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Spontaneous fission of superheavy nuclei

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Abstract. The macroscopic–microscopic method is extended to calculate the deformation energy and penetrability for binary nuclear configurations typical for fission processes. The deformed two-centre shell model is used to obtain single-particle energy levels for the transition region of two partially overlapped daughter and emitted fragment nuclei. The macroscopic part is obtained using the Yukawa-plus-exponential potential. The microscopic shell and pairing corrections are obtained using the Strutinsky and BCS approaches and the cranking formulae yield the inertia tensor. Finally, the WKB method is used to calculate penetrabilities and spontaneous fission half-lives. Calculations are performed for the decay of $^{282,292}120$ nuclei.

Keywords. Cluster decay; alpha decay; spontaneous fission; lifetimes.

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1. Introduction

Fission is a binary phenomenon, and therefore it is necessary to treat it within a two-centre model. When the total deformation energy is calculated along the distance between centres for fission configurations, some valleys appear for different mass asymmetries. These valleys can be obtained as a result of multidimensional minimization of action integral within the space of deformation. To take into account as many deformation parameters as possible, one has to calculate all the terms in the total deformation energy with an appropriate binary model which can describe the stages of the fission process. Such a model has been pioneered and improved by the Frankfurt school in the group of Greiner and collaborators [1,2]. The importance of deformed valleys in the potential energy surfaces (PES) is that they provide the most favoured fission channels for the decay of superheavy nuclei. For the dynamics study, one has to introduce the influence of mass tensor. We use the results from pairing calculations for the occupation probabilities. In this way, the mass tensor components contain binary character of the process, because the pairing parameters are calculated with the two-centre shell model levels. Finally, the penetrabilities and half-lives are calculated within the WKB approximation.

2. The binary macroscopic–microscopic method

The fission-like configurations are used for the total deformation energy calculations. A typical shape is displayed in figure 1, where b_1, a_1 and b_2, a_2 are the small and large semiaxes of the daughter and the emitted fragment respectively, z_s is the position of the separation plane and R is the distance between centres. All these geometrical parameters form the space of deformation, and furtheron one shall work with $\chi_d = b_1/a_1$, $\chi_e = b_2/a_2$, b_2 and R as degrees of freedom.

The microscopic part starts with the binary Hamiltonian written for a single-particle system as

$$H = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\rho, z) + V_{\Omega s} + V_{\Omega^2}, \tag{1}$$

where the potentials are deformation-dependent and m_0 is the nucleon (proton and neutron) mass. The same equation is valid for protons and neutrons. The deformed two-centre oscillator potential for the two fission fragment regions reads as

$$V_{\mathrm{DTCSM}}(\rho, z) = \begin{cases} \frac{1}{2}m_0\omega_{\rho_1}^2\rho^2 + \frac{1}{2}m_0\omega_{z1}^2(z+z_1)^2 \\ \begin{cases} V_{g1}(\rho, z) = 2V_0 - \left[\frac{1}{2}m_0\omega_g^2(\rho-\rho_3)^2 + \frac{1}{2}m_0\omega_g^2(z-z_3)^2\right] \\ V_{g2}(\rho, z) = V_0 \end{cases} \\ \frac{1}{2}m_0\omega_{\rho_2}^2\rho^2 + \frac{1}{2}m_0\omega_{z_2}^2(z-z_2)^2 \end{cases} . \tag{2}$$

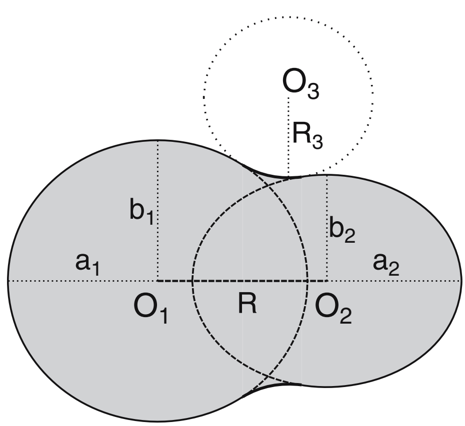

Figure 1. Fission-like configuration for the two ellipsoidal daughter and emitted nuclei. The free geometrical parameters (the semiaxes of the two ellipsoids and the distance between centres) are marked.

