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MICROSCOPIC TREATMENTS OF FISSION INERTIA WITHIN THE WOODS-SAXON TWO CENTER SHELL MODEL

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Abstract. Along the minimal action path for the 234 U fission, the mass parameters are evaluated microscopically with three different models: the cranking model, the gaussian overlap approximation and the semi-diabatic cranking evaluation. All of them give similar fluctuations of the inertia along the minimal action trajectory, approximately the same values in the ground state and after the scission. However, in general the cranking model gives larger values along the minimal action trajectory while the semi-adiabatic evaluation gives the smaller ones.

Key words: Woods-Saxon two center shell model, inertia, fission.

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1. INTRODUCTION

In the macroscopic-microscopic method [1], the whole system is characterized by some collective coordinates that determine approximately the behavior of many other intrinsic variables. The basic ingredient in such an analysis is the shape parametrization that depends on several macroscopic degrees of freedom. The generalized coordinates associated with these degrees of freedom vary in time leading to a split of the nuclear system in two separated fragments. The macroscopic deformation energy is calculated within the liquid drop model. A microscopic potential must be constructed to be consistent with this nuclear shape parametrization. A microscopic correction is then evaluated using the Strutinsky procedure.

The deformation energy is a function of the collective parameters and gives the generalized forces that act on the nuclear shape. For a complete description of the fission process, it is therefore required to know how the nucleus reacts to these generalized forces. This information is contained in the effective mass of the system [2]. The most used approach to calculate the inertia is the cranking model. Recently, the cranking model was generalized by taking into account the intrinsic excitation produced during the fission process itself [3]. In this paper our aim is to compare several

microscopic approaches for the inertia: the cranking model, the generator coordinate method in the gaussian overlap approximation (GOA) and the semi-adiabatic cranking model. A previous comparison between microscopic theories and the Werner-Wheeler method was realized in Refs. [4, 5].

2. MICROSCOPIC MASS PARAMETERS

In a multidimensional deformation space, where the nuclear shape is described by the set of n independent generalized coordinates q_i , the inertia tensor M_{ij} is defined by the equation of the kinetic energy T:

$$T = \frac{1}{2} \sum_{i,j=1}^{n} M_{ij}(q_1, ..., q_n) \frac{\partial q_i}{\partial t} \frac{\partial q_j}{\partial t}$$
(1)

In the adiabatic description of the collective behavior of a nucleus, the nucleons are assumed to move in a average deformed potential. Using a Hamiltonian $H(q_1, ..., q_n)$ that includes pairing interactions, introducing the collective parameters q_i by means of the Lagrange multipliers, it is possible to obtain the response of the nuclear system for slow changes of the shape within the cranking model formula [6]

$$M_{ij}(q_1,...,q_n) = \frac{2}{\hbar^2} \sum_{\nu,\mu} \frac{\left\langle \mu \middle| \frac{\partial H}{\partial q_i} \middle| \nu \right\rangle \left\langle \nu \middle| \frac{\partial H}{\partial q_j} \middle| \mu \right\rangle}{(E_\mu + E_\nu)^3}$$
(2)

$$\times (u_\mu v_\nu + u_\nu v_\mu)^2 + P_{ij}$$

where $|\nu\rangle$ and $|\mu\rangle$ are single particle wave functions, E_{ν} , u_{ν} and v_{ν} are the quasiparticle energy, the vacancy and occupation amplitudes of the state ν , respectively, in the BCS approximation, and P_{ij} is a correction that depends on the variation of the pairing gap Δ and the Fermi energy λ as function of the deformation coordinates. The inertia *B* along a trajectory in the configuration space spanned by the generalized coordinates q_i (*i*=1,*n*) can be obtained within the formula

$$B = \sum_{i=1}^{n} \sum_{j=1}^{n} M_{ij} \frac{\partial q_i}{\partial R} \frac{\partial q_j}{\partial R}$$
(3)

In the previous formula we consider that R is a generalized variable that describe the elongation of the nuclear system, as discussed in the next section. The total inertia is the sum of the contributions that correspond to the proton and to the neutron level schemes. Usually, the matrix elements of the derivatives of the Hamiltonian in Rel. (2) are replaced by the matrix elements of the derivatives of the mean field potential alone.

