

MACROSCOPIC POTENTIAL-ENERGY SURFACES FOR ARBITRARILY ORIENTED, DEFORMED HEAVY IONS

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Note: misprints in Eqs. A.10 and A.17 are corrected here

Abstract

A formalism suitable for numerical evaluation of finite-range liquid-drop model expressions related to the interaction energy of two arbitrarily oriented, deformed heavy ions is developed. The presentation of the formalism is organized to facilitate extensions to alternative parameterizations and energy expressions. The model is applied to specific heavy-ion collisions that illustrate the importance of a multidimensional approach in the study of complete fusion reactions. Potential-energy surfaces related to light-particle emission for heavy, deformed nuclei are also presented.

1 Introduction

Since more than 20 years it has been clear that to account reasonably accurately for the macroscopic interaction energy between two colliding heavy ions it is necessary to include effects related to the finite range of the nuclear force¹). Thus, the potential energy between two colliding heavy ions is usually given as a sum of a Coulomb-energy term and a finite-range surface-energy term¹⁻⁶). The finite-range energy term is a generalization of the proximity potential⁷).

A necessary condition for forming a compound nucleus in a heavy-ion collision is that the fusing system dynamically evolves to a configuration inside the fission saddle point in a multi-dimensional deformation space⁸). To establish the trajectory of the fusing system the solution of the equations of motion⁹⁻¹¹) and a knowledge of the potential energy and the inertia and viscosity tensors as functions of nuclear shape and position are required. These quantities and the relative positions of the fission saddle point and the initial point of touching, determine the optimum energy for fusion in a heavy-ion reaction. For heavy systems an *extra push* over and above the energy of the Coulomb barrier is required to bring the trajectory inside the saddle point and achieve fusion. In the search for the heaviest elements it has been of extreme importance to establish both the optimum target-projectile combination and the most favorable energy for compound nucleus formation.

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Although the solution of the equations of motion is required to calculate cross sections for compound-nucleus formation, potential-energy surfaces are highly useful as a starting point for understanding the general behavior of these equations. Since the equations of motion are normally solved only for very simple initial configurations, for example colliding *spherical* heavy ions, potential-energy surfaces are at present an important tool for quickly analyzing more complex initial conditions. Since one or both of the colliding ions are deformed in many heavy-ion reaction of current interest, we present here calculated potential-energy surfaces for general orientations of colliding, deformed heavy ions.

To allow a systematic evaluation of the potential energy for arbitrarily oriented, deformed heavy ions we develop the integrals that occur in macroscopic expressions for the nuclear and Coulomb interaction energies to a set of expressions that are suitable for numerical evaluation. The presentation of the formalism is organized to facilitate extensions to alternative shape parameterizations and energy expressions.

2 Integrals

Several integrals occur in the finite-range liquid-drop model (FRLDM) and in the finite-range droplet model (FRDM)^{1,4,5,9,12-15}). For our studies of the potential energy in heavy-ion collisions it is sufficient to consider the Coulomb energy and nuclear interaction-energy terms of the 1981 FRLDM^{5,12}). Thus, we obtain for the finite-range surface energy, or as it is also called *nuclear* energy

$$E_n = -\frac{c_s}{8\pi^2 r_0^2 a^3} \iint \left(\frac{\sigma}{a} - 2\right) \frac{e^{-\sigma/a}}{\sigma} d^3r d^3r' \quad (1)$$

and for the direct sharp-surface Coulomb energy

$$E_C = \frac{1}{2} \iint \frac{1}{\sigma} \rho(\vec{r}) \rho(\vec{r}') d^3r d^3r' \quad (2)$$

where

$$\vec{\sigma} = \vec{r} - \vec{r}' \quad (3)$$

and where the charge density at point \vec{r} is given by $\rho(\vec{r})$. The above expressions are appropriate for the self-energy of a single nucleus. When applied to the calculation of the interaction energy between *two* heavy ions the expressions should be multiplied by a factor of 2.

We here develop the expressions for the nuclear and sharp-surface Coulomb interaction energies given in eqs. 1 and 2 to a form suitable for numerical evaluation. The six-dimensional volume integrals that define these energy terms may be reduced to four-dimensional surface integrals by a two-fold application of Gauss theorem^{1,4,9}). One obtains for the nuclear energy^{4,9})

$$E_n = -\frac{c_s}{8\pi^2 r_{01} r_{02}} \oint \oint \left\{ 2 - \left[\left(\frac{\sigma}{a}\right)^2 + 2\left(\frac{\sigma}{a}\right) + 2 \right] e^{-\sigma/a} \right\} \frac{(\vec{\sigma} \cdot d\vec{S}) (\vec{\sigma} \cdot d\vec{S}')}{\sigma^4} \quad (4)$$

The sharp-surface Coulomb energy is given by⁹)

$$E_C = -\frac{\rho_{01} \rho_{02}}{12} \oint \oint \frac{(\vec{\sigma} \cdot d\vec{S}) (\vec{\sigma} \cdot d\vec{S}')}{\sigma} \quad (5)$$

The above formulas should be interpreted slightly differently depending on whether they are applied to the calculation of self energies or interaction energies. Here we will focus on calculating the interaction energy between two heavy ions. Then the above expressions should be multiplied by a factor of 2.

3 Model constants

For the values of the model constants we here choose the determination made by ref.^{5,12}). Thus

$$\begin{aligned}
 c_s &= [c_s(1)c_s(2)]^{1/2} \\
 \rho_{01} &= \frac{3}{4\pi} \frac{Z_1 e}{(r_{01} A_1^{1/3})^3} \\
 \rho_{02} &= \frac{3}{4\pi} \frac{Z_2 e}{(r_{02} A_2^{1/3})^3} \\
 c_s(1) &= a_s(1 - \kappa_s I_1^2) \\
 I_1 &= \frac{N_1 - Z_1}{N_1 + Z_1} \\
 c_s(2) &= a_s(1 - \kappa_s I_2^2) \\
 I_2 &= \frac{N_2 - Z_2}{N_2 + Z_2}
 \end{aligned} \tag{6}$$

where we have assumed constant charge densities ρ_{01} and ρ_{02} in the two ions. In the FRLDM that we use here we choose parameters according to ref.¹²). Thus

$$\begin{aligned}
 a_s &= 21.13 \text{ MeV} \\
 \kappa_s &= 2.30 \\
 e^2 &= 1.439\,976\,4 \text{ MeV fm} \\
 a &= 0.68 \text{ fm} \\
 r_{01} = r_{02} = r_0 &= 1.16 \text{ fm}
 \end{aligned} \tag{7}$$

Finally, we note that we have used the Coulomb energy expression for a sharp-surface shape, instead of the expression for a diffuse-surface shape used in ref.¹²). This represents a slight approximation, but it should be quite sufficient for calculating the *interaction* energy between heavy ions.

For the case the above expressions are applied to obtain the self-energies of a single body, obvious modifications of some of the above quantities should be implemented.

4 Mathematical detail

Before the integrals for the various macroscopic functions can be evaluated they must be brought on a form suitable for numerical integration on a computer. This means that the scalar function to be integrated has to be specified in all its detail. In our case this scalar function will serve as the starting point for constructing a FORTRAN computer subroutine to perform the quadrature of the scalar function. The “only” task that has to be accomplished so that this subroutine can trivially be written is to provide expressions for σ , $\vec{\sigma} \cdot d\vec{S}$, and $\vec{\sigma} \cdot d\vec{S}'$. This is complicated because the vectors occurring in integrals to be evaluated are most easily defined in the body-fixed coordinate systems of shape 1 and 2. To perform the vector operations occurring

in the various integral expressions to be evaluated, we have to express the vector components in a common coordinate system. For definiteness we will express all components in the body-fixed system of shape 1.

We develop the formalism here with the goal that it should facilitate the writing of the computer algorithms required for the numerical evaluation of the integrals. In addition it should be easy to extend the results to more general and to different parameterizations. We therefore proceed in the following steps. In this section we present results that are independent of parameterizations and the curvilinear coordinates eventually chosen as integration variables. These are discussed in subsequent sections. There we discuss the transformations from coordinate system 2 to system 1, and give expressions for σ , $\vec{\sigma} \cdot d\vec{S}$, and $\vec{\sigma} \cdot d\vec{S}'$. These expressions will contain functions that depend on the parameterization and curvilinear coordinate system chosen. The specific functions will then be given in explicit form in the appropriate sections.

