PHYSICAL REVIEW C **74**, 051601(R) (2006)

Relative kinetic energy correction to self-consistent fission barriers

Janusz Skalski
Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA
Physics Division, Oak Ridge National Laboratory, PO Box 2008, Oak Ridge, Tennessee 37831, USA
Sołtan Institute for Nuclear Studies, ul. Hoża 69, PL-00 681, Warsaw, Poland
(Received 9 June 2006; published 16 November 2006)

The effect of spurious relative kinetic energy removal on the fission barriers is discussed within the Skyrme Hartree-Fock method. Calculations for medium-heavy nuclei show that this correction is large and in the right direction.

DOI: 10.1103/PhysRevC.74.051601 PACS number(s): 25.70.Jj, 21.60.Jz

Fusion and fission barriers are crucial to the understanding of nuclear reactions and collective decay. Currently, they can be computed only by using either phenomenological macroscopic-microscopic or self-consistent mean-field methods. Within such models, the barrier height, i.e., the energy difference between the ground state and the spatially deformed lowest saddle configuration of a nucleus, reflects the component of nuclear energy that scales with nuclear surface. Somewhat paradoxically, difficult-to-measure fission barriers in medium-heavy nuclei may better characterize the surface energy term than those in spontaneously fissioning heavy species. This is due to near-scission configurations at the barrier for $A\approx$70–100. To check mean-field models against such experimental data, one needs a precise evaluation of nuclear potential for two separating fragments.

In this work, we consider the effect that the removal of spurious relative kinetic energy of the two nascent fragments has on the self-consistent fission barriers. We have calculated some fusion and conditional fission barriers in medium-heavy nuclei within the self-consistent Skyrme Hartree-Fock method and compared our results with the data. It turns out that by subtracting relative kinetic energy, one can dramatically improve the agreement between the calculated and experimental fission barriers.

The problem we address here may be stated as follows: Kinetic energy of the relative motion of two subsystems contributes to the binding energy of a composed system (by decreasing it), but not to the binding energies of two separate subsystems. Hence, any Hamiltonian or energy functional required to reproduce the binding energy for each configuration of equilibrium must depend on the partition of the system. In fission, as two subsystems separate, the kinetic energy of their relative motion becomes spurious as a part of binding energy and must be subtracted from the energy functional (for tripartition, one should subtract two relative kinetic energies of three fragments, etc.). A precise formula for this subtraction is not known, since for identical nucleons it is difficult to disentangle the energy of the relative motion of two subsystems until they are well separated. This difficulty obscures the definition of the nuclear potential close to scission.

Within nuclear mean-field theory, this difficulty is combined with the breaking of translational symmetry. A localized Slater determinant is a superposition of many momentum eigenstates, and the theory approximately eliminates spurious kinetic energy of the center of mass (c.m.) by means of the so-called c.m. energy correction $E_{\rm c.m.}$ (for a competent review, see Ref. [1]). When we neglect the neutron-proton mass difference, the expectation value of the c.m. kinetic energy for a Slater determinant describing A nucleons reads

$$E_{\rm c.m.}(A) = \frac{1}{2AM}\left(\sum_{k=1}^{A}\langle k|\mathbf{p}^2|k\rangle - \sum_{k\neq l}^{A}|\langle k|\mathbf{p}|l\rangle|^2\right), \quad (1)$$

with k, l labeling the occupied single-particle states, and M the nucleon mass [only exchange two-body terms are present in Eq. (1) as the diagonal matrix elements of momentum vanish in the time-reversal invariant states]. Some Skyrme forces contain the full correction of Eq. (1); others, only the one-body average kinetic energy term $\langle\hat{t}\rangle = \sum_{k-{\rm occ}}\langle k|\mathbf{p}^2|k\rangle/(2AM)$. Crude estimates of both quantities may be obtained from schematic models: For a Fermi gas enclosed in a hard-wall container with a radius $R = r_0A^{1/3}$, $\langle\hat{t}\rangle = 3\epsilon_F/5 \approx 20$ MeV for $r_0 = 1.2$ fm. Assuming an effective harmonic oscillator mean field with the frequency $\hbar\omega = 41A^{-1/3}$ MeV, one obtains $E_{\rm c.m.} \approx 3\hbar\omega/4 \approx 10.5$ MeV for $A = 25$ and 5.25 MeV for $A = 200$. Independent of its form, $E_{\rm c.m.}$ has to be subtracted from the expectation value of the Hamiltonian to obtain the correct binding energy.

