already to 1.9 MeV. This implies that the barrier relevant for the quantum tunneling, while not being higher, becomes shorter.

An estimate of the effect on the fission half-life may be obtained by using the relation $\Delta \log T_{sf} \approx 0.8686 \Delta S$, with action $S = \int \sqrt{2B_{c.f.f}(E - E_{g.s})} \, d\beta_2$, see e.g. 22. For $B_{c.f.f}$ we can use the cranking mass parameters, typical for the appropriate deformation range, calculated with the Woods-Saxon potential. An approximate
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Fig. 2. Barrier configuration in $^{198}$Hg, $Q = 300$ b; density contours 0.01 fm$^{-3}$ apart.

relation between the quadrupole moment and the deformation parameter $\beta_2$, $\beta_2 \approx \sqrt{5\pi Q/(3r_0^2A^{5/3})}$, with the assumed $r_0 = 1.2$ fm, gives $\beta_2 \approx 0.01 \times Q$ for $A = 238$. Between $\beta_2 = 1.8$ and 2.3, where the correction causes an appreciable difference in the integrand of action, the mass parameter $B_{22}$ decreases from about 20 to 5 $\hbar^2$/MeV and is similar to $B_{23}$, while $B_{33}$ increases from about 30 to 60 $\hbar^2$/MeV (subscripts of the mass tensor refer to deformation parameters $\beta_\lambda$, $^{22}$). Taking $B_{eff} = 10\hbar^2$/MeV (as $\beta_3$ increases with $\beta_2$, $B_{eff} > B_{22}$), and estimating $\Delta S$ as $(2.3 - 1.8) \times \sqrt{2B_{eff}E_{av}}$ with $E_{av}$ equal to 1.0 MeV (cf Fig. 3), we obtain a rough estimate $\Delta S = 2.23$ and $\Delta \log T_{sf} = 1.94$. Thus, the expected change in the fission half-life is about two orders of magnitude, compared to the experimental value of $\log T_{sf}$ of 23.4 $^{19}$. The true correction $\Delta \log T_{sf}$ is probably at least that large: The recently calculated selfconsistent cranking inertia parameters $^{23}$ that should be used in the exact calculation, seem larger than the Woods-Saxon cranking mass parameters.

It is worth mentioning that the calculated barriers will be still lowered by the rotational correction. In $^{238}$U, one can expect more than a 1 MeV correction at the first barrier, and more than a 2 MeV correction at the second barrier, based on calculations $^{24}$. An even larger rotational correction should be expected for $^{198}$Hg at the barrier, owing to a larger deformation.
Fig. 3. Fission barrier in $^{238}\text{U}$ without (squares) and with (circles) the $E_{c.m.}(\text{rel, shape})$ correction.

Fig. 4. The barrier ($Q=125$ b, left) and beyond the barrier ($Q=200$ b, right) configurations in $^{238}\text{U}$; density contours 0.01 fm$^{-3}$ apart.

4. Conclusions
Correctly calculated energies of nuclear shapes with constriction become lower than in the standard approach, so such shapes, in particular scission configurations, are less excited with respect to more compact configurations. Here are some consequences of this correction for theoretical predictions:

(i) Fission barriers with configurations close to scission are lowered by aproxi-
mately $E_{\text{c.m.}}$, which weakly depends on the mass number $A$. This brings the calculated fission barriers in relatively light ($A = 70 - 100$) nuclei much closer to the data. 

(ii) A smaller correction is expected for fission barriers in $A \approx 200$ nuclei, e.g. in $^{198}\text{Hg}$ (Fig. 1). This is consistent with very elongated, constricted shapes at the fission saddles in these nuclei, quite different, however, from scission configurations.

(iii) Fission barriers with energy at the scission point close (within a few MeV) to that at the ground state become shorter, and this leads to a moderate decrease in fission half-lives (Fig. 3 for $^{238}\text{U}$).

Modifications are expected for barriers and half-lives for multipartition and multifragmentation; a scission configuration for tripartition will be lowered by $\sim 2E_{\text{c.m.}}$, that for the decay into four fragments by $\sim 3E_{\text{c.m.}}$, etc. One can also notice that the correction to barriers would tend to destabilize hypothetic hyperdeformed minima studied in Ref. 25.

Due to the magnitude of the correction, it lowers substantially fission barriers (up to the actinides) and modifies fission lifetimes, except for the superheavy nuclei. Even there, the correction should be accounted for when considering fission dynamics. A related correction may be necessary in methods other than HF, unless they correctly and smoothly describe binding during fission and fusion.

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