To show when the components of a vector is given in system 2 we use the notation $\{, , \}$ as contrasted to $(, ,)$ for components in system 1. If \vec{r} is the vector from the origin of system 1 to the surface of shape 1, expressed in system 1, and \vec{r}' a vector from the origin of system 2 to the surface of shape 2, expressed in system 2, then

$$\begin{aligned}\vec{r} &= (r_x, r_y, r_z) \\ \vec{r}' &= \{r'_x, r'_y, r'_z\}\end{aligned}\tag{8}$$

Our notation here is introduced with the aim to reduce the possibility of confusion in the subsequent coding of the formalism into computer algorithms. Since we have at this point written such a computer algorithm, we know from practical experience that this approach is extremely useful.

4.1 Coordinate transformations

To specify the location of the coordinate system fixed in shape 2 relative to the system fixed in shape 1, we specify the position and orientation of the second body-fixed system in the following steps. The first element is a translation \vec{R}_{O2} giving the location of the origin of the second system in coordinate system 1. Thus,

$$\vec{R}_{O2} = (R_{O2x}, R_{O2y}, R_{O2z})\tag{9}$$

We now have a coordinate system, translated with respect to system 1 and with coordinate axes parallel to the original system 1. We designate this system x_a, y_a, z_a . Next, a rotation is performed of the second coordinate system around its origin. This rotation is specified in terms of the Eulerian angles of rotation. There are many definitions of Eulerian angles. Here we follow the conventions normally used in quantum mechanics, and build up the complete transformation in terms of three successive transformations around the coordinate axes of the translated system. First, the coordinate system is rotated counterclockwise an angle α about the z_a axis, which rotation is then described by

$$R_{z_a}(\alpha) = \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}\tag{10}$$

yielding the new system x_b, y_b, z_b . Next, the system is rotated an angle β counterclockwise about the y_b axis, which rotation is described by

$$R_{y_b}(\beta) = \begin{pmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{pmatrix} \quad (11)$$

yielding the new system x_c, y_c, z_c . Finally, the system is rotated an angle γ counterclockwise about the z_c axis, which rotation is described by

$$R_{z_c}(\gamma) = \begin{pmatrix} \cos \gamma & \sin \gamma & 0 \\ -\sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (12)$$

yielding the new system x', y', z' . The combined effect of all three rotations is then described by the triple product

$$A = R_{z_c}(\gamma)R_{y_b}(\beta)R_{z_a}(\alpha) \quad (13)$$

The complete transformation is therefore given by

$$A = \begin{pmatrix} \cos \gamma \cos \beta \cos \alpha - \sin \gamma \sin \alpha & \cos \gamma \cos \beta \sin \alpha + \sin \gamma \cos \alpha & -\cos \gamma \sin \beta \\ -\sin \gamma \cos \beta \cos \alpha - \cos \gamma \sin \alpha & -\sin \gamma \cos \beta \sin \alpha + \cos \gamma \cos \alpha & \sin \gamma \sin \beta \\ \sin \beta \cos \alpha & \sin \beta \sin \alpha & \cos \beta \end{pmatrix} \quad (14)$$

The above transformation gives the transformation *from* system 2 with coordinate axes parallel to the coordinate axes of system 1. However, we are interested in the inverse transformation. It is well-known that the inverse of matrices affecting orthogonal transformations is equal to the transpose of the original matrix, that is

$$A^{-1} = \tilde{A} \quad (15)$$

With $T = A^{-1}$ we therefore have for the inverse transformation

$$T = \begin{pmatrix} \cos \gamma \cos \beta \cos \alpha - \sin \gamma \sin \alpha & -\sin \gamma \cos \beta \cos \alpha - \cos \gamma \sin \alpha & \sin \beta \cos \alpha \\ \cos \gamma \cos \beta \sin \alpha + \sin \gamma \cos \alpha & -\sin \gamma \cos \beta \sin \alpha + \cos \gamma \cos \alpha & \sin \beta \sin \alpha \\ -\cos \gamma \sin \beta & \sin \gamma \sin \beta & \cos \beta \end{pmatrix} \quad (16)$$

Therefore the transformation from the body-fixed system of shape 2 to the body-fixed system of shape 1 is given by

$$\begin{pmatrix} r'_x \\ r'_y \\ r'_z \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \begin{Bmatrix} r'_x \\ r'_y \\ r'_z \end{Bmatrix} + \begin{pmatrix} R_{O2x} \\ R_{O2y} \\ R_{O2z} \end{pmatrix} \quad (17)$$

The transformation given in eq. 17 should only be applied to transform *point* coordinates given in the coordinate system 2 to coordinate values in system 1 for the same point. The components of the vector \vec{r}' are specified in terms of a set of such a point coordinates and should therefore be transformed as expressed in eq. 17. However, the components of the surface

area element and the related vector \vec{C} as defined in eqs. 19 and 20 do not represent such a point. The reason is that it does not represent a “point” at all. Instead it is a vector whose magnitude does not depend on the coordinate system used. However, when calculated in the body-fixed system of shape 2, by applying eq. 19 to \vec{r}' its components are given in the rotated system 2. Therefore, the rotational part of the transformation given in eq. 17 must be applied to obtain the correct components in system 1, in which the vector operations are carried out. Thus, for the vector \vec{C}' the following transformation should be applied:

$$\begin{pmatrix} C'_x \\ C'_y \\ C'_z \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \begin{pmatrix} C'_x \\ C'_y \\ C'_z \end{pmatrix} \quad (18)$$

4.2 Surface element

The vector surface area element $d\vec{S}$ is given by

$$d\vec{S} = \frac{\partial \vec{r}}{\partial q_1} \times \frac{\partial \vec{r}}{\partial q_2} dq_1 dq_2 \quad (19)$$

With this order between the partial derivatives the vector $d\vec{S}$ is correctly pointing in the direction away from the volume enclosed by the surface. The variables q_1 and q_2 represent integration variables of some orthogonal, curvilinear system. Specific examples will be discussed below. To develop expressions that are suitable as a starting point for later programming we write

$$d\vec{S} = \vec{C} dq_1 dq_2 \quad (20)$$

Obviously

$$\begin{pmatrix} C_x \\ C_y \\ C_z \end{pmatrix} = \begin{pmatrix} \frac{\partial r_y}{\partial q_1} \frac{\partial r_z}{\partial q_2} - \frac{\partial r_y}{\partial q_2} \frac{\partial r_z}{\partial q_1} \\ \frac{\partial r_z}{\partial q_1} \frac{\partial r_x}{\partial q_2} - \frac{\partial r_z}{\partial q_2} \frac{\partial r_x}{\partial q_1} \\ \frac{\partial r_x}{\partial q_1} \frac{\partial r_y}{\partial q_2} - \frac{\partial r_x}{\partial q_2} \frac{\partial r_y}{\partial q_1} \end{pmatrix} \quad (21)$$

4.3 Scalar products

We are now in a position to write down the expressions for the products $\vec{\sigma} \cdot d\vec{S}$ and $\vec{\sigma} \cdot d\vec{S}'$. It is more convenient to work with expressions that have the infinitesimals dq_1 and dq_2 factored out. Thus we will work with $\vec{\sigma} \cdot \vec{C}$ and $\vec{\sigma} \cdot \vec{C}'$ instead. Two rather distinct cases occur. In one case the two surface integrations are carried out over the same shape, as for instance when a sequence of shapes leading from ground state through the fission barrier are studied. In the other case, two different bodies are involved, as for instance in a heavy-ion collision. To evaluate the total potential energy for such a configuration one interaction integral and two self-energy integrals would be involved. However, the self-energy integrals would not change during the time the two shapes were separated. We therefore here only have to deal with the more complicated interaction integral between two shapes of arbitrary orientation.

We here assume that we are dealing with two distinct shapes. Here the primed vector components will always indicate components in the body-fixed system of the second shape.

