Fission Barriers of Compound Superheavy Nuclei

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(Received 10 December 2008; published 13 May 2009)

The dependence of fission barriers on the excitation energy of the compound nucleus impacts the survival probability of superheavy nuclei synthesized in heavy-ion fusion reactions. In this work, we investigate the isentropic fission barriers by means of the self-consistent nuclear density functional theory. The relationship between isothermal and isentropic descriptions is demonstrated. Calculations have been carried out for ^{264}Fm, ^{272}Ds, ^{278}112, ^{292}114, and ^{312}124. For nuclei around ^{278}112 produced in "cold-fusion" reactions, we predict a more rapid decrease of fission barriers with excitation energy as compared to the nuclei around ^{292}114 synthesized in "hot-fusion" experiments. This is explained in terms of the difference between the ground-state and saddle-point temperatures. The effect of the particle gas is found to be negligible in the range of temperatures studied.

DOI: 10.1103/PhysRevLett.102.192501 PACS numbers: 24.75.+i, 21.60.Jz, 24.10.Pa, 27.90.+b

What are the heaviest nuclei that can exist? To answer this question, nuclear physicists explore superheavy systems at the limit of mass and charge. During recent years, the field has witnessed remarkable progress [1–3] in the production and identification of new elements. The major experimental challenge is to find optimal beam-target combinations and kinematic conditions that would lead to the formation, at reasonable rates, of the species of interest. One of the key problems is the survival probability of a superheavy nucleus synthesized in a heavy-ion fusion reaction that depends on a competition between fission and particle evaporation [4].

The dependence of the fission barrier on the excitation energy is among the key factors determining the production of a superheavy nucleus. Since shell effects, essential for the mere existence of superheavy nuclei, are quenched at high temperatures (see, e.g., Refs. [5,6]), it is expected that the fission barriers in superheavy CN should quickly decrease with energy. In the analysis of experimental data, this is usually accounted for by a phenomenological damping factor [3,7–9] (cf. discussion in Ref. [4]).

Microscopically, shell effects in superconducting heated nuclei can be self-consistently treated by the Finite-Temperature Hartree-Fock-Bogoliubov (FT-HFB) method [6,10–12]. For superheavy nuclei, although there have been extensive self-consistent studies of zero-temperature fission pathways, (see, e.g., [13–15]), studies of CN fission have been virtually nonexistent. Moreover, in the majority of studies, CN fission has been treated as an isothermal process in terms of free energy, $F = E - TS$ at a fixed temperature T. The assumption of $T =$ const is certainly wrong: the fissioning CN is not connected to an external thermal reservoir. Physically, a more appropriate picture of fission is that governed by the isentropic process [16]. The necessary condition for the isentropic scenario is that the collective motion is adiabatic; i.e., no heat energy can be delivered to nor extracted from the system.

The aim of this study is to investigate self-consistent isentropic fission pathways in superheavy CN, with a focus on energy dependence of fission barriers. To this end, we selected several nuclei of current experimental interest: (i) ^{272}Ds and $^{278}112^*$ that have been synthesized in the "cold-fusion" reaction using a ^{208}Pb target at excitation energies E^* of $\sim$10–12 MeV [7]; (ii) the nucleus $^{292}114^*$ produced in the "hot-fusion" reaction $^{48}\mathrm{Ca} + {}^{244}\mathrm{Pu}$ at $E^* \sim 36$–40 MeV [17]; (iii) the nucleus $^{312}124^*$ at $E^* \sim$ 80 MeV studied by means of $^{74}\mathrm{Ge} + {}^{238}\mathrm{U}$ reaction and crystal blocking [18]; and (iv) the ^{264}Fm that is expected to fission symmetrically into two doubly-magic ^{132}Sn nuclei. The FT-HFB calculations are carried out using the two Skyrme-HFB codes: the recently developed axial coordinate-space solver HFB-AX [19] and a symmetry-unrestricted solver HFODD [20]. The description of thermal properties involves significant contributions from high-lying single-particle states which give rise to the particle gas as the temperature increases [21], requiring a very large configuration space to guarantee convergence [22]. In this respect, HFB-AX is an excellent tool as it allows calculations in very large deformed boxes. The finite-temperature formalism has been implemented in HFB-AX and HFODD in the usual way [11] by introducing the thermal-averaged particle and pairing densities through the Fermi distribution function.