In the generator coordinate method [7-10] the inertia must be calculated sepa-

rately for proton and neutron working spaces:

$$M_{n(p)} = 2\hbar^2 \frac{\left[\sum_{\nu,\mu} P_{\nu\mu} P_{\mu\nu} (u_{\nu}v_{\mu} + u_{\mu}v_{\nu})^2\right]^2}{\sum_{\nu,\mu} (E_{\nu} + E_{\mu}) P_{\nu\mu} P_{\mu\nu} (u_{\nu}v_{\mu} + u_{\mu}v_{\nu})^2}$$
(4)

The quantities $P_{\nu\mu}$ are given by the next formula that depends on a specific trajectory in the collective configuration space

$$P_{\nu\mu} = \sum_{i}^{n} P_{\nu\mu}(q_i) \frac{\partial q_i}{\partial R}$$
(5)

where [8]

$$P_{\nu\mu}(q_i) = - \langle \nu \mid \frac{\partial H}{\partial q_i} \mid \mu \rangle \frac{u_{\nu}v_{\mu} + u_{\mu}v_{\nu}}{E_{\mu} + E_{\nu}} + \delta_{\nu\mu}\frac{\Delta}{2E_{\nu}^2} \left(\frac{\partial\lambda}{\partial q_i} + \frac{\epsilon_{\nu} - \lambda}{\Delta}\frac{\partial\Delta}{\partial q_i}\right)$$
(6)

Here, ϵ_{ν} is the single particle energy of the state ν . The inertia of the nuclear system is obtained as follows:

$$B = \frac{M_n M_p}{4(M_n + M_p)} \tag{7}$$

where the index n stands for the neutron level scheme while the index p is for protons.

In the case of the semi-adiabatic cranking model, the tensor elements of the inertia are:

$$M_{ij} = 2\hbar^2 \sum_{\nu \neq \mu} \frac{\left(E_{\nu\mu} - E_0\right) \left(\frac{|\kappa_{\nu}\sqrt{\rho_{\nu}}|\kappa_{\mu}|}{|\kappa_{\nu}|\sqrt{\rho_{\mu}}} - \frac{\kappa_{\mu}\sqrt{\rho_{\mu}}|\kappa_{\nu}|}{|\kappa_{\mu}|\sqrt{\rho_{\nu}}|^2}\right) < \mu \mid \frac{\partial H}{\partial q_i} \mid \nu > < \nu \mid \frac{\partial H}{\partial q_j} \mid \mu > \\ (E_{\nu\mu} - \sum_{\gamma \neq \nu,\mu} T_{\gamma}^{\nu\mu} - E_0 + \sum_{\gamma} T_{\gamma})^2$$
(8)

where $\kappa_{\nu} = u_{\nu}v_{\nu}$ is the paring moment component, $\rho_{\nu} = v_{\nu}^2$ is the occupation probability of the level ν in the seniority zero state. The energies of the seniority two states are:

$$E_{\nu\mu} = \sum_{\gamma \neq \nu,\mu} \rho_{\gamma}^{\nu\mu} \epsilon_{\gamma} - \frac{|\Delta_{\nu\mu}|^2}{G} - G \sum_{\gamma \neq \nu,\mu} (\rho_{\gamma}^{\nu\mu})^2 + \epsilon_{\nu} + \epsilon_{\mu}$$
(9)

where the levels ν and μ are blocked, the values of $\rho_{\gamma}^{\nu\mu}$ address occupation probabilities for the seniority two states and

$$T_{\gamma}^{\nu\mu} = 2\rho_{\gamma}^{\nu\mu}\epsilon_{\gamma} - 2G(\rho_{\gamma}^{\nu\mu})^2 + \frac{\kappa_{\gamma}^{\nu\mu}\Delta_{\nu\mu}^* + (\kappa_{\gamma}^{\nu\mu})^*\Delta_{\nu\mu}}{2} \left(\frac{(\rho_{\gamma}^{\nu\mu})^2}{|\kappa_{\gamma}^{\nu\mu}|^2} - 1\right)$$
(10)