It follows from the above that one c.m. correction should be applied for a system in one piece, while two c.m. corrections, one for each fragment, are required for separated entities. The magnitude of $E_{\rm c.m.}$, although depending on the approximation, does not depend strongly on the nuclear mass A (except for light systems). Thus, to obtain a potential correct in both limits of one- and two-piece systems (i) the outer part of the fission barrier should be reduced by $\sim E_{\rm c.m.}$ with respect to the prediction obtained for one undivided system, or (ii) the inner part of the fusion barrier should be raised by $\sim E_{\rm c.m.}$ with respect to the prediction based on separate fragments. Unfortunately, a discontinuity results close to the scission point.

To relate this to barriers, consider a static potential $V(R)$ between nuclei 1 and 2 at zero orbital angular momentum, defined by

$$V(R) = E(R) + B_1 + B_2, \tag{2}$$

where $E(R)$ is the (negative) Hartree-Fock (HF) energy of a dinuclear complex at the distance R, and B_i are the (positive) binding energies of separate fragments. For two separated fragments of A_1 and A_2 nucleons, $A_1 + A_2 = A$, with vanishing mutual momentum overlaps, $\langle k_1|\mathbf{p}|l_2\rangle = 0$, one obtains from Eq. (1) the relation

$$E_{\text{c.m.}}(A_1) + E_{\text{c.m.}}(A_2) = E_{\text{c.m.}}(A) + \frac{A_2 E_{\text{c.m.}}(A_1) + A_1 E_{\text{c.m.}}(A_2)}{A}. \tag{3}$$

The second term on the right-hand side is just the expectation value of kinetic energy of the fragments' relative motion, $E_{\text{c.m.}}(\text{rel})$, which becomes spurious for a two-piece system. Observe, that $V(R)$ tends to $E_{\text{c.m.}}(\text{rel})$ when R tends to infinity. The usual meaning of the entrance channel potential and fusion barrier requires that this asymptotic term be subtracted from Eq. (2). This has been noted by Berger and Gogny [2] who tried to obtain within collective theory a deformation-dependent correction that would tend to $E_{\text{c.m.}}(\text{rel})$ for large fragment distances—apparently without success. In the frozen density calculations of fusion barriers [3,4], $E_{\text{c.m.}}(\text{rel})$ was simply subtracted without touching upon the question, How much of it is really required for a barrier corresponding to an undivided one-piece shape? On the other hand, to the best of our knowledge, the spurious kinetic term was never subtracted in calculations of fission barriers.

One may ask whether fission data actually call for any such correction, even if the correction itself seems pretty obvious. It happens that a correction of similar properties and magnitude, but based on completely different grounds, has been introduced in macroscopic-microscopic calculations [5,6]. It originated from terms in macroscopic energy that are roughly constant for all or a majority of nuclei, such as the "congruence" or "Wigner" energy. To assure a unique definition of potential energy, such a term has to double during fission or diminish by half during fusion. To make its change continuous during fusion and fission its dependence on nuclear shape was evoked [7]. It was then argued that the shape-dependent congruence energy lowers the calculated fission barriers in light- and medium-heavy nuclei just enough to remove the discrepancy between the calculations and the data. (In fact, some discrepancies of a few MeV remain, see Fig. 15 in Ref. [8]). Quite independent of the macroscopic-microscopic studies, the recent work [9] shows that the self-consistent Skyrme HF calculations without such a correction severely overestimate conditional fission barriers in ^{70}Se.

