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Computer modelling of the decay of atomic compound nuclei

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Abstract

We present numerical algorithm which describes the decay of hot, rotating compound nuclei. This algorithm treats the fission dynamics in conjunction with light-particle (n, p, α) evaporation. The detailed results are given for the ^{188}Pt nucleus at the excitation energy of 100 *MeV*.

1. Introduction

Properties of highly excited nuclei being in thermal equilibrium are of great physical interest. This is the reason for construction of a numerical program able to simulate the decay of such complex objects. Indeed, good computer programs are not only to reproduce or predict experimental data but they often also serve as a guideline to prepare new experiments. Such a computer modelling can then save a lot of time (and money) for scientists working in this field.

We would like to describe the dynamics of the nuclear fission process from an initial state in which the compound nucleus is formed with an almost spherical shape to the saddle and finally the scission configurations where the nucleus separates into two fragments. The simultaneous possible des-excitation of the compound nucleus through the emission of light particles is included throughout the deformation process. The decision about the decay path of a compound nucleus is made by a computer program written in FORTRAN-77, which is based on the algorithm described below.

The paper is organized as follows: after presenting the physical background of our model in Section 2, we show in Section 3 how to determine the decay of the compound nucleus and we explain how we couple the emission of light particles to the dynamical evolution of the system. We finally present some typical CPU times obtained with our program on different platforms on which we have performed our simulations.

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2. Physical model

2.1. Shape parametrization and definition of the fission path

For the description of the a variety of nuclear shapes encountered along the fission path we need a flexible enough description of the nuclear surface. We first used the very general parametrization proposed by Trentalange, Koonin and Sierk [1] which, unfortunately, turns out to be numerically unstable. We are therefore now using a new parametrization which belongs to the generalized Funny-Hill family of shapes [2-3], based on the Lorentz function. For axially symmetric nuclear shapes it is given by:

$$r_s^2(z) = c^2 \mathrm{R}_0^2 \left(1-u^2\right)\left[A + \mathrm{sign}\left(\mathrm{B}\right)\left(1 - \frac{1}{1+|B|u^2}\right)\right], \tag{1}$$

where r_s^2 is the square distance from the z-axis to the surface and $u = z/z_0$ with $2z_0 = 2\mathrm{R}_0 c$ the elongation of the nucleus along the *z*-axis, *B* being related to the neck size. Imposing volume conservation as the nucleus deforms one obtains a relation which expresses *A* as a function of the other parameters *B* and *c*.It is known that rapidly rotating nuclei can exhibit nonaxial shapes. We have therefore introduced an additional parameter *h* which describes such shapes [3]. For the case that sections perpendicular to the *z*-axis produce ellipses with half-axis of lengths *a* and *b*, *h* is given by:

$$h = \frac{b^2 - a^2}{\max\left(a^2, b^2\right)}.$$

The expression (1) for the nuclear surface can then be rewritten as:

$$\hbar^2 = \begin{cases} r_s^2 \dfrac{\sqrt{1+h}}{1+h\cos^2 j}, & h \in (-1,0) \\ r_s^2 \dfrac{\sqrt{1-h}}{1-h\cos^2 j}, & h \in (0,1) \end{cases} \tag{2}$$

where j denotes the azimuthal angle in the cylindrical coordinates.

The fission path is obtained by minimization with respect to the neck parameter *B* and the non-axiality *h* of the collective potential [4] defined as the Helmholtz free energy [4] at given deformation for the fixed temperature *T* and the angular momentum *L*. This collective potential can be written as:

$$V(def) = E_u + E_s(def) + E_k(def) + E_c(def) + E_r(def), \tag{3}$$

where E_u, E_s, E_k, E_c and E_r are volume, surface, curvature, Coulomb and rotational energies respectively. These terms are evaluated within the temperature-dependent liquid-drop model by performing multiple Gauss quadratures over the *z* and j coordinates.

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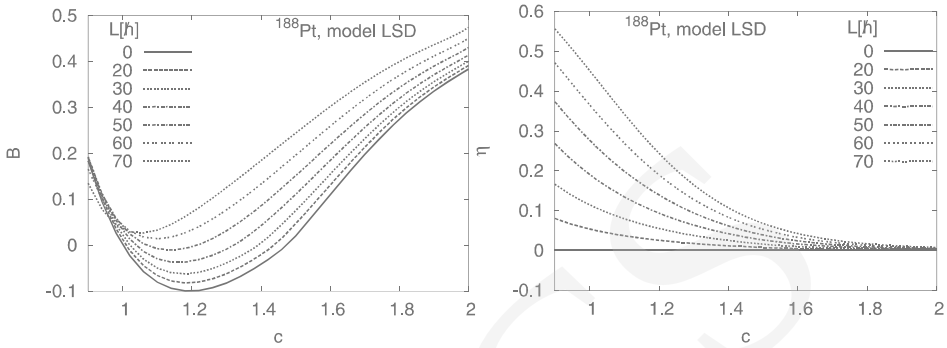

Fig. 1. Deformation parameters corresponding to the fission path of ^{188}Pt

The minimization of the potential surface was performed using the subroutine ZXMIN [5]. The parameters B and h along the fission path are shown in Fig. 1 for ^{188}Pt for different angular momenta.

