## Nuclear temperature effects in the scission-point model of nuclear fission

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According to the scission-point model, the probability for a particular fission event can be expressed in terms of the collective potential and the collective kinetic energy at the scission point. Two additional assumptions make the scission-point model an easily calculable model: the assumption of equal collective kinetic energies for constant distances d between the tips of the fragments, and the assumption that one is able to characterize the excitation energy of the fragments with a nuclear temperature T, independent of both the mass ratio and the charge ratio, and of the deformations of the fragments. It is pointed out that the latter assumption violates energy conservation. A modified, recursive procedure is proposed, resulting in an "energy conservation consistent" scission-point method. Mass and charge distributions for the fission of <sup>235</sup>U and <sup>252</sup>Cf compound systems have been calculated and compared with distributions following the "standard" scission-point method of Wilkins, Steinberg, and Chasman.

NUCLEAR REACTIONS Scission-point model. Collective potential and intrinsic excitation energy. Nuclear temperature T. Mass and charge distributions. Fission of <sup>235</sup>U and <sup>252</sup>C.

#### I. INTRODUCTION

During the past decennium, the theoretical aspects of the nuclear fission phenomenon received much attention.<sup>1,2</sup> From such studies,<sup>3,4</sup> it has become clear that the various distributions of induced fission are mainly determined between the outer saddle point and the scission point (Fig. 1). In spontaneous fission, an additional role is played by the penetration of the fission barrier between the ground state and the exit point. In some, more constrained studies, one only considers the saddle point or the scission point itself as the most important configuration in determining the fission characteristics.

The "scission-point model" 5-7 basically assumes that there exists an equilibrium among the collective degrees of freedom, near the scission point, which can be characterized by a collective temperature  $T_{col}$ . As the most important collective degrees of freedom one considers the following: the mass ratio  $A_1/A_2$ , the charge ratio  $Z_1/Z_2$ , and the deformation parameters sets  $\{\beta_1\}$  and  $\{\beta_2\}$  of the nascent complementary fragments. According to statistical mechanics, the probability  $P(A_i, Z_i, \{\beta_i\})$  for a particular fission event then becomes proportional to  $\exp[-E_{col}/T_{col}]$ . Here  $E_{col}(A_i, Z_i, \{\beta_i\})$  expresses the total collective energy available to the collective degrees of freedom at the scission point. This collective energy remains constant after the scission point and can be calculated for each scission configuration as the sum of the collective potential energy and the collective kinetic energy.

Taking into account energy conservation (see Fig. 1), an equivalent formulation of the scission-point model assumption results in

$$P(A_i, Z_i, \{\beta_i\}) \sim \exp[+E_{\text{int}}/T_{\text{col}}].$$
<sup>(1)</sup>

Here  $E_{int}(A_i, Z_i, \{\beta_i\})$  stands for the energy absorbed by

the intrinsic nucleonic motion during the fission process from saddle point to scission. Thereby, the equivalent amount is dissipated from the collective degrees of freedom. Consequently, a precise knowledge of the collective potential energy and of the ratio of the intrinsic nucleon excitation energy to the collective kinetic energy, at a moment after the scission point, is necessary for a wellfounded description of the fission characteristics. When calculating the collective potential energy, no particular



FIG. 1. Energy conservation, illustrated schematically for the fission process between saddle point and scission point.

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<u>28</u>

1640

difficulties arise (cf. the detailed calculation of fission barriers<sup>8,9</sup>). In order to obtain the collective kinetic and the intrinsic excitation energy, however, one has to study the process between saddle point and scission point by solving a time-dependent Schrödinger equation. This implies, in general, enormous numerical efforts.<sup>10,11</sup>

#### II. ENERGY CONSERVATION CONSISTENT SCISSION-POINT MODEL

In the scission-point model of Wilkins *et al.*,<sup>6,7</sup> simple numerical calculations become possible by the introduction of two additional assumptions:

(i) One replaces the factor

$$\exp[-(E_{col,pot}+E_{col,kin})/T_{col}]$$

by the factor

-

$$\exp[-E_{\text{col,pot},d}/T_{\text{col}}]$$
,

where  $E_{col,pot,d}(A_i, Z_i, \{\beta_i\})$  describes the collective potential energy of the post-scission configuration, with a distance d between the tips of the produced fragments. The distance d is assumed to be constant, independent of the particular scission configuration. Only under the condition that the collective kinetic energy, calculated with a constant value of d, is independent of both the mass ratio and charge ratio, and of the deformations of the fragments, can the factor

$$\exp[-E_{\rm col,kin}/T_{\rm col}]$$

be taken out of the total exponential and considered as a constant for the particular fission process.