The largest effect of eliminating spurious relative kinetic energy on fission barriers is expected for relatively light nuclei, with barriers so close to the scission point that (nearly) the whole asymptotic value of $E_{\text{c.m.}}(\text{rel})$ should be subtracted (see Fig. 1). In this work, we study the conditional fission barriers in nuclei ^{70}Se, ^{96}Zr, ^{90}Mo, and ^{98}Mo for the following partitions: ^{38}Ar + ^{32}S, ^{58}Ni + ^{12}C, ^{48}Ca + ^{48}Ca, ^{50}Ti + ^{40}Ca, and ^{50}Ti + ^{48}Ca. Our basic assumption is that the configuration of the conditional saddle for a given partition is the same as that at the top of the fusion barrier of the inverse reaction. This assumption is consistent with the results of the liquid drop studies [10], with the recent mean-field results [9] for ^{70}Se, and with our checks: Compact fusionlike scission configurations in these nuclei have energies lower than or very close to those of more elongated saddles. However, one has to admit that our assumption, although very plausible, is not proven; our calculations considered only nearly axially symmetric nuclear shapes.

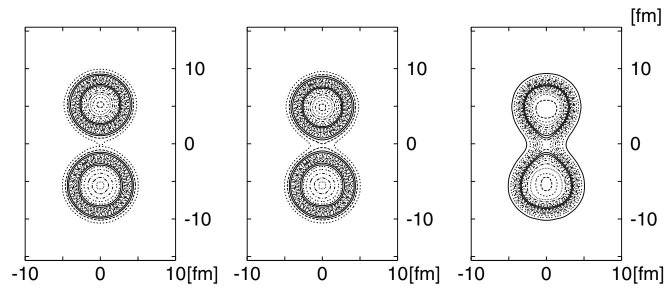

FIG. 1. Density profiles for ^{38}Ar + ^{32}S system around fusion barrier at (from left to right) $R = 10.77$, 10.40, and 9.84 fm, obtained with the Skyrme force SLy6. Contour lines are 0.01 fm^{-3} apart. The middle distance corresponds to the barrier top.

Our calculations of adiabatic fusion barriers for the reactions ^{38}Ar + ^{32}S, ^{58}Ni + ^{12}C, ^{48}Ca + ^{48}Ca, ^{50}Ti + ^{40}Ca, and ^{50}Ti + ^{48}Ca were based on Eq. (2). We used two realistic Skyrme forces with very different c.m. correction methods: SkM* [11] with $E_{\text{c.m.}} = 16$–19 MeV given by the one-body term alone, and SLy6 [12] with typical $E_{\text{c.m.}} = 5$–8 MeV given by the whole expression (1). To have a numerically consistent treatment, $B_i, i = 1, 2$, and $E(R)$ in Eq. (2) were calculated with the same HF code. We note that the calculated binding energies B_i depend on the Skyrme functional and usually differ from the experimental values by a few MeV. Pairing is included as given by the delta interaction with the energy cutoff defined in Ref. [13], which allows for a smooth transition between one- and two-piece nuclear configurations. We fixed the strength of the delta interaction for neutrons and protons at the values from another study that reproduce experimental gaps in ^{252}Fm ($V_n = 272$, $V_p = 315$ MeV fm^3 for SkM* $V_n = 316$, $V_p = 322$ MeV fm^3 for SLy6). The potential $V(R)$ and the fusion barriers were calculated by subtracting the total value of $E_{\text{c.m.}}(\text{rel})$ from the expression in Eq. (2), $V(R) = E(R) + B_1 + B_2 - E_{\text{c.m.}}(\text{rel})$.

The HF plus BCS equations have been solved on a spatial mesh. Initially, two sets of wave functions corresponding to two fragments at their ground states are placed at a chosen distance. We use a uniform step in initial distances of 0.345 fm, half of the step of the spatial mesh. During HF iterations, the constraints are imposed on the center of mass of the total system and its quadrupole moment. The adiabatic potential is built by the local minima of the energy functional to which the initial configuration converged. The distance R between two fragments is calculated as the distance between the mass centers of two half-spaces containing A_1 and A_2 nucleons.

The HF iterations show two distinct patterns depending on whether the initial distance R (or the quadrupole moment Q) is greater or smaller than some distance $R_c(Q_c)$ close to or a little smaller than the position of the top of the barrier $R_b(Q_b)$.