Thus, we obtain for the product involving the surface element of the first shape, by use of the transpose of eq. 17

$$\vec{\sigma} \cdot \vec{C} = \left((r_x \ r_y \ r_z) - \left[\left\{ r'_x \ r'_y \ r'_z \right\} \tilde{T} + (R_{O2x} \ R_{O2y} \ R_{O2z}) \right] \right) \begin{pmatrix} C_x \\ C_y \\ C_z \end{pmatrix} \quad (22)$$

An evaluation of eq. 22 yields

$$\begin{aligned} \vec{\sigma} \cdot \vec{C} = & (r_x - r'_x T_{11} - r'_y T_{12} - r'_z T_{13} - R_{O2x}) C_x \\ & + (r_y - r'_x T_{21} - r'_y T_{22} - r'_z T_{23} - R_{O2y}) C_y \\ & + (r_z - r'_x T_{31} - r'_y T_{32} - r'_z T_{33} - R_{O2z}) C_z \end{aligned} \quad (23)$$

For the integration over the primed variable, which in this case involves the surface area of shape 2 we find the following expression for the product involving the surface area of the second shape

$$\vec{\sigma} \cdot \vec{C}' = \left((r_x \ r_y \ r_z) - \left[\left\{ r'_x \ r'_y \ r'_z \right\} \tilde{T} + (R_{O2x} \ R_{O2y} \ R_{O2z}) \right] \right) \left[T \begin{pmatrix} C'_x \\ C'_y \\ C'_z \end{pmatrix} \right] \quad (24)$$

Note that we here only performed a pure rotational transformation of the surface element vector components as discussed in connection with eq. 18. Evaluation of eq. 24 yields

$$\begin{aligned} \vec{\sigma} \cdot \vec{C}' = & (r_x - r'_x T_{11} - r'_y T_{12} - r'_z T_{13} - R_{O2x})(C'_x T_{11} + C'_y T_{12} + C'_z T_{13}) \\ & + (r_y - r'_x T_{21} - r'_y T_{22} - r'_z T_{23} - R_{O2y})(C'_x T_{21} + C'_y T_{22} + C'_z T_{23}) \\ & + (r_z - r'_x T_{31} - r'_y T_{32} - r'_z T_{33} - R_{O2z})(C'_x T_{31} + C'_y T_{32} + C'_z T_{33}) \end{aligned} \quad (25)$$

5 Curvilinear coordinates

The choice of coordinate system for evaluating the integrals occurring in the macroscopic energy expression is normally based on the parameterization used to generate the nuclear shapes. For the perturbed-spheroid ϵ parameterization used in the Nilsson^{16,17)} and folded-Yukawa single-particle models¹⁸⁾, this choice is spherical polar coordinates, for the three-quadratic-surface parameterization used in studies with the folded-Yukawa single-particle potential¹⁹⁾ the choice is cylindrical coordinates. In our first study here, we consider only the perturbed-spheroid ϵ parameterization, since it best describes the nuclear ground-state¹⁸⁾, which is the relevant shape to consider in heavy-ion collisions.

5.1 Spherical polar coordinates

The spherical polar coordinates are defined by

$$\begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned} \quad (26)$$

It is common to parametrize the nuclear surface by giving r as a function of θ and ϕ . With the most general assumption in which \vec{r} and \vec{r}' may refer to different surfaces labeled by “1” and “2” we obtain

$$\vec{r} = (R_1(\theta, \phi) \sin \theta \cos \phi, R_1(\theta, \phi) \sin \theta \sin \phi, R_1(\theta, \phi) \cos \theta) \quad (27)$$

$$\vec{r}' = \{R_2(\theta', \phi') \sin \theta' \cos \phi', R_2(\theta', \phi') \sin \theta' \sin \phi', R_2(\theta', \phi') \cos \theta'\} \quad (28)$$

Here we have for definiteness assumed that the primed coordinates refer to a shape “2” that is different from shape “1”. We have also given the components of the vector \vec{r}' to the surface of the second shape in the body-fixed primed coordinate system of the second shape. That the vector components are given in this system is indicated by the notation $\{ \}$. We have previously given the transformations of the primed components to the unprimed system and expressions for $\vec{\sigma} = \vec{r} - \vec{r}'$ and $\vec{\sigma} \cdot d\vec{S}'$.

$$\begin{aligned} \frac{\partial \vec{r}}{\partial \theta} &= \left(\frac{\partial R_1(\theta, \phi)}{\partial \theta} \sin \theta \cos \phi + R_1(\theta, \phi) \cos \theta \cos \phi, \right. \\ &\quad \left. \frac{\partial R_1(\theta, \phi)}{\partial \theta} \sin \theta \sin \phi + R_1(\theta, \phi) \cos \theta \sin \phi, \frac{\partial R_1(\theta, \phi)}{\partial \theta} \cos \theta - R_1(\theta, \phi) \sin \theta \right) \\ \frac{\partial \vec{r}}{\partial \phi} &= \left(\frac{\partial R_1(\theta, \phi)}{\partial \phi} \sin \theta \cos \phi - R_1(\theta, \phi) \sin \theta \sin \phi, \right. \\ &\quad \left. \frac{\partial R_1(\theta, \phi)}{\partial \phi} \sin \theta \sin \phi + R_1(\theta, \phi) \sin \theta \cos \phi, \frac{\partial R_1(\theta, \phi)}{\partial \phi} \cos \theta \right) \end{aligned} \quad (29)$$

6 Parameterizations

We now present explicit expressions for derivatives and other functions required for numerical evaluation of the double surface integrals. Each parameterization and coordinate system leads to a specific set of equations. As mentioned earlier we develop as a first application only the perturbed-spheroid ϵ parameterization in spherical polar coordinates.

6.1 ϵ parameterization in spherical polar coordinates

The ϵ parameterization was used originally¹⁶⁾ in the Nilsson modified oscillator model. It was introduced to simplify the calculation of matrix elements between nuclear single-particle wave functions. Here we employ its extension to higher multipole distortions and to axially asymmetric shapes^{20–22)}. Note that there is a factor $\sqrt{\frac{4\pi}{9} \frac{1}{2}}$ missing in front of the $V_4(\gamma)$ function in eq. 3 of ref.²²⁾. As a first step a “stretched” representation is introduced. The stretched coordinates ξ , η and ζ are defined by

$$\begin{aligned} \xi &= \left\{ \frac{m\omega_0}{\hbar} \left[1 - \frac{2}{3} \epsilon_2 \cos \left(\gamma + \frac{2}{3} \pi \right) \right] \right\}^{1/2} x \\ \eta &= \left\{ \frac{m\omega_0}{\hbar} \left[1 - \frac{2}{3} \epsilon_2 \cos \left(\gamma - \frac{2}{3} \pi \right) \right] \right\}^{1/2} y \\ \zeta &= \left\{ \frac{m\omega_0}{\hbar} \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \right] \right\}^{1/2} z \end{aligned} \quad (30)$$

where $\hbar\omega_0$ is the normally Z and N -dependent oscillator energy, ϵ_2 the ellipsoidal deformation parameter, and γ the non-axiality angle. It is then convenient to define a “stretched” radius vector ρ_t by

$$\rho_t = (\xi^2 + \eta^2 + \zeta^2)^{1/2} \quad (31)$$

a stretched polar angle θ_t by

$$u = \cos \theta_t = \frac{\zeta}{\rho_t} = \left[\frac{1 - \frac{2}{3}\epsilon_2 \cos \gamma}{1 - \frac{1}{3}\epsilon_2 \cos \gamma (3 \cos^2 \theta - 1) + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin \gamma \sin^2 \theta \cos 2\phi} \right]^{1/2} \cos \theta \quad (32)$$

and a stretched azimuthal angle ϕ_t by

$$v = \cos 2\phi_t = \frac{2\eta}{(\xi^2 + \eta^2)^{1/2}} = \frac{\left[1 + \frac{1}{3}\epsilon_2 \cos \gamma\right] \cos 2\phi + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin \gamma}{1 + \frac{1}{3}\epsilon_2 \cos \gamma + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin \gamma \cos 2\phi} \quad (33)$$

The Nilsson modified-oscillator potential is now defined by

$$\begin{aligned} V = \frac{1}{2}\hbar\omega_0\rho_t^2 \left\{ 1 + 2\epsilon_1 P_1(\cos \theta_t) \right. \\ - \frac{2}{3}\epsilon_2 \cos \gamma P_2(\cos \theta_t) + \frac{1}{3}\epsilon_2 \sin \gamma \left(\frac{8}{5}\pi\right)^{1/2} [Y_{22}(\theta_t, \phi_t) + Y_{2-2}(\theta_t, \phi_t)] \\ + 2\epsilon_3 P_3(\cos \theta_t) + 2\epsilon_4 V_4(\cos \theta_t, \cos 2\phi_t) + 2\epsilon_5 P_5(\cos \theta_t) + 2\epsilon_6 P_6(\cos \theta_t) \left. \right\} \\ - \kappa\hbar\omega_0 [2\vec{l}_t \cdot \vec{s} + \mu(\vec{l}_t^2 - \langle \vec{l}_t^2 \rangle)] \end{aligned} \quad (34)$$

where

$$V_4(u, v) = a_{40}P_4 + \sqrt{\frac{4\pi}{9}} [a_{42}(Y_4^2 + Y_4^{-2}) + a_{44}(Y_4^4 + Y_4^{-4})] \quad (35)$$