In the previous formalism, E_0 and all quantities without indices $\nu\mu$ correspond to the seniority zero state. The inertia along the trajectory is obtained within Rel.(7). The final value of B is a sum of the quantities obtained for protons and neutrons as in the classical cranking model and the relation (3) is used.

3. THE FISSION TRAJECTORY

In order to calculate the microscopic inertia for the fissioning system, the first step is the determination of a fission path that satisfies the minimal action criteria [2]. The sequence of shapes that follows a nucleus when it passes from the ground state to the scission point depend principally on the potential energy surface and the inertia. In the macroscopic-microscopic model, first of all, it is required to define a nuclear shape parametrization. In the following, an axial symmetric nuclear shape is obtained by smoothly joining two spheroids of semi-axis a_i and b_i (i=1,2) with a neck surface generated by the rotation of a circle around the axis of symmetry. By imposing the condition of volume conservation we are left by five independent generalized coordinates $\{q_i\}$ (i=1,5) that can be associated to five degrees of freedom: the elongation R given by the distance between the centers of the spheroids; the necking parameter $C = S/R_3$ related to the curvature of the neck, the eccentricities ϵ_i associated with the deformations of the nascent fragments and the mass asymmetry parameter $\eta = a_1/a_2$. This parametrization was widely used in investigating fission processes [11–16] and the formation of superheavy elements [17, 18]. This parametrization is described in detail in Refs. [19].

If we consider that the elongation $q_1 = R$ is the main coordinate, the dependencies of the other generalized coordinates $q_i = f_i(R)$ (i = 2, 5) must be obtained. As specified in Ref. [2], such trajectories emerge by minimizing the action functional.

$$P = -\frac{2}{\hbar} \int_{R_i}^{R_f} \sqrt{2B(q_i, \partial q_i/\partial R)V(q_i)} dR \tag{11}$$

where $B(q_i, \partial q_i/\partial R)$ is the inertia along the trajectory and $V(q_i)$ is the deformation energy. R_i and R_f stand for the elongation associated to the ground state and the exit from the barrier, respectively. In our calculation the reference of the deformation energy is always taken as the energy in the ground state. So the next condition is fulfilled $V(R_i) = V(R_f) = 0$. As it can be seen in formula (11), as the fissioning nucleus passes from its ground state to the scission configuration, the sequences of shapes depends mainly on the deformation energy and the inertia. The deformation energy is obtained in the frame of the macroscopic-microscopic model [1] while the inertia is computed within the cranking approximation. The deformation energy was obtained by summing the liquid drop energy E_{LDM} with the shell and the pairing corrections δE . The macroscopic energy E_{LDM} is obtained in the framework of the Yukawa - plus - exponential model [20] extended for binary systems with different charge densities [21] as detailed in Ref. [22]. The shell corrections are obtained within the two center Woods-Saxon model [19]. They are many methods to minimize dynamically the action integral [23–26]. We will use the method initiated in [23] and used extensively in fission calculations [27-30].

4. SINGLE PARTICLE LEVELS



Fig. 1 – The potential barrier V for the 234 U fission along the minimal action trajectory as function of the elongation R. The ground state is located close to a distance between the centers of fragments of about 4 fm.