A moderate number of iterations leads to a unique potential value when $R > R_c$, with the final values of R and V close to the initial ones. A possible difficulty in this regime occurs when the Fermi levels in the two fragments are unmatched and nucleons redistribute between the fragments during HF iterations. Then one obtains the potential value that corresponds to another entrance channel. A shift in the mass and charge partition by quite a few units is possible, up to 10 mass units for the reaction $^{50}\mathrm{Ti} + {}^{40}\mathrm{Ca}$ with SkM*. The required entrance channel can be obtained only by imposing additional constraints. To fix the mass and charge partition, we adjust pairing separately in each fragment which keeps occupations of single-particle levels close to the initial ones. This works as long as the fragment densities do not overlap substantially, which for the considered nuclei means up to and a little inward of the scission point. We further refer to such a calculation as the constrained one.

Starting HF iterations from the initial distance a little smaller than R_c, which means somewhat smaller than at the configuration of two touching fragments, one obtains after many HF iterations the final minimum with the values of R and V much smaller than the initial ones. This reflects the onset of the buildup of the neck between the two fragments, associated with the increase in the hexadecapole moment Q_{40} at the constant Q. This change in the HF iteration pattern signals that the barrier has been crossed from the outside.

Our calculations with the SLy6 force are illustrated in Fig. 2. Two kinds of points, open and solid squares, for three