In the particle-hole channel, we use the SkM* energy density functional [23] that has been optimized at large deformations; hence it is often used for fission barrier predictions. In the pairing channel, we adopted the density-dependent δ interaction in the mixed variant [24]. The pairing strengths, $V_p = -332.5$ MeV fm^{-3} (protons) and $V_n = -268.9$ MeV fm^{-3} (neutrons) have been fitted to reproduce the pairing gaps in ^{252}Fm. The details of HFB-AX calculations follow Ref. [19]. We used $M = 13$ order B splines, and the maximum mesh size $h = 0.6$ fm. The cylindrical box employed depends on the total quadrupole moment of the system, Q_{20}. That is, for $Q_{20} \leq 30$ b we used a square box of $R_\rho = R_z = 20.4$ fm; for $30 < Q_{20} \leq 80$ b we took $R_\rho = 19.2$ fm and $R_z = 21.6$ fm; and for $Q_{20} > 80$ b we took $R_\rho = 18$ fm and $R_z = 22.8$ fm. The calculations with HFODD were carried out in a space of the lowest 1161 stretched oscillator states originating from the 31 principal oscillator shells.

As pointed out in Ref. [16], isothermal and isentropic descriptions can be related by making use of the thermodynamical identity $(\frac{\partial E}{\partial Q_{20}})_S = (\frac{\partial F}{\partial Q_{20}})_T$ which is reminiscent of the well-known relation $(\frac{\partial E}{\partial V})_S = (\frac{\partial F}{\partial V})_T$. Indeed, Q_{20} enters the variations dF and dE via the term $-q_{20} dQ_{20}$, where q_{20} is the Lagrange multiplier corresponding to the constraint on the quadrupole moment. Figure 1 displays isothermal and isentropic axial fission pathways of ^{292}114 as a function of Q_{20}. In the isentropic description, S was fixed at the value $S = S(T)$ corresponding to the free energy minimum at temperature T. This was done by performing constrained FT-HFB calculations for a number of temperatures and inverting the relation $S = S(T)$ numerically by using interpolation. It is seen that the isothermal and isentropic curves are very close. It is worth noting that in the macroscopic-microscopic calculations of Ref. [16] the isentropic barriers are predicted to be significantly higher than the isothermal ones. The reason for this is the violation of self-consistency in the macroscopic-macroscopic theory. Figure 1 shows that the variational principle behind FT-HFB guarantees practical equivalence of isothermal and isentropic pictures. The remaining small discrepancy is due to the numerical interpolation error caused by extraction of (E, S) values from the original (F, T) mesh.

The behavior of temperature $T = T(S)$ is shown in Fig. 2 along the fission pathways of ^{278}112 and ^{292}114. The entropy corresponds to the ground-state (g.s.) value at $T_{\text{g.s.}} \sim 750$ keV. It is seen that T changes as a function of Q_{20}. In particular, the barrier temperature is significantly lower than $T_{\text{g.s.}}$. In the following, we shall stick to the isentropic description; i.e., the temperature will be related to the g.s. excitation energy.

Figure 3 displays the energy curves of ^{264}Fm as functions of Q_{20} at different entropies corresponding to different values of $T_{\text{g.s.}}$. At $S(kT_{\text{g.s.}} = 0.5)$, the barrier increases by about 0.6 MeV as compared to $S = 0$, due to the reduction of pairing correlations [6,10–12]. (In our calculations, pairing energies are unimportant above $kT = 0.7$ MeV.) At higher excitation energies, the barrier is gradually reduced to 0.9 MeV at $S(kT_{\text{g.s.}} = 1.5)$, due to the thermal quenching of shell effects. In order to estimate the reduction of the fission barrier due to triaxiality expected in the Fm isotopes [15,25], we performed symmetry-unrestricted calculations with HFODD. The result is shown in Fig. 3 by a dashed line. At low excitation energies, triaxiality reduces the fission barrier by ~3–4 MeV, but the triaxial shell effect is washed out with increasing entropy and becomes negligible at the largest excitations considered. For the systematic calculations of triaxial and reflection-asymmetric deformations along the isentropic fission pathways of superheavy nuclei, we refer the reader to Ref. [26].