The potential energy surface of ^{188}Pt minimized with respect to the neck parameter B is presented in Fig. 2 for the angular momenta $L = 0\mathbf{h}$ and $L = 60\mathbf{h}$. The different shapes corresponding to the white points on the fission path are shown in the lower part of Fig. 2.

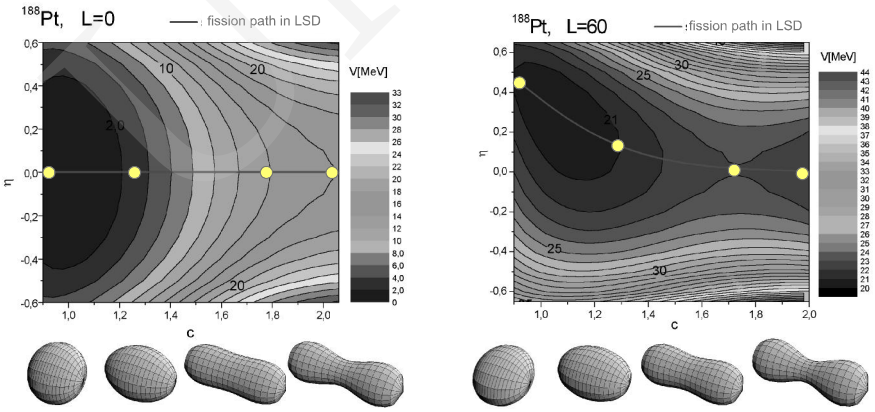

Fig. 2. Maps of collective potential for ^{188}Pt at $L = 0\mathbf{h}$ and $L = 60\mathbf{h}$ and the nuclear shapes corresponding to the different points along the fission paths

2.2. Equations of motions

The time evolution of the nuclear system from its initial (almost spherical) state to its final state corresponding to the scission configuration is described by the following equations of motion [6]:

$$\frac{dq}{dt} = \frac{p}{M(q)}, \tag{4}$$

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$$\frac{dp}{dt} = \frac{1}{2}\left(\frac{p}{M(q)}\right)^2 \frac{dM(q)}{dq} - \frac{dV(q)}{dq} - \frac{g(q)}{M(q)}p + E_L(t), \tag{5}$$

where *p(t)* is the momentum associated with the collective coordinate *q(t)*, *M(q)* the collective mass evaluated in the irrotational fluid approximation [7], *g(q)* the friction coefficient calculated in the wall-and-window friction model [8], and *V(q)* the collective potential. Explicit expressions of these quantities have been presented and discussed in detail in Ref. [4]. The quantity $F_L(t)$ represents the random Langevin force which depends on the nuclear diffusion, the time steps used in the numerical code and a normally distributed (Gaussian) random variable. To solve these equations of motion we have used their discretised form with a sufficiently small time step t [6, 9].

2.3. Particle emission

The probability for emitting any particle in a (small enough) time step of length t is given by

$$P(t) = 1 - e^{-\Gamma t} \approx \Gamma t \ , \tag{6}$$

where $\Gamma = \Gamma_n + \Gamma_p + \Gamma_a$ and Γ_n is the total emission rate for the particles of type n integrated over their energies e_k and the angular momenta l_l. The partial width Γ_n^{kl} which determines the number of particles of type n with given energy and angular momentum emitted per unit time from a nucleus with the excitation energy E^* and the total angular momentum L are described by the Weisskopf formula [10, 6] or by a more microscopic determination which we presented in Ref. [9].

3. Fission and emission algorithm

The fission and emission program is based on the Monte Carlo algorithm. For random numbers we use the generator RAN3 which returns a uniform random number between 0 and 1 and a function GASDEV which returns a normally distributed random number [11].

The initial conditions related to the formation process of the compound nucleus describe the distribution of the initial points of the trajectories in the *(q,p)* space. These conditions are defined by the input data. The decision whether fission and/or emission occurs is taken at each time step *[t,t+t]* when solving Eqs. (4, 5). To proceed towards fission one draws a random number h from a Gaussian distribution which defines the fluctuating force in Eq. (5) and thus generates the next point of the trajectory. Each trajectory can either lead to fission if it overcomes the fission barrier and continues to the scission point or ends up as a rather cold nucleus (evaporation residuum) if too much energy has

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been lost on emission. To decide whether a light particle is emitted at a given time step one draws another random number h_1. If $h_1 < P(t)$ a particle is emitted. In this case one needs to decide on which type this particle is. For this purpose one draws a random number h_2. Covering the interval [0,1] by the 3 bins P_n/P, P_p/P and P_α/P the localisation of h_2 in either of the 3 bins decides on whether a neutron, a proton or an α particle is emitted, as shown in Fig. 3.