Angular momentum-dependent potentials, $V_{\Omega s}$ and V_{Ω^2} are constructed to comply to the $V(\rho, z)$-dependence and hermiticity of the operators, so that

$$V_{\rm so} = \begin{cases} -\left\{\dfrac{\hbar}{m_0\omega_{0T}}\kappa_T(\rho, z), (\nabla V^{(r)} \times \mathbf{p})\mathbf{s}\right\}, & v_T\text{-region} \\ -\left\{\dfrac{\hbar}{m_0\omega_{0P}}\kappa_P(\rho, z), (\nabla V^{(r)} \times \mathbf{p})\mathbf{s}\right\}, & v_P\text{-region} \end{cases}$$

and a similar potential for the V_{Ω^2} term. The matrix diagonalization of H generates the level scheme of the fission configuration, for spheroidally deformed nuclei, at any given distance R between centres and intermediary independent b_2, $\chi_{\rm d}$ and $\chi_{\rm e}$. The level scheme sequence from the compound nucleus (CN) up to complete separation is the input data for the Strutinsky method [3], and calculations are performed separately for protons and neutrons. The shell correction energy is obtained as the difference between the simple sum of level energies and the smoothed part of the same scheme:

$$E_{\rm sh} = \sum_i E_i - \tilde{U}, \tag{3}$$

where the summation is performed for all occupied levels. The main part of the calculation consists of obtaining the smoothed term $\tilde{U}$. A smoothed-level distribution density $\tilde{g}(\epsilon)$ is defined by averaging the actual distribution over a finite interval γ (here equal to 1.2 in $\hbar\omega$ units). If the level energies in units of $\hbar\omega$ are denoted by ϵ_i, one can write the integral which replaces the discrete sum and obtains the smoothed distribution

$$\begin{aligned} \tilde{g}(\epsilon) &= \frac{1}{\gamma}\int_{-\infty}^{\infty} \zeta\left(\frac{\epsilon - \epsilon'}{\gamma}\right) g(\epsilon')\mathrm{d}\epsilon' \\ &= \frac{1}{\gamma}\sum_{i=1}^{\infty} \zeta\left(\frac{\epsilon - \epsilon_i}{\gamma}\right). \end{aligned} \tag{4}$$

This work utilizes a smoothing function ζ of the form

$$\zeta(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2) f_m(x), \tag{5}$$

where $x = (\epsilon - \epsilon')/\gamma$ and the smoothing function f is taken as a polynomial sum:

$$f_m(x) = \sum_{k=0}^{m} a_{2k} H_{2k}(x), \tag{6}$$

where $H_n(x)$ are the Hermite polynomials, and the maximum degree m (here 3) is taken such as $\mathrm{d}\tilde{U}/\mathrm{d}\gamma$ = constant (the plateau condition). The maximum level is chosen such that $|x_i| \geq 3$. Beyond this limit, the contribution of more remote levels is negligible. Once the density of smooth levels $\tilde{g}(\epsilon)$ is obtained by this smearing procedure, the smoothed part of the energy is given by

$$\tilde{u} = \tilde{U}/\hbar\omega = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon)\epsilon \mathrm{d}\epsilon, \tag{7}$$

where the Fermi level $\tilde{\lambda}$ for smoothed distribution is obtained from the conservation of the total number of nucleons:

$$N_{\mathrm{e}} = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon)\mathrm{d}\epsilon. \tag{8}$$