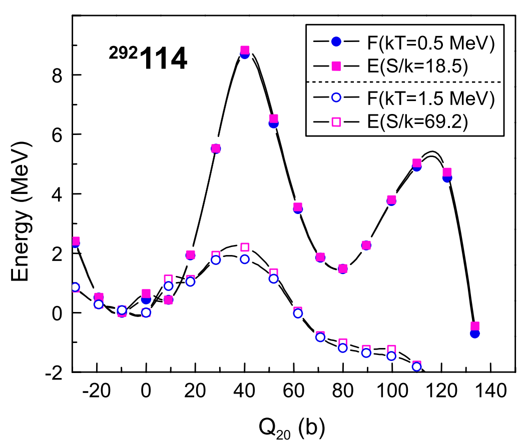

FIG. 1 (color online). Calculated isothermal (F at constant T) and isentropic (E at constant S) axial symmetric fission pathways for ^{292}114 as a function of the total quadrupole moment Q_{20}. The isothermal calculations were carried out at $kT = 0.5$ and 1.5 MeV. In the isentropic description, S was fixed at the free energy minimum, i.e., $S/k = 18.5(69.2)$ at $kT = 0.5(1.5)$ MeV.

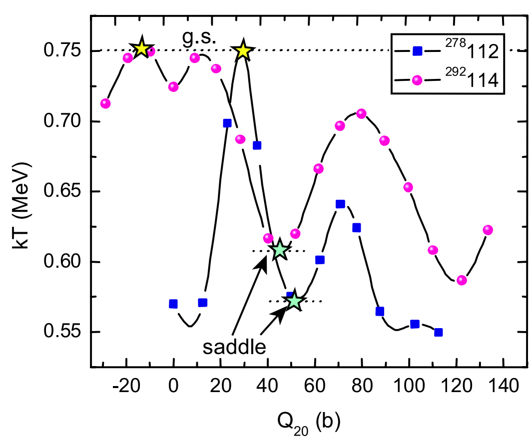

FIG. 2 (color online). The temperature along the isentropic symmetric fission pathways of ^{278}112 and ^{292}114. The g.s. and saddle-point configurations are marked by stars. The g.s. temperature was assumed to be $T_{\text{g.s.}} \sim 750$ keV and $S = S(T_{\text{g.s.}})$. The temperature at the saddle point is considerably lower than $T_{\text{g.s.}}$.

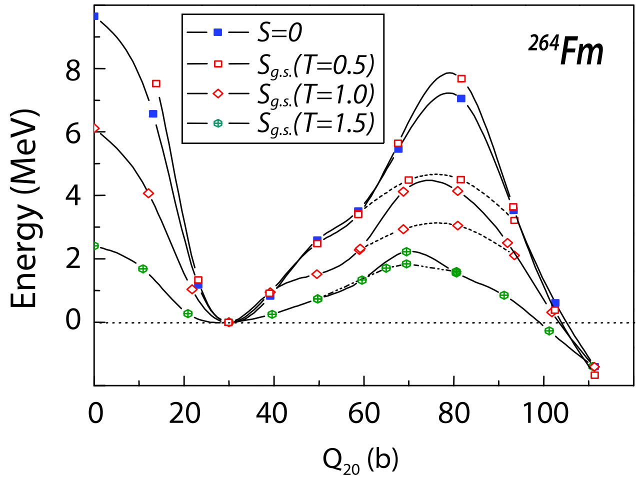

FIG. 3 (color online). Symmetric isentropic fission pathways of ^{264}Fm at the values of S corresponding to $kT_{\text{g.s.}} = 0$, 0.5, 1.0, and 1.5 MeV The energy has been normalized to zero at the ground-state minimum. The effect of triaxial degrees of freedom on the first barrier is marked by dashed lines.