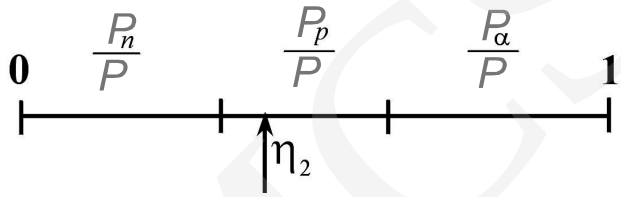

Fig. 3. Determination of the type of emitted particle

To determine the energy with which this particle is emitted one introduces the probability $\Pi_n(e_k)$ that a particle of type n is emitted with an energy smaller than e_k [6]. The function Π_n covers the interval [0,1]. Subdividing this interval into a certain number of equal bins the drawing of a third random number h_3 decides with which energy the light particle is emitted. Inverting this function, $\Pi_n^{-1}(h_3) \in [e_a - \Delta e_a/2, e_a + \Delta e_a/2]$ determines into which energy bin the evaporated particle falls (see Fig. 4).

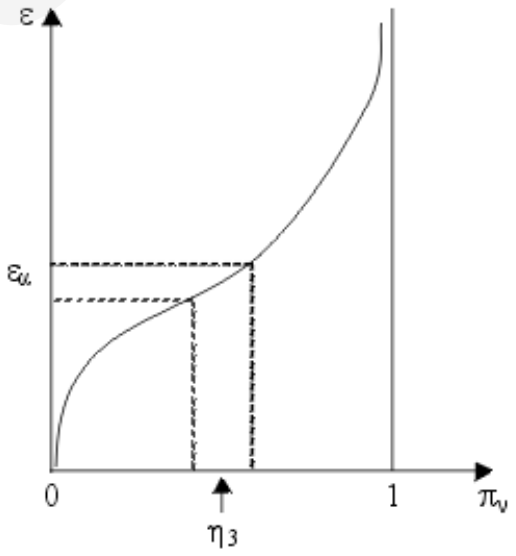

Fig. 4. Determination of the energy with which the particle is emitted.

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Emitted particles and their energies are registered. It is evident from the conservation of the total energy and angular momentum that each particle emission carries away excitations energy and angular momentum. As the height of a fission barrier depends on these quantities, it is evident that hereby the height of the fission barrier of the residual nucleus is increased which, in turn, renders fission less and less probable. The dependence of the height of the fission barrier for different values of the temperatures and different values of the angular momentum is shown in Fig. 5.

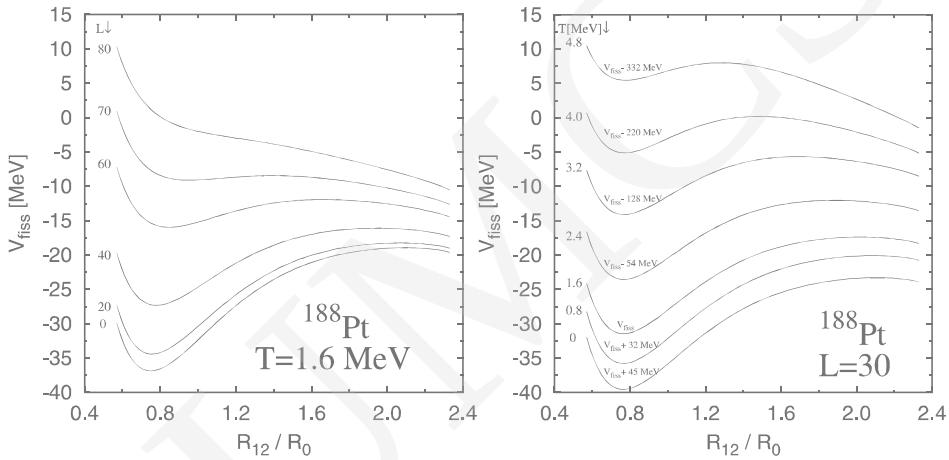

Fig. 5. Collective potential V_{fiss} for ^{188}Pt as the function of the center-of-mass distance between the fragments $\boldsymbol{R}_{12}/\boldsymbol{R}_0$ from oblate deformation up to the scission point. The left-hand side of the figure corresponds to different values of the angular momentum L and T = 1.6 MeV, while the right-hand side shows V for different temperatures T and $L = 30\mathbf{h}$. The different curves are shifted vertically in order to make the relative changes more visible

To be able to make reliable predictions on the fission yields and the multiplicity and energy distribution of the emitted light particles such dynamical calculations which follow the nuclear system from the initial state to the final configuration has to be carried out for a very large number ($\mathrm{NTRAJ} \approx 10^4$) of trajectories, each of these trajectories being subdivided into a very large number ($\mathrm{NTIME} \approx 10^5$ NTIME 10^5) of time intervals.

To get a feeling about the involved computation times we give in the table below the involved CPU times for a typical set of the parameters $\mathrm{NTRAJ} = 1000$ and $\mathrm{NTIME} = 800000$ and for 2 different processors which we used.

PROCESOR	RAM	CPU TIME
Aplha 600 MHz	256 MB RAM	5h
Athlon MP 1700	512 MB RAM	2h

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We would finally like to mention that our model was recently extended [12-13] by including the mass-asymmetry degree of freedom as an additional dynamical variable and was used to predict properties of superheavy nuclei as e.g. synthetized at the JINR in Dubna.

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