Here the hexadecapole potential $V_4(u, v)$ is made dependent on γ in such a way that axial symmetry is maintained when $\gamma = 0, 60^\circ, -120^\circ$, and -60° . This is accomplished by choosing the coefficients a_{4i} so that they have the transformation properties of a hexadecapole tensor. Thus²²⁾

$$\begin{aligned} a_{40} &= \frac{1}{6}(5 \cos^2 \gamma + 1) \\ a_{42} &= -\frac{1}{12}\sqrt{30} \sin 2\gamma \\ a_{44} &= \frac{1}{12}\sqrt{70} \sin^2 \gamma \end{aligned} \quad (36)$$

The usual assumption is now to assume that the shape of the nuclear surface is equal to the shape of an equipotential surface given by eq. (34). By neglecting the $\vec{l}_t \cdot \vec{s}$ and \vec{l}_t^2 terms and solving for ρ_t and then using eqs. (30–33) to derive an expression for r in the non-stretched laboratory system the following expression is obtained

$$\begin{aligned}
 r(\theta, \phi) = & \frac{R_0}{\omega_0/\overset{\circ}{\omega}_0} \left\{ \left[1 - \frac{2}{3}\epsilon_2 \cos \left(\gamma + \frac{2}{3}\pi \right) \right] \left[1 - \frac{2}{3}\epsilon_2 \cos \left(\gamma - \frac{2}{3}\pi \right) \right] \left[1 - \frac{2}{3}\epsilon_2 \cos \gamma \right] \right\}^{-1/2} \\
 & \times \left[1 - \frac{1}{3}\epsilon_2 \cos \gamma - \frac{2}{9}\epsilon_2^2 \cos^2 \gamma + \epsilon_2 \left(\cos \gamma + \frac{1}{3}\epsilon_2 \cos 2\gamma \right) u^2 \right. \\
 & \quad \left. - \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \left(1 - \frac{2}{3}\epsilon_2 \cos \gamma \right) (1 - u^2)v \right]^{1/2} \\
 & \times \left[1 - \frac{2}{3}\epsilon_2 \cos \gamma \frac{1}{2}(3u^2 - 1) + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - u^2)v \right. \\
 & \quad \left. + 2\epsilon_1 P_1(u) + 2\epsilon_3 P_3(u) + 2\epsilon_4 V_4(u, v) + 2\epsilon_5 P_5(u) + 2\epsilon_6 P_6(u) \right]^{-1/2} \quad (37)
 \end{aligned}$$

The quantity $\omega_0/\overset{\circ}{\omega}_0$ is determined by the volume conservation condition, which gives

$$\begin{aligned}
 \left(\frac{\omega_0}{\overset{\circ}{\omega}_0} \right)^3 = & \frac{1}{4\pi} \left\{ \left[1 - \frac{2}{3}\epsilon_2 \cos \left(\gamma + \frac{2}{3}\pi \right) \right] \left[1 - \frac{2}{3}\epsilon_2 \cos \left(\gamma - \frac{2}{3}\pi \right) \right] \left[1 - \frac{2}{3}\epsilon_2 \cos \gamma \right] \right\}^{-1/2} \\
 & \times \int_0^\pi d\theta_t \int_0^{2\pi} d\phi_t \sin \theta_t \left[1 - \frac{2}{3}\epsilon_2 \cos \gamma P_2(u) + \epsilon_2 \sin \gamma \left(\frac{8\pi}{45} \right)^{1/2} (Y_{22} + Y_{2-2}) \right. \\
 & \quad \left. + 2\epsilon_1 P_1(u) + 2\epsilon_3 P_3(u) + 2\epsilon_4 V_4(u, v) + 2\epsilon_5 P_5(u) + 2\epsilon_6 P_6(u) \right]^{-3/2} \quad (38)
 \end{aligned}$$

The above equation is derived by determining the volume inside the nuclear surface given by eq. 37 by evaluating the integral $\int d^3r$ inside the surface. This integration is carried out in terms of the “non-stretched” coordinates θ and ϕ , naturally. It is after a variable substitution that one arrives at the expression in eq. 38. The Legendre polynomials and spherical harmonics that occur in the above expressions are given in the Appendix.

6.1.1 Partial derivatives

In spherical polar coordinates evaluation of expression 21 requires expressions for the partial derivatives occurring in eq. 29, that is partial derivatives of $r(\theta, \phi)$ given in eq. 37. We observe that

$$\begin{cases} \frac{\partial r}{\partial \theta} = \frac{\partial r}{\partial \cos \theta} \frac{\partial \cos \theta}{\partial \theta} + \frac{\partial r}{\partial \cos 2\phi} \frac{\partial \cos 2\phi}{\partial \theta} \\ \frac{\partial r}{\partial \phi} = \frac{\partial r}{\partial \cos \theta} \frac{\partial \cos \theta}{\partial \phi} + \frac{\partial r}{\partial \cos 2\phi} \frac{\partial \cos 2\phi}{\partial \phi} \end{cases} \quad (39)$$

Equation 39 simplifies to

$$\begin{cases} \frac{\partial r}{\partial \theta} = -\sin \theta \frac{\partial r}{\partial \cos \theta} \\ \frac{\partial r}{\partial \phi} = -2 \sin 2\phi \frac{\partial r}{\partial \cos 2\phi} \end{cases} \quad (40)$$

which can be further developed to

$$\begin{cases} \frac{\partial r}{\partial \theta} = -\sin \theta \left[\frac{\partial r}{\partial \cos \theta_t} \frac{\partial \cos \theta_t}{\partial \cos \theta} + \frac{\partial r}{\partial \cos 2\phi_t} \frac{\partial \cos 2\phi_t}{\partial \cos \theta} \right] \\ \frac{\partial r}{\partial \phi} = -2 \sin 2\phi \left[\frac{\partial r}{\partial \cos \theta_t} \frac{\partial \cos \theta_t}{\partial \cos 2\phi} + \frac{\partial r}{\partial \cos 2\phi_t} \frac{\partial \cos 2\phi_t}{\partial \cos 2\phi} \right] \end{cases} \quad (41)$$

which simplifies to

$$\begin{cases} \frac{\partial r}{\partial \theta} = -\sin \theta \frac{\partial r}{\partial u} \frac{\partial u}{\partial \cos \theta} \\ \frac{\partial r}{\partial \phi} = -2 \sin 2\phi \left[\frac{\partial r}{\partial u} \frac{\partial u}{\partial \cos 2\phi} + \frac{\partial r}{\partial v} \frac{\partial v}{\partial \cos 2\phi} \right] \end{cases} \quad (42)$$

We further observe that $r(\theta, \phi)$ may be written

$$r(\theta, \phi) = C \left[\frac{f(u, v)}{g(u, v)} \right]^{1/2} \quad (43)$$

with

$$\begin{aligned} C &= \frac{R_0}{\omega_0/\dot{\omega}_0} \left\{ \left[1 - \frac{2}{3} \epsilon_2 \cos \left(\gamma + \frac{2}{3} \pi \right) \right] \left[1 - \frac{2}{3} \epsilon_2 \cos \left(\gamma - \frac{2}{3} \pi \right) \right] \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \right] \right\}^{-1/2} \\ f(u, v) &= \left[1 - \frac{1}{3} \epsilon_2 \cos \gamma - \frac{2}{9} \epsilon_2^2 \cos^2 \gamma + \epsilon_2 \left(\cos \gamma + \frac{1}{3} \epsilon_2 \cos 2\gamma \right) u^2 \right. \\ &\quad \left. - \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \left(1 - \frac{2}{3} \epsilon_2 \cos \gamma \right) (1 - u^2) v \right] \\ g(u, v) &= \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \frac{1}{2} (3u^2 - 1) + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - u^2) v \right. \\ &\quad \left. + 2\epsilon_1 P_1(u) + 2\epsilon_3 P_3(u) + 2\epsilon_4 V_4(u, v) + 2\epsilon_5 P_5(u) + 2\epsilon_6 P_6(u) \right] \end{aligned} \quad (44)$$