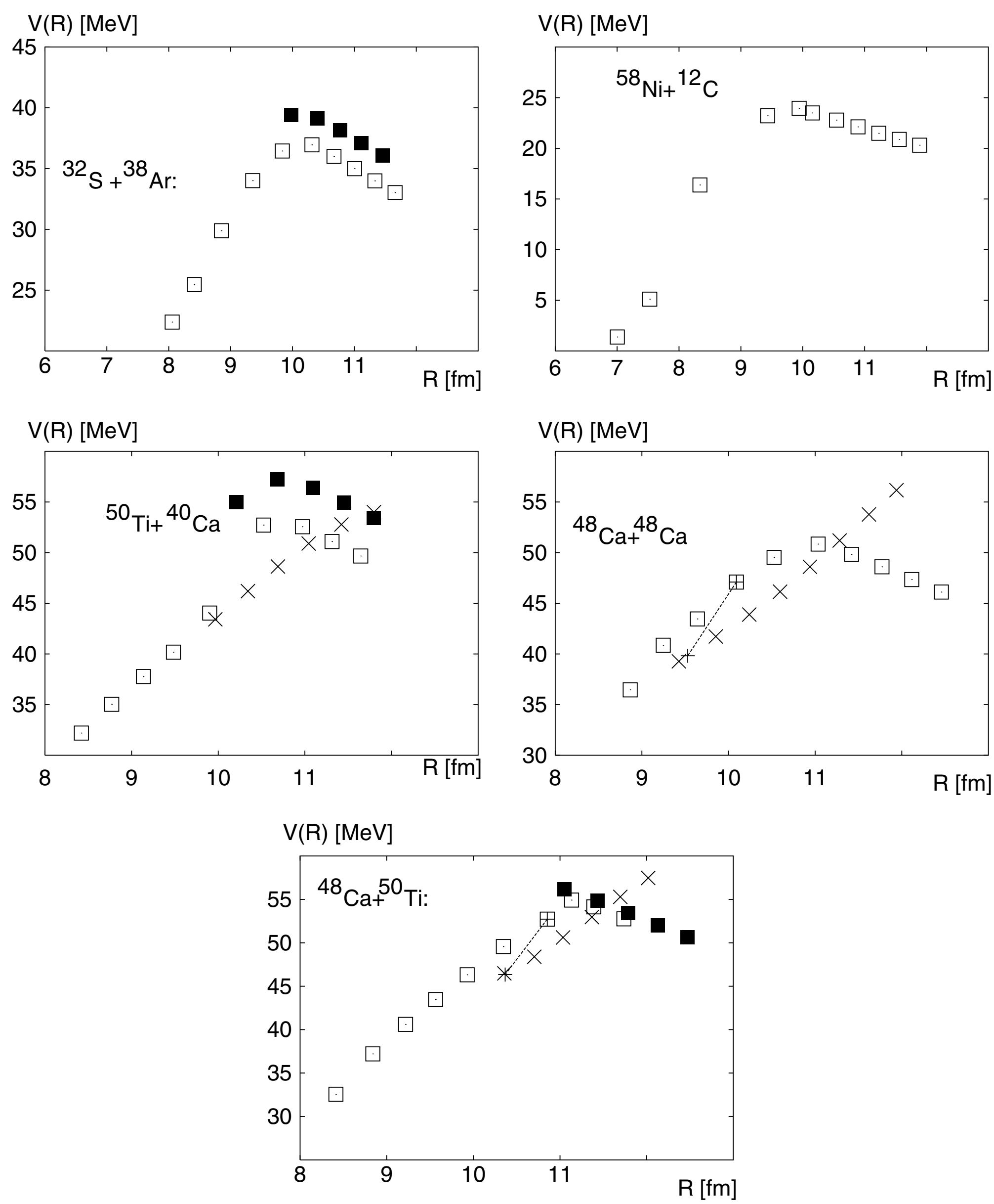

FIG. 2. Fusion barriers (squares) and mass-symmetric fission valleys of compound nuclei (crosses) obtained with the Skyrme force SLy6. For other explanations, see text.

asymmetric reactions can be seen for large distances. These correspond to the calculations without (lower points) and with the imposed constraint on the mass and charge partition (upper points). The magnitude of the energy differences between them varies from 1 MeV for the ^{38}Ar+^{32}S system to 4 MeV for the ^{50}Ti+^{40}Ca reaction. Clearly, this induces some arbitrariness in the value of $V(R)$ at the barrier, related to the uncertainty of the point at which one switches from the constrained to the unconstrained results. Consider as an example the system ^{38}Ar+^{32}S. With the SLy6 force, we obtain from the unconstrained calculation $V(R = 10.31\text{fm}) = 36.95$ MeV and from the constrained one $V(R = 10.40\text{ fm}) = 39.13$ MeV ($Q = 37.5$ b). In both calculations, the system is nearly completely divided at this distance, see Fig. 1. Since the unconstrained calculation changes the mass partition to a more asymmetric one, we choose the potential value given by the constrained calculation. For the smaller distances, the neck develops (see Fig. 1), so only the values of $V(R)$ from the unconstrained calculations are relevant there. Since they are all smaller than 39.13 MeV (cf. Fig. 2), the latter value gives the height of the fusion barrier. Similar reasoning applies to the other cases. For the reactions ^{48}Ca+^{48}Ca and ^{58}Ni+^{12}C, the unconstrained calculations give the correct partition, and the barrier height may be read out from the $V(R)$ curve. As mentioned above, only the constrained calculations give the asked mass division for the reaction ^{50}Ti+^{40}Ca, and we take as the fusion barrier the value of $V(R)$ at the touching distance $R = 11.1$ fm.

The unconstrained (in mass and charge partition) minima at distances $R < R_c$ shown in Fig. 2 are, in general, conditional. They have been obtained within the described method of calculations after a reasonably long iteration. With decreasing Q, their moments Q_{40} smoothly interpolate between the fusion barrier and the fission valley. The latter defines the absolute minima for $R < R_c$, with much larger Q_{40}, for three heavier compound nuclei. These minima, shown as crosses in three lower panels in Fig. 2, were obtained by the conventional method of stretching the nucleus. The change from the conditional minimum to the one at the same Q in the fission valley corresponds to an abrupt shape change and decrease in R and V, as depicted by points (pluses) connected by lines for two reactions with ^{48}Ca in Fig. 2. It should be emphasized that the part of the potential curve for $R < R_c$ is arbitrary to some degree, as a choice of a descent path from the given elevation over the fission valley. This reflects the arbitrariness of the inside part of the fusion potential in the static approach. At the same time, the height of the adiabatic fusion barrier is defined (up to the uncertainty discussed above) as long as large deformations of separate fragments are forbidden.