By substituting this expression for $\tilde{g}(\epsilon)$ one obtains

$$N_{\mathrm{e}} = \frac{2}{\sqrt{\pi}} \sum_{1}^{\infty} \int_{-\infty}^{x_{iF}} f_m(x_i^2) \exp(x_i^2)\mathrm{d}x_i, \tag{9}$$

where $x_{iF} = (\tilde{\lambda} - \epsilon_i)/\gamma$. The summation is in fact reduced to the levels around the Fermi limit. The latter equation yields the Fermi level for smoothed distribution $\tilde{\lambda}$, and is solved numerically. We consider a set of doubly degenerate energy levels $\{\epsilon_i\}$ expressed in units of $\hbar\omega_0^0$. Calculations for neutrons and protons are similar and hence for the moment we shall consider only protons. In the absence of a pairing field, the first $Z/2$ levels are occupied, from a total number of n_t levels available. Only for a few levels below (n) and above (n'), the Fermi energy contributes to the pairing correlations. Usually, $n' = n$. If $\tilde{g}_{\mathrm{s}}$ is the density of states at the Fermi energy obtained from the shell correction calculation $\tilde{g}_{\mathrm{s}} = \mathrm{d}Z/\mathrm{d}\epsilon$, expressed as the number of levels per $\hbar\omega_0^0$ spacing, the level density is half of this quantity: $\tilde{g}_n = \tilde{g}_{\mathrm{s}}/2$.

We can choose as computing parameter, the cut-off energy (in units of $\hbar\omega_0^0$), $\Omega \simeq 1 \gg \tilde{\Delta}$. Let us take the integer part of the following expression:

$$\Omega\tilde{g}_{\mathrm{s}}/2 = n = n'. \tag{10}$$

When we obtain $n > Z/2$ from the calculation we consider $n = Z/2$ and similarly if $n' > n_t - Z/2$ we consider $n' = n_t - Z/2$.

The gap parameter $\Delta = |G| \sum_k u_k v_k$ and the Fermi energy with pairing correlations λ (both in units of $\hbar\omega_0^0$) are obtained as solutions of a nonlinear system of two BCS equations

$$n' - n = \sum_{k=k_i}^{k_f} \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}, \tag{11}$$

$$\frac{2}{G} = \sum_{k=k_i}^{k_f} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}, \tag{12}$$

where $k_i = Z/2 - n + 1$; $k_f = Z/2 + n'$.

The pairing interaction G is calculated from a continuous distribution of levels

$$\frac{2}{G} = \int_{\tilde{\lambda}-\Omega}^{\tilde{\lambda}+\Omega} \frac{\tilde{g}(\epsilon)\mathrm{d}\epsilon}{\sqrt{(\epsilon - \tilde{\lambda})^2 + \tilde{\Delta}^2}}, \tag{13}$$

where $\tilde{\lambda}$ is the Fermi energy deduced from the shell correction calculations and $\tilde{\Delta}$ is the gap parameter obtained from a fit to experimental data, usually taken as $\tilde{\Delta} = 12/\sqrt{A}\hbar\omega_0^0$.

Both Δ_p and Δ_n decrease with increasing asymmetry $(N-Z)/A$. From the above integral we get

$$\frac{2}{G} \simeq 2\tilde{g}(\tilde{\lambda}) \ln\left(\frac{2\Omega}{\tilde{\Delta}}\right). \tag{14}$$

Real positive solutions of BCS equations are allowed if

$$\frac{G}{2} \sum_k \frac{1}{|\epsilon_k - \lambda|} > 1 \tag{15}$$

i.e., for a pairing force (G-parameter) large enough at a given distribution of levels.