To study the excitation energy dependence of fission barriers in more detail, in Fig. 4 we plot the height of the inner axial fission barrier of ^{264}Fm, ^{272}Ds, ^{278}112, ^{292}114, and ^{312}124 as a function of the excitation energy $E^* = E(S) - E(S = 0)$. Above $kT_{\text{g.s.}} = 0.5$ MeV, fission barriers E_B are damped exponentially with E^*: $E_B \propto e^{-\gamma_D E^*}$. The value of the damping parameter γ_D is not known well (see discussion in Ref. [9]) but γ_D^{-1} is usually taken in the range of 8–20 MeV [8,9]. According to our calculations, in the CN ^{272}Ds and ^{278}112 synthesized in cold-fusion reaction $\gamma_D^{-1} = 17.2$ and 10.8 MeV, respectively, while it is 30 MeV in ^{292}114 and 20.2 MeV in ^{312}124.

The appreciable change in γ_D with N and Z, e.g., when going from ^{278}112 to ^{292}114, can be traced back to shell effects. As seen in Fig. 2, in the isentropic picture, the saddle-point temperature T_B is *lower* than $T_{\text{g.s.}}$, i.e., $\Delta T = T_{\text{g.s.}} - T_B > 0$ (in a nice analogy to an adiabatically expanding gas). Because of shell effects, $\Delta T(^{278}112) > \Delta T(^{292}114)$ and the thermodynamical identity $(\frac{\partial E}{\partial S})_{Q_{20}} = kT$ implies a larger γ_D in ^{278}112, thus explaining the pattern seen in Fig. 4.

As discussed in Ref. [27], the FT-HFB solution in a confined box (or in a finite localized basis) corresponds to a nucleus located at the center surrounded by the external gas. The gas produces the pressure necessary to obtain an equilibrium with the particle-decaying hot nucleus; the corresponding particle-decay lifetime is in fact inversely proportional to the density of the external gas [21]. Figure 5 illustrates the effect of the gas for spherical configuration in ^{292}114 at different temperatures. In order to separate gas contributions, we applied the procedure of Refs. [21,28]. It is seen that with increasing temperature, the gas gradually appears. As expected, the neutron gas is uniformly distributed within the volume of the box while the proton gas appears outside the nuclear surface due to the effect of the Coulomb barrier. The contribution from the gas to the kinetic energy is very small: it is about 0.2 (0.9) MeV at $kT = 1.25(1.5)$ MeV. The number of gas neutrons is very small; it increases from $N_{\text{gas}} = 0.01$ at $kT = 1$ MeV to 0.21 at $kT = 1.5$ MeV; cf. Fig. 5. Consequently, the gas contribution to the deformation energy is practically negligible in the range of temperatures consid-

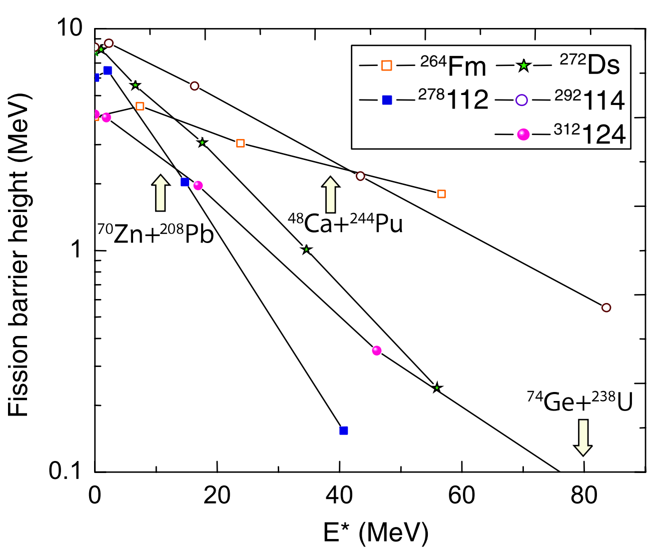

FIG. 4 (color online). The height of the inner fission barrier in ^{264}Fm, ^{272}Ds, ^{278}112, ^{292}114, and ^{312}124 as a function of excitation energy E^*. The effect of triaxiality on the fission barrier has been included. The experimental values of E^* corresponding to CN formed in the reactions indicated are marked by arrows.