(ii) One assumes that the intrinsic excitation of the fis-

sion fragments can be described by one-quasiparticle excitations, so that the occupation probabilities of the proton and neutron single particle levels satisfy Fermi distributions with parameters  $T_p(A_i, Z_i, \{\beta_i\})$  and  $T_n(A_i, Z_i, \{\beta_i\})$ for protons and neutrons, respectively. Moreover, one assumes that both  $T_p$  and  $T_n$  equal the nuclear temperature T. The parameter T is assumed to be independent of the collective degrees of freedom at the scission point, and is expected to be only a function of the extra excitation energy at the saddle point (Fig. 1).

Using these additional assumptions, it becomes possible to calculate, in a simple way, scission probabilities  $P(A_i, Z_i, \{\beta_i\})$  starting from the following:

(a) temperature independent quantities: Coulomb and nuclear interaction energies between the fragments and liquid-drop energies of the fragments;

(b) temperature dependent microscopic corrections: proton and neutron shell and pairing corrections.

Although both assumptions (i) and (ii) are essential to make the scission-point model a calculable model, they are subject to fundamental criticism. In the following, we concentrate on the aspects related to nuclear temperature in the scission-point model. Assumption (i) of constancy of collective kinetic energy will be discussed in detail in a subsequent paper.

In the scission-point model calculations of Wilkins et al.,<sup>7</sup> the excitation energy is assumed to be described by the nuclear temperature  $T(A_i, Z_i, \{\beta_i\})$ . Moreover, for each mass ratio and charge ratio, and for each deformation of the scission configuration, one imposes the condition  $T(A_i, Z_i, \{\beta_i\}) = T$ . At low nuclear temperatures  $T(A_i, Z_i, \{\beta_i\})$ , the excitation energy  $E_{int}(A_i, Z_i, \{\beta_i\})$  (Refs. 12 and 13),

$$E_{\text{int}} = \sum_{\nu=0}^{\infty} \left\{ 1 - th \left[ \frac{\epsilon_{\nu,p} - \epsilon_F(T_p)}{2T_p} \right] \right\} \epsilon_{\nu,p} - E_p(T_p = 0) + \sum_{\nu=0}^{\infty} \left\{ 1 - th \left[ \frac{\epsilon_{\nu,n} - \epsilon_F(T_n)}{2T_n} \right] \right\} \epsilon_{\nu,n} - E_n(T_n = 0) , \qquad (2)$$

is strongly dependent on the collective parameters:

(a) the single particle states  $\epsilon_v$  are mainly dependent on the deformation parameters  $\{\beta_i\}$  of the fragments;

(b) the Fermi levels  $\epsilon_F$  are mainly dependent on the fragment mass neutron and proton numbers,  $(A - Z)_i$  and  $Z_i$ .

At higher temperatures, more and more terms in (2) contribute to  $E_{int}(A_i, Z_i, \{\beta_i\})$  and the variation of the excitation energy as a function of the collective degrees of freedom becomes less pronounced. One obtains the approximate relation

$$E_{\text{int}} \sim (A_1 + A_2) \cdot T^2 . \tag{3}$$

Whatever the precise relation  $E_{int}(A_i, Z_i, \{\beta_i\})$  vs  $T(A_i, Z_i, \{\beta_i\})$  is, it becomes clear that one cannot satisfy the fundamental law of energy conservation during the fission process, assuming a constant value for  $T(A_i, Z_i, \{\beta_i\})$ .

Therefore, we propose the following modified procedure: Once the parameter d has been determined (d is

the distance between the fragments for which all possible configurations are supposed to have the same collective kinetic energy), the collective potential energy is also fixed sharply. One has to derive the intrinsic excitation energy from energy conservation for each possible combination of the collective degrees of freedom. Moreover, if one assumes that one-quasiparticle excitations determine the occupation probability of the single particle states, the associated temperatures must be fixed so that they correspond to the intrinsic excitation energies derived from energy conservation. The collective potential and intrinsic excitation energies must then be calculated again with the derived temperatures. This recursive method has to be carried through for each fission event until the probabilities  $P(A_i, Z_i, \{\beta_i\})$  converge. With these probabilities and the corresponding excitation energies  $E_{int}(A_i, Z_i, \{\beta_i\})$  one finally is able to derive the averaged excitation energy  $E_{av}$ :

$$E_{\rm av} = \sum_{A_i} \sum_{Z_i} \sum_{\{\beta_i\}} P(A_i, Z_i, \{\beta_i\}) E_{\rm int}(A_i, Z_i, \{\beta_i\}) . \tag{4}$$

This quantity  $E_{av}$  is very important when comparing cal-

culated and experimental results because of its relationship with the experimental known excitation energy of the compound system.