As a consequence of pairing correlation, the levels situated below the Fermi energy are only partially filled, while those above the Fermi energy are partially empty; a probability is given for each level to be occupied by a quasiparticle

$$v_k^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\right] \tag{16}$$

or a hole

$$u_k^2 = 1 - v_k^2. \tag{17}$$

Only the levels in the near vicinity of the Fermi energy (in a range of the order of Δ around it) are influenced by the pairing correlations. For this reason, it is only sufficient for the cut-off parameter value to exceed a given limit $\Omega \gg \tilde{\Delta}$, the value in itself having no significance. The shell and pairing corrections calculated for the splitting of $^{292}120$ in the Sn fission channel are displayed in figure 2 along the reduced distance between centres. One observes large fluctuations of proton and neutron shell corrections opposite to the pairing corrections; maxima for shell corrections correspond to minima for pairing corrections and vice-versa.

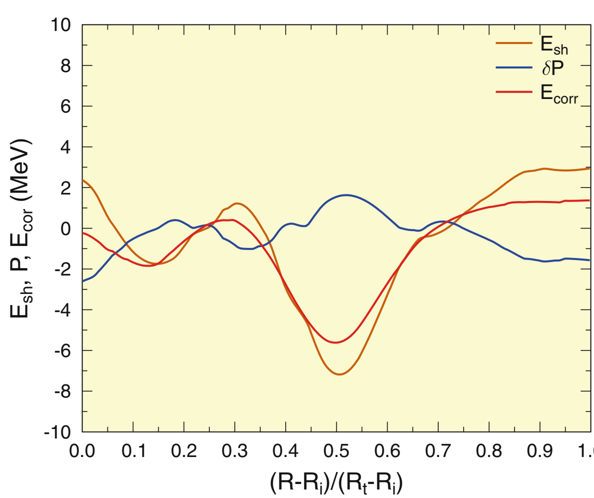

Figure 2. Shell and pairing corrections for neutrons and protons, and their sum for the symmetric splitting of ^{236}Pu.

The macroscopic part is obtained using the Yukawa-plus-exponential method, specific to binary processes. The Coulomb term E_C [4] and the nuclear surface term E_Y [5] are computed as

$$E_C = \frac{2\pi}{3}\left(\rho_{e_d}^2 F_{C_d} + \rho_{e_e}^2 F_{C_e} + 2\rho_{e_d}\rho_{e_e} F_{C_{de}}\right) \tag{18}$$

and

$$E_Y = \frac{1}{4\pi r_0^2}[c_{s_d} F_{EY_d} + c_{s_e} F_{EY_e} + 2(c_{s_d} c_{s_e})^{1/2} F_{EY_{de}}], \tag{19}$$

where ρ_{ei} is the charge density and c_{si} the surface coefficient. F_{C_i} and F_{EY_i} are shape-dependent integrals. The peculiarity resides in the last term of both formulae, $F_{C_{de}}$ and $F_{EY_{de}}$, which account for the interaction between non-overlapped parts of the overlapping configuration. Details of these terms are given in [6].

The total deformation-dependent macroscopic energy is calculated as the sum of the Coulomb and surface terms:

$$E_{\text{macro}} = (E_C - E_C^{(0)}) + (E_Y - E_Y^{(0)}), \tag{20}$$

where $E_C^{(0)}$ and $E_Y^{(0)}$ are the values for the corresponding spherical CN. Finally, the deformation energy is computed as the sum of the macroscopic part, the shell correction and pairing energies:

$$E_{\text{def}} = E_{\text{macro}} + E_{\text{sh}} + P. \tag{21}$$

3. Dynamics

To obtain the penetrabilities for different reaction channels, the action integral must be computed. Besides the usual deformation energy, nuclear inertia tensor which accounts for the reaction of nucleus to deformation along a given degree of freedom, needs to be computed. This uses the cranking approach to obtain mass tensor components within the four-dimensional space of (b_e, χ_d, χ_e, R). According to the cranking model, after including the BCS pairing correlations [7], the inertia tensor is given by [8]

$$B_{ij} = 2\hbar^2 \sum_{\nu\mu} \frac{\langle\nu|\partial H/\partial\beta_i|\mu\rangle\langle\mu|\partial H/\partial\beta_j|\nu\rangle}{(E_\nu + E_\mu)^3}(u_\nu v_\mu + u_\mu v_\nu)^2 + P_{ij}, \tag{22}$$

where H is the two-centre single-particle Hamiltonian which allows the determination of energy levels and the wave functions $|\nu\rangle$, u_ν, v_ν are the BCS occupation probabilities, E_ν is the quasiparticle energy and P_{ij} gives the contribution of occupation number variation when the deformation is changed (terms include variation of the gap parameter, Δ, and the Fermi energy, λ, $\partial\Delta / \partial\beta_i$ and $\partial\lambda / \partial\beta_i$).