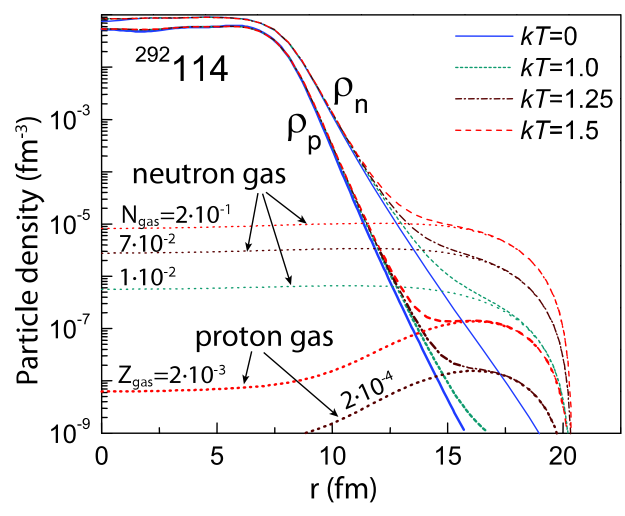

FIG. 5 (color online). Proton (thick lines) and neutron (thin lines) spherical density distributions in ^{292}114 calculated at different temperatures (in MeV). The external gas contributions are marked by dotted lines. The number of nucleons in the gas is indicated by numbers. The size of the box in HFB-AX was 20.4 fm.

ered. At very high temperatures, however, the gas is expected to significantly change the Coulomb energy, the total entropy, and the chemical potentials, and its contribution should be properly removed [21].

In conclusion, we performed self-consistent calculations of isentropic fission barriers of compound superheavy nuclei based on a coordinate-space FT-HFB method. We first demonstrated the relationship between the isothermal and isentropic description of fission and emphasized the role of self-consistency. The conclusion, important for practical applications, is that the surfaces of $F(T = T_0)$ and $E(S = S_0)$ in the space of collective coordinates are identical for $S_0 = S(T_0)$ if the self-consistency condition is met. It is to be noted, however, that this formal connection does not indicate that the isothermal and isentropic pictures of fission are similar. The isothermal approach to fission is clearly incorrect as the nucleus is not connected to a thermal bath; i.e., the temperature of the g.s. configuration and the barrier obviously differ. On the other hand, if the fission process is adiabatic, the isentropic description should be closer to reality.

Second, we demonstrate that the dependence of isentropic fission barriers on excitation energy changes rapidly with particle number, pointing at the importance of shell effects even at large excitation energies characteristic of compound nuclei. For instance, fission barriers for ^{272}Ds and ^{278}112, produced in a cold-fusion reaction, and ^{292}114, synthesized in a hot-fusion reaction, are predicted to exhibit markedly different behavior. For the CN ^{312}124, we calculate no isentropic fission barrier at $E^* \sim 80$ MeV.

Finally, we show that the external particle gas has no effect on the fission barriers up to at least $kT = 1.5$ MeV. The barrier damping parameters extracted from our FT-HFB calculations, as well as the neutron decay rates extracted from the magnitude of the neutron gas component [21] can be used to provide reliable theoretical estimates of CN survival probability. Work along these lines is in progress.

Useful discussions with W. Loveland, J. Skalski, and A. Staszczak are gratefully acknowledged. This work was supported in part by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through Grant DE-FG03-03NA00083; by the U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963 (University of Tennessee), and DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory), and DE-FC02-07ER41457 (UNEDF SciDAC Collaboration). Computational resources were provided by the National Center for Computational Sciences at Oak Ridge National Laboratory.

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