Calculated fusion barriers are given in Table I. Whether obtained with the SkM* or SLy6 force, they are remarkably similar in spite of the very different $E_{\text{c.m.}}$(rel) corrections. Experimental values mentioned in Table I correspond to the peak positions in the measured barrier distributions [14,15]. The low-energy edges of these distributions lie lower by $\sim$2 MeV. Probably, some intermediate barrier height would be relevant when comparing with our adiabatic HF results.

Conditional fission barriers, with and without the relative kinetic energy subtraction, are presented in Table II, together with the existing data. Note that, unlike Eq. (2), they involve binding B_c (taken as positive) of the compound nucleus, $B_{\text{fis}} = E(R) + B_c$ or $E(R) + B_c - E_{\text{c.m.}}$(rel). This is determined by the same HF code for consistency. The salient feature of the results in Table II is that the subtraction of $E_{\text{c.m.}}$(rel) brings the calculated conditional fission barriers closer to their experimental values, while without this subtraction they are considerably overestimated. The latter fact was previously established for ^{70}Se and SkM* force [9]. The barrier of 51.5 MeV for the ^{39}K+^{31}P partition found there (without any additional corrections) agrees well with the value 49.8 MeV without $E_{\text{c.m.}}$(rel) correction for the close channel ^{38}Ar+^{32}S (Table II). (In fact, the barrier of 50 MeV should be reported in Ref. [9], cf. the panel for 39 b in Fig. 8 there, in even closer agreement with our result.) The agreement for the ^{58}Ni+^{12}C partition is worse: 35.1 MeV (Table II) vs 40.9 MeV [9], but the latter is an upper bound rather than the barrier (cf. Fig. 17 in Ref. [9]).

TABLE I. Calculated fusion barriers vs data (in MeV).

System	B_{fus}(SkM*)	B_{fus}(SLy6)	B_{fus}(exp)
^{38}Ar+^{32}S	38.97	39.13	–
^{58}Ni+^{12}C	23.62	23.95	–
^{50}Ti+^{40}Ca	56.14	56.38	57 [14]
^{48}Ca+^{48}Ca	50.35	50.84	51.2 [15]
^{50}Ti+^{48}Ca	54.75	54.85	–

Fission barriers including the $E_{\text{c.m.}}$(rel) correction with the SkM* force are systematically lower than those with the SLy6. This might look like a correlation with the larger magnitude of the $E_{\text{c.m.}}$ correction for the SkM* force. In fact, the differences between the fission barriers for both forces are equal, within 0.5 MeV, to the differences in the calculated reaction Q values, $B_1 + B_2 - B_c$ (Table II, the difference between the last two columns). Thus, the differences in B_{fis} reflect the quality of each force in reproducing the ground state binding energies: One may expect that the calculated barrier is by $\Delta Q = Q - Q_{\text{exp}}$ too low. For the studied nuclei, the SLy6 force better reproduces the reaction Q values. We also note that the barriers obtained with the SLy6 force leave some room for additional corrections that lower the fission barrier (like the rotational one, see Ref. [9]).

The conditional fission barrier for ^{90}Mo is definitely too high with both forces, while the corresponding fusion barrier agrees well with the data. Perhaps, the fission and fusion barriers are different in this case. One also has to mention that the experiment [8,16] determined only the charge partition, while the mass partition was not measured and might differ from the one assumed here.

In summary, we have shown that the removal of spurious relative kinetic energy considerably lowers fission barriers in medium-mass nuclei. This brings the self-consistent results closer to the experimental data and solves a big part of the problem of too high barriers reported in Ref. [9]. Moreover, the necessity of the applied correction is evident in contrast to the concept of the deformation-dependent congruence term used in the macroscopic energy plus Strutinsky shell correction

TABLE II. Calculated conditional fission barriers vs data and differences $\Delta Q = Q - Q_{\mathrm{exp}}$ between calculated and experimental reaction Q values (in MeV, $Q = B_1 + B_2 - B_c$). In parentheses: barriers without relative kinetic energy correction.