To calculate the inertia, we need a microscopic potential. The microscopic potential must be constructed to be consistent within our nuclear shape parametrization. The simplest way it to use a semi-phenomenological Woods-Saxon potential. In order to take into account nuclear deformations going over to separate shapes and obtain two separated fragments, a two-center shell model with a Woods-Saxon potential was developed recently [19]. Other recipes that allows to treat strongly deformed nuclei are presented in Refs. [31,32]. The mean field potential is defined in the frame of the Woods-Saxon model:

$$V_0(\rho, z) = -\frac{V_c}{1 + \exp\left[\frac{\Delta(\rho, z)}{a}\right]}$$
(12)

where $\Delta(\rho, z)$ represents the distance between a point (ρ, z) and the nuclear surface. This distance is measured only along the normal direction on the surface and

it is negative if the point (ρ, z) is located in the interior of the nucleus. V_c is the depth of the potential while a is the diffuseness parameter. In our work, the depth is $V_c = V_{0c}[1 \pm \kappa (N_0 - Z_0)/N_0 + Z_0)]$ with plus sign for protons and minus sign for neutrons, V_{0c} = 51 MeV, a=0.67 fm, κ =0.67. Here A_0 , N_0 and Z_0 represent the mass number, the neutron number and the charge number of the parent, respectively. This parametrization, referred as the Blomqvist-Walhlborn one in Ref. [33], is adopted because it provides the same radius constant r_0 for the mean field and the pairing field. That ensures a consistency of the shapes of the two fields at hyperdeformations, *i.e.*, two tangent ellipsoids. The Hamiltonian is obtained by adding the spin-orbit and the Coulomb terms to the Woods-Saxon potential. The eigenvalues are obtained by diagonalization of the Hamiltonian in the semi-symmetric harmonic two center basis [34,35]. In this work, the major quantum number used is $N_{max}=12$. The two center Woods-Saxon model will be used to compute shell and pairing corrections together with inertia in this work. The two center shell model represents a valuable instrument to investigate the role of individual orbitals for the treatment of a wide variety of superasymmetric disintegration processes, pertaining to cluster- and alpha-decays [36-38].



Fig. 2 – Family of nuclear shapes, from the spherical configuration up to scission, along the minimal action trajectory. The distances between the center of the fragments are marked on the plot.

5. RESULTS

The calculations were performed for the fission of 234 U having as final partition 102 Zr+ 132 Te. The fission barrier taking as reference the ground state of the parent located at approximately R = 4 fm is displayed in Fig. 1 as function of the distance between the centers of the fragments. The potential barrier exhibits the well known two humped shape. The sequence of nuclear shapes along the minimal action trajectory is plotted in Fig. 2. In the caption the distances between the centers of the M. Mirea



Fig. 3 – The inertia B along the minimal action trajectory as function of the distance between the centers of the fragments R. Full line: the semi-adiabatic cranking evaluation. Dot-dashed line: cranking approximation. Dashed line: gaussian overlap approximation.

fragments are also marked. It can be seen that the shapes become asymmetric when the second barrier is penetrated.

In Fig. 3, the three inertia obtained within our microscopic approaches are plotted as function of R. After scission, it can be be observed that the reduced mass is reached. Our results are in line with those given in Refs. [8,9] concerning the comparison between the cranking model and the gaussian overlap approximation. The cranking model gives values always larger than the gaussian overlap approximation with a factor 1/3 in average. The two models show a similar shell structure when the deformation is modified. The semi-adiabatic approach gives lower values than the two other models and a similar shell structure with deformation. The maximal values of the inertia are obtained in the region of the second barrier and in the second well. Similar values of the inertial are obtained in the ground state. The penetration of the first barrier is characterized by a small effective mass.

The microscopic inertia was calculated for large scale amplitude motion that

characterizes the fission process, at moderate asymmetries. We have used in the past the two center shell model to treat alpha-decay and cluster emission as superasymmetric fission processes and the model is proved valid. Therefore an analysis of the effective mass behavior in very asymmetric processes, including the alpha decay of superheavy elements [39,40] is planned in the future.

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