Thus

$$\begin{cases} \frac{\partial r(u, v)}{\partial u} = C \frac{f'_u(u, v)g(u, v) - f(u, v)g'_u(u, v)}{2f^{1/2}g^{3/2}} \\ \frac{\partial r(u, v)}{\partial v} = C \frac{f'_v(u, v)g(u, v) - f(u, v)g'_v(u, v)}{2f^{1/2}g^{3/2}} \end{cases} \quad (45)$$

From eqs. 32, 33 and 44 we are now able to determine the required derivatives. The partial derivatives of $f(u, v)$ and $g(u, v)$ are given by

$$f'_u(u, v) = \left[2\epsilon_2 \left(\cos \gamma + \frac{1}{3} \epsilon_2 \cos 2\gamma \right) u + 2 \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \left(1 - \frac{2}{3} \epsilon_2 \cos \gamma \right) uv \right]$$

$$\begin{aligned}
 f'_v(u, v) &= - \left[\left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \left(1 - \frac{2}{3} \epsilon_2 \cos \gamma \right) (1 - u^2) \right] \\
 g'_u(u, v) &= \left[- 2\epsilon_2 \cos \gamma u - 2 \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma uv \right. \\
 &\quad \left. + 2\epsilon_1 \frac{dP_1(u)}{du} + 2\epsilon_3 \frac{dP_3(u)}{du} + 2\epsilon_4 \frac{dV_4(u, v)}{du} + 2\epsilon_5 \frac{dP_5(u)}{du} + 2\epsilon_6 \frac{dP_6(u)}{du} \right] \\
 g'_v(u, v) &= \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - u^2) + 2\epsilon_4 \frac{\partial V_4(u, v)}{\partial v} \tag{46}
 \end{aligned}$$

The derivatives of the Legendre polynomials occurring above are given in the Appendix. The partial derivatives of $u(\cos \theta, \cos 2\phi)$ in eq. 32 are determined by observing that

$$\begin{aligned}
 u(\cos \theta, \cos 2\phi) &= C_{\text{pol}} \left[\frac{1}{h(\cos \theta, \cos 2\phi)} \right]^{1/2} \cos \theta \\
 \frac{\partial u(\cos \theta, \cos 2\phi)}{\partial \cos \theta} &= \frac{C_{\text{pol}}}{2} \left[2h(\cos \theta, \cos 2\phi) - \frac{\partial h(\cos \theta, \cos 2\phi)}{\partial \cos \theta} \cos \theta \right] \left[\frac{1}{h(\cos \theta, \cos 2\phi)} \right]^{3/2} \\
 \frac{\partial u(\cos \theta, \cos 2\phi)}{\partial \cos 2\phi} &= - \frac{C_{\text{pol}}}{2} \frac{\partial h(\cos \theta, \cos 2\phi)}{\partial \cos 2\phi} \left[\frac{1}{h(\cos \theta, \cos 2\phi)} \right]^{3/2} \cos \theta \tag{47}
 \end{aligned}$$

where

$$\begin{aligned}
 C_{\text{pol}} &= \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \right]^{1/2} \\
 h(\cos \theta, \cos 2\phi) &= \left[1 - \frac{1}{3} \epsilon_2 \cos \gamma (3 \cos^2 \theta - 1) + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - \cos^2 \theta) \cos 2\phi \right] \tag{48}
 \end{aligned}$$

We obtain

$$\begin{aligned}
 \frac{\partial h(\cos \theta, \cos 2\phi)}{\partial \cos \theta} &= - 2\epsilon_2 \cos \gamma \cos \theta - \left(\frac{1}{3} \right)^{1/2} 2\epsilon_2 \sin \gamma \cos \theta \cos 2\phi \\
 \frac{\partial h(\cos \theta, \cos 2\phi)}{\partial \cos 2\phi} &= \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - \cos^2 \theta) \tag{49}
 \end{aligned}$$

and

$$\begin{aligned}
 \frac{\partial u(\cos \theta, \cos 2\phi)}{\partial \cos \theta} &= \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \right]^{1/2} \\
 &\quad \times \left[1 + \frac{1}{3} \epsilon_2 \cos \gamma + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \cos 2\phi \right] \\
 &\quad \times \left[1 - \frac{1}{3} \epsilon_2 \cos \gamma (3 \cos^2 \theta - 1) + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \sin^2 \theta \cos 2\phi \right]^{-3/2} \\
 \\
 \frac{\partial u(\cos \theta, \cos 2\phi)}{\partial \cos 2\phi} &= -\frac{1}{2} \left[1 - \frac{2}{3} \epsilon_2 \cos \gamma \right]^{1/2} \cos \theta \\
 &\quad \times \left[\left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma (1 - \cos^2 \theta) \right] \\
 &\quad \times \left[1 - \frac{1}{3} \epsilon_2 \cos \gamma (3 \cos^2 \theta - 1) + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \sin^2 \theta \cos 2\phi \right]^{-3/2}
 \end{aligned} \tag{50}$$

For the function $v = \cos 2\phi_t$ in eq. 33 we only need to calculate the derivative with respect to $\cos 2\phi$ since this function does not depend on $\cos \theta$. To facilitate the derivation of the derivative we write

$$v = \frac{s}{t} \tag{51}$$

where

$$\begin{aligned}
 s &= \left[1 + \frac{1}{3} \epsilon_2 \cos \gamma \right] \cos 2\phi + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \\
 t &= 1 + \frac{1}{3} \epsilon_2 \cos \gamma + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \cos 2\phi
 \end{aligned} \tag{52}$$

We need to calculate

$$\frac{\partial v}{\partial \cos 2\phi} = \frac{s't - st'}{t^2} \tag{53}$$

We find that

$$\begin{aligned}
 \frac{\partial s}{\partial \cos 2\phi} &= 1 + \frac{1}{3} \epsilon_2 \cos \gamma \\
 \frac{\partial t}{\partial \cos 2\phi} &= \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma
 \end{aligned} \tag{54}$$

This gives

$$\begin{aligned}
 \frac{\partial s}{\partial \cos 2\phi} t &= 1 + \frac{1}{3} \epsilon_2 \cos \gamma + \left(\frac{1}{3} \right)^{1/2} \epsilon_2 \sin \gamma \cos 2\phi \\
 &\quad + \frac{1}{3} \epsilon_2 \cos \gamma + \frac{1}{9} \epsilon_2^2 \cos^2 \gamma + \left(\frac{1}{3} \right)^{3/2} \epsilon_2^2 \cos \gamma \sin \gamma \cos 2\phi
 \end{aligned}$$

$$s \frac{\partial t}{\partial \cos 2\phi} = \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin \gamma \cos 2\gamma + \left(\frac{1}{3}\right)^{3/2} \epsilon_2^2 \sin \gamma \cos \gamma \cos 2\phi + \frac{1}{3} \epsilon_2^2 \sin^2 \gamma \quad (55)$$

Thus we find for the derivative

$$\frac{\partial v}{\partial \cos 2\phi} = \frac{1 + \frac{2}{3} \epsilon_2 \cos \gamma + \frac{1}{9} \epsilon_2^2 \cos^2 \gamma - \frac{1}{3} \epsilon_2^2 \sin^2 \gamma}{\left[1 + \frac{1}{3} \epsilon_2 \cos \gamma + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin \gamma \cos 2\phi\right]^2} \quad (56)$$

7 Implementation

When a model of a physical phenomenon is developed, the project commonly evolves in the following steps:

1. An idea of a project emerges. The ideas are developed as a set of handwritten notes. A computer code is written, based on the handwritten notes.
2. The model is explored by use of the computer code. Both model and code are debugged.
3. Based on the experience from the initial model formulation and its computer implementation a revised, final model and a revised, final computer code are developed. This latter process is usually a multi-step process. In each step new sets of hand-written notes are produced.
4. A manuscript, which defines the model and discusses the results obtained from the computer implementation is prepared.