System	B_{fis}(SkM*)	B_{fis}(SLy6)	B_{fis}(exp)	ΔQ(SkM*)	ΔQ(SLy6)
^{70}Se $\to$ ^{38}Ar + ^{32}S	(49.8) 32.7	(49.3) 40.8	35.35 [16]	7.5	−0.4
^{70}Se $\to$ ^{58}Ni + ^{12}C	(35.1) 18.2	(38.4) 28.2	25.3 [16]	7.3	−2.4
^{90}Mo $\to$ ^{50}Ti + ^{40}Ca	(64.2) 47.2	(59.8) 51.7	41.5 [8]	2.9	−1.45
^{96}Zr $\to$ ^{48}Ca + ^{48}Ca	(56.8) 39.2	(51.5) 43.4	–	8.16	4.4
^{98}Mo $\to$ ^{50}Ti + ^{48}Ca	(57.4) 39.6	(53.2) 45.1	44.5 [8]	7.7	2.15

method (as long as it is not sure that congruence energy extends over the whole nuclear chart as a global term). Thus, the correction should be used in the self-consistent studies of fission barriers.

The lowering of the potential energy by $\sim E_{\mathrm{c.m.}}$(rel) around the scission point will lower fission barriers in nuclei with the scission configuration lying above or a little below the ground state energy. Modifications may be expected for medium-heavy and some actinide nuclei. Short barriers, such as those in super-heavy species, should not be affected. However, it is clear that to improve predictions of fission barriers, one has to specify some satisfactory prescription to account for a gradual transformation of kinetic energy of the fragments' relative motion into potential energy of the combined system.

Finally, since the macroscopic-microscopic approach is an approximate version of the self-consistent HF, the relative kinetic energy problem, although hidden, is pertinent to it as well.

This work was supported in part by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through the U.S. Department of Energy Research Grant No. DE-FG03-03NA00083; by the U.S. Department of Energy under Contract No. DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory); and by the Polish Committee for Scientific Research (KBN) Grant Nos. 1P03B06427 and 1P03B05927.

[1] M. Bender, K. Rutz, P.-G. Reinhard, and J. A. Maruhn, Eur. Phys. J. A **7**, 467 (2000).
[2] J. F. Berger and D. Gogny, Nucl. Phys. **A333**, 302 (1980).
[3] V. Yu Denisov and W. Nörenberg, Eur. Phys. J. A **15**, 375 (2002).
[4] A. Dobrowolski, K. Pomorski, and J. Bartel, Nucl. Phys. **A729**, 713 (2003).
[5] P. Möller, J. R. Nix, and W. J. Swiatecki, Nucl. Phys. **A492**, 349 (1989).
[6] P. Möller and A. Iwamoto, Phys. Rev. C **61**, 047602 (2000); P. Möller, D. G. Madland, A. J. Sierk, and A. Iwamoto, Nature (London) **409**, 785 (2001); P. Möller, A. J. Sierk, and A. Iwamoto, Phys. Rev. Lett. **92**, 072501 (2004).
[7] W. D. Myers and W. J. Swiatecki, Nucl. Phys. **A612**, 249 (1997).
[8] K. X. Jing *et al.*, Nucl. Phys. **A645**, 203 (2000).
[9] L. Bonneau and P. Quentin, Phys. Rev. C **72**, 014311 (2005).
[10] S. Cohen and W. J. Swiatecki, Ann. Phys. (NY) **22**, 406 (1963).
[11] J. Bartel *et al.*, Nucl. Phys. **A386**, 79 (1982).
[12] E. Chabanat *et al.*, Nucl. Phys. **A635**, 231 (1998).
[13] M. Bender, K. Rutz, P.-G. Reinhard, and J. A. Maruhn, Eur. Phys. J. A **8**, 59 (2000).
[14] A. A. Sonzogni, J. D. Bierman, M. P. Kelly, J. P. Lestone, J. F. Liang, and R. Vandenbosch, Phys. Rev. C **57**, 722 (1998).
[15] M. Trotta *et al.*, Phys. Rev. C **65**, 011601(R) (2001).
[16] T. S. Fan *et al.*, Nucl. Phys. **A679**, 121 (2000).