### **III. CALCULATIONS**

Detailed calculations of fission characteristics have been carried out using the Wilkins method and the "energy conservation consistent" method as outlined in Sec. II. We have used the liquid-drop mass formula of Seeger and Howard<sup>14</sup> for describing the macroscopic part of the collective energy. The Coulomb interaction energy was calculated using expansions in the charge moments of various order.<sup>15</sup> The nuclear interaction energy has been obtained using expressions as given by Krappe and Nix.<sup>16</sup> A value of 1.5 fm was taken for the parameter d, while for the parameter  $T_{col}$  the value 1.0 MeV was used. Special attention was given to the calculation of the microscopic corrections. The single particle energies were calculated starting from a Nilsson Hamiltonian.<sup>17,18</sup> In contrast with previous scission-point model calculations, a temperature independent pairing strength was used, and pairing corrections as well as the pairing gaps were obtained by solving the temperature dependent Bardeen-Cooper-Schrieffer (BCS) equations.<sup>9</sup> In calculating the temperature dependence of the shell corrections we did not use the less precise method outlined by Bohr and Mottelson<sup>20</sup>; the shell corrections were calculated by applying the Strutinsky renormalization method to single particle states with a temperature dependent Fermi-occupation probability.<sup>12,13</sup> In the Appendix, we discuss in some detail the numerical solution to this problem. No attempts have been undertaken to modify calculated potential energies by adjusting towards the experimental known ground state masses.

In Fig. 2(a) we illustrate the calculated mass distributions for the fission of a  $^{235}$ U compound nucleus using the energy conservation consistent scission-point method. The resulting mass distributions correspond to different values of the averaged intrinsic excitation energy  $E_{av}$  at the scission point (no temperatures can be specified any longer). In these calculations, we assumed that, for a particular fragment configuration:

(a) The proton single particle states of the light and heavy fragments could be described by the same temperature  $T_p(A_i, Z_i, \{\beta_i\})$  (analogous for the neutron single particle states).

(b) The proton and neutron nuclear temperatures,  $T_p(A_i, Z_i, \{\beta_i\})$  and  $T_n(A_i, Z_i, \{\beta_i\})$ , could be fixed so that the excitation energies absorbed by each type of nucleons becomes proportional to the number of nucleons available.

In Fig. 3, we compare the averaged nuclear temperature for neutrons,

$$T_{\text{av,n}}(A_i) = \sum_{Z_i} \sum_{\{\beta_i\}} P(A_i, Z_i, \{\beta_i\}) T_n(A_i, Z_i, \{\beta_i\}) , \quad (5)$$

with the nuclear temperature value according to the "standard" scission-point method. The relation  $T_{av,n}$  vs  $A_i$  is obviously very similar to the corresponding mass distribution, as is expected from combining relations (1) and (3).

In order to make the comparison with the standard scission-point model calculations,<sup>7</sup> carried out at different

constant temperatures T, one must also calculate each time the averaged intrinsic excitation energy  $E_{av}$  using Eqs. (2) and (4). Figure 2(b) gives the result of these calculations for the fission of <sup>235</sup>U. Although the standard scission-point calculations are completely contradictory to energy conservation, no spectacular differences between the two methods result at high averaged excitation energies. This observation is expected: The relation expressing temperature versus intrinsic excitation energy (3) becomes less steep at higher excitation energies. Moreover, the temperature dependence of the shell corrections  $\delta S$  is not very pronounced  $[|d(\delta S)/dT|| < 5]$ , and the pairing corrections only depend on temperature below the critical temperature. The temperature dependence of the pairing gap is only significant in the neighborhood of the critical temperature.