This, rather common development process makes it difficult to ascertain the correctness of the computer model and of the model specification in the manuscript, for two reasons. First, the incremental nature of the development process usually leads to non-optimal, non-transparent code, because an existing code is modified to include the additions to the model. Second, when the manuscript presenting the model is prepared as a final step, errors may occur in the manuscript, even after careful proof-reading, precisely because the manuscript *is* the *final* step. The manuscript itself is therefore not subject to particularly challenging tests of correctness.

To avoid these difficulties we have proceeded in a different manner. We *first* wrote the model specification sections of this manuscript and *then* wrote the corresponding computer code. The specific steps involved were the following.

The model specification presented in this paper was written in L^AT_EX on a 386SL laptop computer. A FORTRAN computer code was then developed on the same laptop, *after* the complete model specification was available as a L^AT_EX manuscript, which served as the specification of the code.

The code was tested in several ways. If a discovered error was caused by a misprint in the manuscript, the misprint was corrected and the new manuscript version served as the specification for the code, which excluding write and format statements is about 1100 lines long.

The computer code was first tested by evaluating the derivatives occurring in the model specifications both by use of the analytical expressions derived in this paper and by numerical differentiation. In double precision we were able to assure the agreement between these two derivatives to more than 10 digits. Second, we tested the code by evaluating the potential energy for several, equivalent spatial configurations of deformed nuclei. Third, one notes that

with slight modifications one can use the current formalism to evaluate the Coulomb energy of a single, charged, deformed nucleus. We compared the result of such an evaluation for axially asymmetric shapes with results obtained by Ingemar Ragnarsson by use of a completely different code and obtained agreement to desired accuracy, depending on the number of integration points selected.

At present we are running the code on an HP-Apollo 9000-735 computer. The running time depends on the number of integration point in the four-dimensional surface integrals. With the specific choice of 24 steps in each of the four angles we obtain a total of 331776 integration points, for which case the energy evaluation takes 1.5 s for one configuration.

Although some normal coding procedures for obtaining high-speed code have been observed, the most obvious one being the storage of often used function values in matrices, our major concern has been to write the code for clarity, not for speed.

8 Applications

We now apply the above formalism to four representative physical situations of current interest. We first consider subbarrier fusion, which we follow by a study of a reaction used in an attempt to synthesize superheavy elements. We then consider α emission from deformed nuclei and finally the potential energy for a system where both the target and projectile are well deformed.

8.1 Subbarrier fusion

As the first example of a calculated potential-energy surface we display in fig. 1 the interaction energy in the $^{184}\text{W}+^{16}\text{O}$ reaction. The ^{184}W target is shown in the center as a dark shaded area. The shape of ^{184}W in its ground state is taken from the calculation of ref. ¹⁵⁾. The calculated interaction energy is given as a function of the location of the center of ^{16}O . Since the energy can only be calculated to the point of touching of the two ions, there will be an area outside the surface of ^{184}W for which the energy is undefined, at least for the separated-system configuration which we consider here. This area is shaded in light gray. To show the shape and relative sizes of both target and projectile without obscuring the potential-energy surface we show the projectile as a magenta-colored shape *inside* the target. Of course, such an overlapping configuration is not considered in our calculations here.

Because the ^{184}W target is not spherical, the calculated potential energy for $^{184}\text{W}+^{16}\text{O}$ is not nearly spherically symmetric, in particular near the top of the Coulomb barrier. Instead, the highest region of the Coulomb barrier resembles a mountain ridge with valleys and peaks. The highest peaks, at 75 MeV, are located, as should be expected, in directions where the closest approach to the center occurs, in this case along the ρ axis. Conversely, the lowest saddle points on the ridge, at 69 MeV, at about $z = 10$ fm and $\rho = 6$ fm, for example, occur in the directions of the most distant closest approach. For the nuclear shape investigated here this corresponds to directions at angles of approximately 45° with respect to the vertical. The barrier heights calculated here agree very well with the values obtained in ref. ²³⁾ with a different interaction potential. With that potential the maximum Coulomb barrier was about 74 MeV and the minimum was about 67 MeV.

We note that the energy difference between the highest and lowest points on the ridge is 6 MeV. Consequently, one must conclude that Coulomb-barrier calculations based on simple spherical models of target and projectile are only correct to within about this magnitude. Or, more precisely, a one-dimensional Coulomb barrier calculation is in many realistic reactions a

Table 1: Comparison between ground-state deformations determined from fusion cross-section and Coulomb-excitation experiments and calculated deformation parameters.

Nucleus	^{154}Sm		^{186}W	
	β_2	β_4	β_2	β_4
Fusion	0.30	0.05	0.30	-0.02
Coulomb Excitation	0.30	0.11	0.24	-0.09
Mass Calculation	0.27	0.11	0.23	-0.11

considerable approximation both because its energy cannot be well defined, and because the “barrier” is in reality a multi-dimensional surface.

Nuclei in the beginning of the rare-earth region have a positive hexadecapole moment, in contrast to nuclei like ^{184}W at the end of the rare-earth region, where negative hexadecapole moments are the norm¹⁵⁾. In fig. 2 we show a potential-energy surface for a heavy-ion collision where the target has a large positive hexadecapole deformation. In this case the maxima and minima on the ridge around the target are located along the ρ and z axes with energies of about 63 MeV and 57 MeV respectively. Also these values agree well with an earlier calculation²⁴⁾.

In several papers^{23–26)} the sign and magnitude of β_4 for rare-earth nuclei is discussed, in particular the degree of fusion enhancement for positive and negative β_4 . In ref.²⁴⁾ it is pointed out that quite different results are obtained for the values of β_2 and β_4 in analysis of Coulomb excitation data and fusion cross-section data. For ^{184}W we find that a large, positive value of β_4 yields a lower fusion barrier. We obtain barrier heights of 73 MeV and 67 MeV in the equatorial and polar regions, respectively. This lower barrier can be expected to yield a larger enhancement to the fusion cross section, relative to the value $\beta_4 = 0$ than the negative $\beta_4 = -0.095$ corresponding to the shape investigated in fig. 1.

We compare for two nuclei in the beginning and at the end of the rare-earth region the deformations deduced from fusion cross-section and Coulomb excitation experiments, as summarized in ref.²⁶⁾, to deformations obtained in a nuclear mass calculation¹⁵⁾. The calculations agree very well with results from Coulomb excitation experiments. However, it is pointed out in ref.²⁶⁾ that a more elaborate analysis of the fusion data, which takes into account couplings to vibrational states, will yield deformations in better agreement with Coulomb excitation data.

8.2 Superheavy elements

In studies of heavy-ion reactions leading to compound heavy and superheavy nuclei it is of interest to consider if particular relative orientations of target and projectile may enhance the cross section for complete fusion. One reaction that has been studied experimentally²⁷⁾ is $^{248}\text{Cm} + ^{48}\text{Ca}$. In fig. 3 we display the potential-energy surface for this reaction. The 15 MeV difference between the barrier in the equatorial and polar regions stands out clearly. At first sight collisions in the polar regions may seem preferable since such reactions are possible at energies leading to lower excitation energies of the compound system. However, this reaction would also lead to the most elongated of all the possible initial configurations. A collision in the equatorial region would have to take place at a 15 MeV higher energy, but would represent a more compact initial touching configuration. Thus, the amount of extra push required to bring the system to a sufficiently compact shape for complete fusion, that is to inside the fission saddle point, may be so much less than in the polar regions that it more than compensates for

the higher Coulomb barrier in the equatorial region.

8.3 Light-particle emission

It has been a longstanding problem that the observed barriers for charged-particle emission are lowered from their observed absorption barriers²⁸⁾. A simple explanation of this difference is that the parent nuclei are more deformed than the ground states of their daughter nuclei. This deformation effect was observed in the energy spectra and α -emission angular distributions following heavy-ion fusion reactions^{29,30)}. However, the explanation of this effect is not yet confirmed, partly because the results are obtained only after a complicated statistical-model analysis³¹⁾. Another requirement, necessary to confirm this interpretation is a more realistic calculation of the emission-barrier heights for charged particles from arbitrarily deformed nuclei. If a compound nucleus deforms in the emission process, the lowest energy part of the emission is greatly influenced³²⁾, and we can expect to see the effect in some of the data. A previous model calculation³²⁾ was not precise enough in this respect. Thus, it is of interest to calculate the distribution of barrier heights for charged-particle emission for various deformed nuclei using our new model for the interaction barrier.