The penetrability P for a given fusion path is calculated as

$$P = \exp(-K_{\text{ov}}), \tag{23}$$

where K_{ov} is the overlapping action integral. The barriers are supposed to be tunnelled at the level of ground-state energy of the CN. This is the minimum value of kinetic energy

Table 1. The fission channels with the lowest half-lives from $^{282}120$.

Reaction	log P	log T
$^{140}Nd+^{142}Nd$	−5.0	3.51
$^{120}Cd+^{162}Hf$	−5.35	3.92
$^{112}Pd+^{170}Wf$	−5.9	4.22

Table 2. The fission channels with the lowest half-lives from $^{292}120$.

Reaction	log P	log T
$^{146}Nd+^{146}Nd$	−8.27	5.78
$^{120}Sn+^{172}Yb$	−6.98	4.8
$^{116}Cd+^{176}Hf$	−7.41	5.1

in this study where fission reactions are intended to take place at the lowest energy. K_{ov} is calculated numerically as

$$K_{\text{ov}}(b_2, \kappa_{\text{d}}, \kappa_{\text{e}}; R) = \frac{2}{\hbar} \int_{(\text{fis})} [2B(R)_{b_2,\kappa_{\text{d}},\kappa_{\text{e}}} E_{\text{def}}(R)_{b_2,\kappa_{\text{d}},\kappa_{\text{e}}}]^{1/2} \text{d}R. \tag{24}$$

As K_{ov} is calculated for every set $(b_2, \kappa_{\text{d}}, \kappa_{\text{e}})$ at every point R, the penetrability appears as multidimensional. The final value of P for every channel reaction is the result of the minimization of action integral K_{ov} over the whole range of $(b_2, \kappa_{\text{d}}, \kappa_{\text{e}}, R)$. The multi-dimensional minimization of the action integral is performed over the grid in the space of $I(b_2, \kappa_{\text{d}}, \kappa_{\text{e}}; R)$, where I is the integrand.

4. Results and discussion

The method described here is used in the decay of $^{282,292}120$ nuclei. For every superheavy system, the entire possible range of mass asymmetry has been considered. The daughter–emitted fragment pairs start from the symmetry $\eta_A = 0$ ($A_{\text{d}} \simeq A_{\text{e}}$) up to the maximum asymmetry value. Once static barriers are obtained from the minima on the potential energy surface, the mass asymmetry is completed by finding the charge asymmetry, by repeating the calculations for all possible $(Z_{\text{d}}, Z_{\text{e}})$ for the same $(A_{\text{d}}, A_{\text{e}})$. Finally the mass tensor and penetrability are calculated for all $(A_{\text{d}}, Z_{\text{d}}) - (A_{\text{e}}, Z_{\text{e}})$ reaction channels by preserving R as the main free variable. The numerical results for the most favoured fission channels (lowest half-life) are presented in tables 1 and 2.

5. Conclusions

A binary configuration model was used within a large number of degrees of freedom to calculate the barriers and penetrabilties towards the calculation of fission lifetimes in

$^{282,292}120$ superheavy isotopes. Dynamical multidimensional minimization of the action integral yielded the penetrabilities and half-lives by the WKB method. The barriers are larger and higher, and penetrabilities are lower as the system becomes neutron-rich. Highest values of log P for every superheavy isotope are obtained for spherically emitted and/or daughter nucleus.

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