In even-even fissioning systems, the difference between standard and energy conservation consistent calculations is expected to be larger. Indeed there, more than in the fission of odd-even systems, odd-even effects do show up manifestly. Consider, for instance, three configurations (one with four, one with two, and one with no odd numbers of nucleons) which would have the same potential energy, not taking into account odd-even effects (Fig. 4). The energy conservation consistent calculation generates three different temperatures  $T_4 < T_2 < T_0$ , of which the lowest belongs to the configuration with the strongest odd-even effects, so that these disappear in a retarded manner when rising the excitation energy. On the contrary, the standard calculations would have produced the same averaged excitation energy for a single temperature  $T_{\rm st}$ , higher than both  $T_4$  and  $T_2$ , and consequently the odd-even effects would be much smaller at the same averaged excitation energy. From Fig. 5, in which we compare the standard and energy conservation consistent scission-point model calculated mass distributions for the fission of <sup>252</sup>Cf at various averaged excitation energies, these intuitive arguments are fully confirmed. The dominance of odd-even effects in the mass distributions disappears quite suddenly in the standard calculations at an averaged excitation energy of about 11 MeV. In energy conservation consistent calculations, however, the dominance only disappears very slowly.

The difference between both approaches comes out even more pronounced when comparing charge distributions. In Fig. 6, we compare the  $(Z_p - Z_{ucd})$  values, calculated according to the standard (T = 0.832 MeV) and using the energy conservation consistent treatment, at an averaged intrinsic excitation energy of 15.3 MeV per <sup>235</sup>U fission event for both . The standard curve contains an oscillation with a period of 3.5 mass units, as well as a strongly pronounced N = 82 shell effect. On the other hand, the energy conservation consistent curve contains the same pattern as the well-known experimental  $(Z_p - Z_{ucd})$  curve for the thermal neutron induced fission<sup>21</sup> of <sup>235</sup>U: An oscillation with a period of five mass units.

### **IV. CONCLUSION**

According to the scission-point model, the probability of a particular fission event, characterized by a given set



MASS NUMBER A

FIG. 2. Mass distributions for the fission of  $^{235}$ U, calculated in (a) the energy conservation consistent (left-hand side) and (b) the standard scission-point model (right-hand side).

of collective parameters, is determined by the sum of the collective potential and collective kinetic energy of the post-scission configuration characterized by the same parameters. The precise knowledge of the collective kinetic energy can only be obtained by studying the dynamics of the fission process between the saddle point and the scission point. Calculations do simplify much, imposing a relation between the collective kinetic energy and the vari-



FIG. 3. Comparison between the neutron nuclear temperature  $T_{av,n}(A_i)$  according to the energy conservation consistent scissionpoint model, and the constant nuclear temperature T according to the standard scission-point model, at a particular value of the averaged intrinsic excitation energy  $E_{av}$  (fission of <sup>235</sup>U).

ous collective degrees of freedom at the scission point (mass ratio, charge ratio, and deformations of the fragments).

Whether the collective kinetic energy is imposed or cal-



culated, the value of the intrinsic excitation energy (absorbed by the nucleons) is fixed unambiguously by energy conservation. If one describes the excitation of the fragments by one-quasiparticle excitations, then the values of the parameters  $T(A_i, Z_i, \{\beta_i\})$  of the Fermi occupation probability of the single particle levels become fixed for each combination of the collective degrees of freedom. They cannot be chosen freely, as was the case in the standard scission-point model of Wilkins et al.<sup>7</sup> The difference between energy conservation consistent and standard scission-point model calculations of charge distributions is quite pronounced for a given value of the averaged intrinsic excitation energy. The difference between the two approaches is not very spectacular when comparing mass distribution calculations: Differences only occur when comparing odd-even effects. The dominance of those odd-even effects disappears quite suddenly in the standard calculations, but disappears very slowly in energy conservation consistent calculations.

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FIG. 4. Schematic representation of the disappearance of odd-even effects, for a particular choice of the (constant) collective kinetic energy, using the energy conservation consistent and the standard scission-point model, respectively.

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# APPENDIX: NUMERICAL CALCULATION OF TEMPERATURE DEPENDENT SHELL CORRECTIONS ACCORDING TO THE STRUTINSKY RENORMALIZATION METHOD