We calculate the two-dimensional potential-energy surface for α -particle emission as a typical example. We choose ^{240}Pu as a compound nucleus because the change of the barrier height caused by deformation is larger for heavier compound nuclei than for lighter systems. In figs. 4–8 we show the two-dimensional Coulomb barrier for shapes corresponding to a hypothetical spherical nucleus, to the ground state ($\epsilon_2 = 0.20$, $\epsilon_4 = -0.067$), to the first saddle ($\epsilon_2 = 0.40$, $\epsilon_4 = 0.04$), to the second minimum ($\epsilon_2 = 0.56$, $\epsilon_4 = 0.07$), and to the second, asymmetric saddle ($\epsilon_2 = 0.85$, $\epsilon_4 = 0.12$, $\epsilon_3 = 0.16$, $\epsilon_5 = -0.064$).

The barrier for the hypothetical spherical ^{236}U plus an α particle in fig. 4 is spherically symmetric, as it should be. The peak of barrier is located about 2 fm away from the touching point and its height is between 23 and 24 MeV. However, since the ground state of the nucleus ^{236}U is deformed fig. 4 does not represent the barrier for α absorption to ^{236}U . When the nucleus ^{236}U is highly excited, however, the shell effect is at least partially washed out, which may well result in a spherical ^{236}U . This figure corresponds to such situation, i.e., an α emission from spherical compound nucleus, and thus it plays the role of a reference configuration for the next four calculations.

The potential energy corresponding to the ground-state shape of ^{236}U plus an α particle is shown in fig. 5. Due to the combined effect of β_2 and β_4 , we observe a well-developed deformation in the figure. The potential-energy surface has changed relative to fig. 4 so that the barrier is now higher for the equatorial region of the nucleus in the upper and lower part of the figure, and lower in the polar regions. The $^{236}\text{U} + \alpha$ configuration is rotationally symmetric about the z axis. Thus, the potential energy has the same rotational symmetry, which is also maintained in figs. 6–8. The height of the tallest peak of the potential-energy surface is almost the same as the height of the ridge in the potential energy corresponding to the hypothetical spherical configuration shown in fig. 4. The low point on the ridge around the deformed ^{236}U nucleus is a saddle configuration which is about 2 MeV lower in height relative to the height of the ridge for the spherical configuration in fig. 4. This difference is rather big and one can expect to see the effect in the α absorption data.

Figure 6 shows the potential energy corresponding to the first saddle-point deformation. The β_2 deformation has increased relative to its ground-state value and the potential energy, in consequence, deviates still further from spherical symmetry than does the potential corresponding to the ground-state configuration in fig. 5. The potential energy becomes maximum in the

equatorial region and is here about 1 MeV higher than the ridge for the spherical configuration. On the other hand, the barrier saddle points in the polar regions are 3 MeV lower than the highest regions of the potential-energy surface.

The potential energy corresponding to α emission from a fission-isomeric configuration is shown in fig. 7. The β_2 deformation has increased further, but the potential energy has not changed much relative to the previous figure. The highest potential-energy region is qualitatively the same. In the polar regions we notice a reduction of about 1 MeV of the saddle-point height compared to fig. 6. The difference between the highest and the lowest barrier height is here about 4 MeV, which should be detectable if α isomer absorption is observed.

Figure 8 shows the potential energy for the second-saddle-point configuration. In this case, both the β_2 and β_4 deformations and the left-right asymmetric deformation β_3 are important. Consequently, the structure of the potential energy is quite complicated. The lowest part of the ridge around the saddle point shape is located somewhat outside the left tip of the nucleus. The height of this saddle region is about 17 MeV. The highest barrier near the middle, equatorial region of the saddle-point shape is as high as 24 MeV so the difference between the highest and lowest points on the barrier ridge around the nucleus is about 7 MeV. The saddle-point height on the right part of the ridge around the saddle-point shape is about 19.5 MeV in height.

As we have seen in figs. 4–8, the potential-energy surfaces for α emission depend rather sensitively on the deformation of the parent nucleus. When the compound nucleus is heavy, the difference in energy between the highest and lowest point on the ridge around the daughter nucleus is not at all negligible. Thus, it may be possible to find a definite effect of deformation in the experimental data. This goal is not simple to achieve, because a complicated statistical model analysis is required to interpret the experimental data. In addition, a model for the emission rate from highly deformed nuclei, similar to a preliminary formulation investigated in ref. ³²⁾ is required. Nevertheless, we expect that it will be possible in the near future, to obtain more definite results related to this longstanding problem of charged-particle emission, because coincidence experiments with fission fragments developed recently³³⁾ will give us more detailed information on the deformation of compound nucleus.

8.4 Deformed target and projectile

All potential-energy surfaces studied above involved one deformed nucleus and one spherical nucleus. When the deformed nucleus is axially symmetric a two-dimensional potential-energy surface defines the potential completely. If axial symmetry is broken the problem becomes three-dimensional.

When both target and projectile are deformed the potential becomes considerably more complex. For axially symmetric nuclei the problems becomes four-dimensional; when axial symmetry is broken it is six-dimensional.

We illustrate this complexity by presenting four representative potential-energy surfaces for $^{24}\text{Mg}+^{24}\text{Mg}$. Since the ^{24}Mg nucleus is strongly deformed, with a calculated deformation $\epsilon_2 = 0.333$ ¹⁵⁾, four degrees of freedom are required to completely specify the potential for this system. For reference we first show the potential energy of a hypothetical spherical configuration in fig. 9. We also show in figs. 10–12 calculated potential-energy surfaces for colliding, deformed ^{24}Mg nuclei for three representative relative orientations of the colliding nuclei. In fig. 10 the relative orientations of the two nuclei are such that the z axes of the two systems are always at right angles and *not* in the same plane, except for $y = 0$. In fig. 11 the axes are parallel and in the same plane. Finally, in fig. 12 the z axes are again at right angles, but in contrast to the configuration studied in fig. 10 the two symmetry axes are here always in the same plane.

For this light system the energy along the ridge around the target nucleus only varies by about 2 MeV. The variation in ridge height between figs. 9–12 is also only about two MeV.

It is of interest to note that certain points in figs. 10–12 represent equivalent configurations and should therefore have the same energy. For example, in fig. 12 the z and x axes represent equivalent configurations, and the energy is also identical along these two axes. The z axis in fig. 10 is also equivalent to the z and x axes in fig. 12 and the energy along all three of these axes is indeed identical.

Complex potentials of similar structure as the potential in figs. 10–12 can also be expected in molecular collisions. In modelling of such collisions it can therefore be expected that a consideration of the full, multidimensional problem is necessary to establish if molecular resonances correspond to local minima in the potential, near the point of touching of the colliding molecules.

9 Summary

We have shown that deformation of target and projectile in heavy-ion collisions and of the daughter nuclei after particle emission, such as α -emission, has a dramatic effect on the nature of the Coulomb barrier.

The simple concept of a one-dimensional Coulomb barrier is clearly inadequate for many applications. We saw, for example, that the Coulomb barrier for the reaction $^{48}\text{Ca} + ^{248}\text{Cm}$ was 15 MeV lower in the polar regions as compared to the barrier in the equatorial region. This reaction was studied experimentally in an attempt to form compound systems in the region of superheavy nuclei. The complex structure of the Coulomb barrier clearly influences the optimum reaction energy for compound nucleus formation.

The enhancement of subbarrier fusion, which has been observed for lighter target-projectile combinations, can be qualitatively understood by noting that for a deformed target the Coulomb barrier is several MeV lower in some directions than the one-dimensional “Coulomb barrier” obtained from considering purely spherical target and projectile nuclei. For spherical nuclei subbarrier fusion may also be enhanced due to vibrational motion.

The model presented here allows the calculation of the potential energy for completely general configurations of two separated nuclei. It can also be generalized to alternative parameterizations in a straightforward manner.