Assuming an occupation of the single particle levels of the Fermi type (with nuclear temperature T), one obtains<sup>12</sup> for the shell correction (for instance,  $\gamma = 1.3\hbar\omega_0$  and p = 6):

$$\delta S = U - \tilde{U} = \int_{-\infty}^{+\infty} \epsilon \left\{ \sum_{\kappa=1}^{\infty} \left[ 1 - th \left[ \frac{\epsilon - \epsilon_F}{2T} \right] \right] \delta(\epsilon - \epsilon_{\kappa}) \right\} d\epsilon$$
$$- \int_{-\infty}^{+\infty} \epsilon \left\{ \frac{1 - th \left[ \frac{\epsilon - \tilde{\epsilon}_F}{2T} \right]}{\sqrt{\pi}\gamma} \sum_{\kappa=1}^{\infty} \sum_{\substack{n=0\\\text{even}}}^{p} \frac{H_n(0)H_n \left[ \frac{\epsilon - \epsilon_{\kappa}}{\gamma} \right]}{2^n n!} \exp \left[ - \left[ \frac{\epsilon - \epsilon_{\kappa}}{\gamma} \right]^2 \right] \right\} d\epsilon .$$
(A1)

Here  $H_n(x)$  denotes the Hermite polynomial of degree *n*;  $\epsilon_F$  and  $\tilde{\epsilon}_F$  are the solutions of, respectively,

$$A = \sum_{\kappa=1}^{\infty} \left[ 1 - th \left[ \frac{\epsilon_{\kappa} - \epsilon_F}{2T} \right] \right]$$
(A2)

and

$$A = \frac{2}{\sqrt{\pi}} \sum_{\substack{n=0\\\text{even}}}^{p} \frac{H_n(0)}{2^n n!} \sum_{\kappa=1}^{\infty} p_n \left[ \frac{\widetilde{\epsilon}_F - \epsilon_\kappa}{\gamma}, T \right], \qquad (A3)$$

and the functions  $q_n(x,T)$  and  $p_n(x,T)$  stand for

$$p_n(x,T) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{-t^2} H_n(t) \left[ 1 - th \left[ \frac{t-x}{2T/\gamma} \right] \right] dt , \qquad (A4)$$

$$q_n(x,T) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{-t^2} H_n(t) \left[ 1 - th \left[ \frac{t-x}{2T/\gamma} \right] \right] t \, dt \quad .$$
(A5)

Only in the limiting case T=0, can expressions (A4) and (A5) be calculated independent of the x value. One obtains

$$p_n(x,0) = -e^{-x^2} H_{n-1}(x)$$
, (A6)



FIG. 6.  $(Z_p - Z_{ucd})$  values in the charge distribution of the fission of <sup>235</sup>U, calculated in the energy conservation consistent scission-point model (denoted with a solid line) and in the standard scission-point model (denoted with a dashed line).

$$q_n(x,0) = -e^{-x^2} \left[ \frac{1}{2} H_n(x) + n H_{n-2}(x) \right], \qquad (A7)$$

assuming conventionally

$$H_{-1}(x) = -\frac{\sqrt{\pi}}{2}e^{+x^2}[1 + \operatorname{erf}(x)].$$
 (A8)

For an arbitrary value of T, the integrals (A4) and (A5) have to be calculated numerically. This is extremely time consuming, in view of the fact that, in solving fission problems, tens of thousands of shell corrections have to be calculated. However, after iteratively repeated partial integrations of expressions (A4) and (A5), one obtains a series expansion in powers of T:

$$p_n(x,T) = p_n(x,0) - \sum_{\substack{k=2\\\text{even}}}^{\infty} \beta_k \left[ \frac{T}{\gamma} \right]^k H_{n+k-1}(x) e^{-x^2}, \quad (A9)$$
$$q_n(x,T) = q_n(x,0)$$

$$-\sum_{\substack{k=2\\\text{even}}}^{\infty} \beta_k \left[\frac{T}{\gamma}\right]^k \left[\frac{1}{2}H_{n+k}(x) + nH_{n+k-2}(x)\right]e^{-x^2}, \quad (A10)$$

with

$$\beta_k = \frac{(2^k - 2)\pi^k}{k!} |B_k| , \qquad (A11)$$

 $B_k$  is the Bernoulli number of order k. Since  $\lim_{k\to\infty}\beta_k = +2$ , expansions (A9) and (A10) are oscillating divergent, but of the asymptotic type, owing to the  $e^{-x^2}$  factor: Up to a certain k value, K, the successive terms in (A9) and (A10) become smaller and smaller; for



FIG. 7. Schematic representation of the effect of truncating the series expansion of  $p_n(x, T)$  at any order k.

k > K, they become larger with alternating signs (see Fig. 7). Consequently, truncation of these series ever yields finite errors. These errors are obviously totally negligible as far as  $T/\gamma < 1/10$ , which corresponds with tempera-

tures up to 1.0 MeV. Shell correction calculations at arbitrary temperature T, relying on this method, only require about three times as much time as required by shell correction calculations at zero temperature.

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