10 Appendix

10.1 Legendre polynomials and spherical harmonics

The Legendre polynomials

$$P_l, \quad l = 0, 1, 2, \dots, \infty \quad (57)$$

are defined by

$$P_l(u) = \frac{1}{2^l l!} \frac{d^l}{du^l} (u^2 - 1)^l \quad (58)$$

The associated Legendre functions

$$P_l^m, \quad l = 0, 1, 2, \dots, \infty; \quad m = 0, 1, 2, \dots, l \quad (59)$$

are defined by

$$P_l^m(u) = \frac{(1 - u^2)^{m/2}}{2^l l!} \frac{d^{l+m}}{du^{l+m}} (u^2 - 1)^l \quad (60)$$

The first six Legendre polynomials are

$$\begin{aligned}
 P_0(u) &= 1 \\
 P_1(u) &= u \\
 P_2(u) &= \frac{1}{2}(3u^2 - 1) \\
 P_3(u) &= \frac{1}{2}(5u^3 - 3u) \\
 P_4(u) &= \frac{1}{8}(35u^4 - 30u^2 + 3) \\
 P_5(u) &= \frac{1}{8}(63u^5 - 70u^3 + 15u) \\
 P_6(u) &= \frac{1}{16}(231u^6 - 315u^4 + 105u^2 - 5)
 \end{aligned} \tag{61}$$

The spherical harmonics may be determined from the following relations

$$Y_l^m(\theta, \phi) = (-)^m \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\phi} \tag{62}$$

and

$$Y_l^{m*}(\theta, \phi) = (-)^m Y_l^{-m}(\theta, \phi) \tag{63}$$

For the functions used here we obtain

$$\begin{aligned}
 Y_2^2(\theta, \phi) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{2i\phi} \\
 Y_2^{-2}(\theta, \phi) &= \sqrt{\frac{315}{32\pi}} \sin^2 \theta e^{-2i\phi} \\
 Y_4^4(\theta, \phi) &= \sqrt{\frac{315}{512\pi}} \sin^4 \theta e^{4i\phi} \\
 Y_4^{-4}(\theta, \phi) &= \sqrt{\frac{315}{512\pi}} \sin^4 \theta e^{-4i\phi} \\
 Y_4^2(\theta, \phi) &= \sqrt{\frac{45}{128\pi}} \sin^2 \theta (7 \cos^2 \theta - 1) e^{2i\phi} \\
 Y_4^{-2}(\theta, \phi) &= \sqrt{\frac{45}{128\pi}} \sin^2 \theta (7 \cos^2 \theta - 1) e^{-2i\phi}
 \end{aligned} \tag{64}$$

It is the sums

$$\begin{aligned}
 SY_{22} &= Y_2^2(\theta, \phi) + Y_2^{-2}(\theta, \phi) \\
 SY_{44} &= Y_4^4(\theta, \phi) + Y_4^{-4}(\theta, \phi) \\
 SY_{42} &= Y_4^2(\theta, \phi) + Y_4^{-2}(\theta, \phi)
 \end{aligned} \tag{65}$$

that are required in the expression for the single-particle potential and in the corresponding equation for the nuclear surface. We obtain

$$SY_{22} = \sqrt{\frac{15}{8\pi}} \sin^2 \theta \cos 2\phi = \sqrt{\frac{15}{8\pi}} (1 - u^2) v$$

$$\begin{aligned}
SY_{44} &= \sqrt{\frac{315}{128\pi}} \sin^4 \theta \cos 4\phi = \sqrt{\frac{15}{128\pi}} (1-u^2)^2 (2v^2-1) \\
SY_{42} &= \sqrt{\frac{45}{32\pi}} \sin^2 \theta (7 \cos^2 \theta - 1) \cos 2\phi = \sqrt{\frac{45}{32\pi}} (1-u^2)(7u^2-1)v
\end{aligned} \tag{66}$$

10.2 Partial derivatives

The partial derivatives of the Legendre polynomials $P_l(u)$ are

$$\frac{dP_1(u)}{du} = 1 \tag{67}$$

$$\frac{dP_2(u)}{du} = 3u \tag{68}$$

$$\frac{dP_3(u)}{du} = \frac{1}{2}(15u^2 - 3) \tag{69}$$

$$\frac{dP_4(u)}{du} = \frac{1}{2}(35u^3 - 15u) \tag{70}$$

$$\frac{dP_5(u)}{du} = \frac{1}{8}(315u^4 - 210u^2 + 15) \tag{71}$$

$$\frac{dP_6(u)}{du} = \frac{1}{8}(693u^5 - 630u^3 + 105u) \tag{72}$$

We also need the partial derivatives of $V_4(u, v)$ defined in eq. 35. Obviously

$$\begin{aligned}
\frac{\partial V_4(u, v)}{\partial u} &= a_{40} \frac{dP_4(u)}{du} + \sqrt{\frac{4\pi}{9}} \left[a_{42} \frac{\partial SY_{42}}{\partial u} + a_{44} \frac{\partial SY_{44}}{\partial u} \right] \\
\frac{\partial V_4(u, v)}{\partial v} &= \sqrt{\frac{4\pi}{9}} \left[a_{42} \frac{\partial SY_{42}}{\partial v} + a_{44} \frac{\partial SY_{44}}{\partial v} \right] \\
\frac{\partial SY_{44}}{\partial u} &= -\sqrt{\frac{315}{128\pi}} 4u(1-u^2)(2v^2-1) \\
\frac{\partial SY_{42}}{\partial u} &= +\sqrt{\frac{45}{32\pi}} (16u - 28u^3)v \\
\frac{\partial SY_{44}}{\partial v} &= +\sqrt{\frac{315}{128\pi}} 4(1-u^2)^2v \\
\frac{\partial SY_{42}}{\partial v} &= +\sqrt{\frac{45}{32\pi}} (1-u^2)(7u^2-1)
\end{aligned} \tag{73}$$

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Figure captions

- Fig. 1 Potential-energy surface for the reaction $^{184}\text{W}+^{16}\text{O}$. The energy in the light-gray area, outside the ^{184}W nucleus in the center was not calculated, because the points in this region correspond to points inside the touching configuration. The magenta-colored shape inside the ^{184}W nucleus has been drawn to show the relative size of the projectile to the target. This overlapping configuration is not considered in actual calculations. Note the ridge with passes and peaks around the target nucleus. The minimum pass (saddle point) on the ridge is about 69 MeV and occurs at about $z = 10$ fm and $\rho = 6$ fm. The maximum Coulomb barrier is about 75 MeV and occurs in the $z = 0$ plane.
- Fig. 2 Potential-energy surface for the reaction $^{154}\text{Sm}+^{16}\text{O}$. Here the minimum in the Coulomb barrier is about 57 MeV and occurs at $z = \pm 12$ fm and $\rho = 0$. The maximum is about 63 MeV and occurs in the $z = 0$ plane.
- Fig. 3 Potential-energy surface for the reaction $^{248}\text{Cm}+^{48}\text{Ca}$. The Coulomb barrier in the equatorial region is about 15 MeV higher than in the polar regions. Which region is the most favorable for complete fusion depends on the amount of extra push required in the two regions, see discussion in text.
- Fig. 4 Potential-energy surface for α emission from ^{240}Pu with spherical shape. Since both ^{240}Pu and the daughter nucleus ^{236}U are deformed, this calculation is shown mainly to serve as a reference configuration that can be compared to realistic calculations with deformation effects included.
- Fig. 5 Potential-energy surface for α emission from the ground-state configuration of ^{240}Pu . Here a small deviation from spherical symmetry has developed so that the Coulomb barrier in the equatorial region is 2 MeV higher than in the polar regions.
- Fig. 6 Potential-energy surface for α emission from the first saddle point configuration of ^{240}Pu . The Coulomb barrier in the equatorial region is now about 3 MeV higher than in the polar regions.
- Fig. 7 Potential-energy surface for α emission from the fission-isomeric configuration of ^{240}Pu . The difference between the Coulomb barrier in the equatorial and polar regions is now 4 MeV.
- Fig. 8 Potential-energy surface for α emission from the second, mass-asymmetric saddle configuration of ^{240}Pu . Because of the asymmetry there is a difference of about 2 MeV between Coulomb barriers in the two polar regions. In the equatorial region the barrier is 7 MeV higher than the lower of the two polar-region barriers.
- Fig. 9 Potential-energy surface for the reaction $^{24}\text{Mg}+^{24}\text{Mg}$. Although these nuclei are deformed in their ground states, we show the potential energy calculated for spherical shapes, so that we can compare this configuration to the realistic, deformed calculations in figs. 10–12.
- Fig. 10 Potential-energy surface for the reaction $^{24}\text{Mg}+^{24}\text{Mg}$ for ground-state nuclear shapes. The symmetry axes of the two nuclei are at right angles, that is the

Eulerian angles (α, β, γ) are $\alpha = 0$, $\beta = 90^\circ$, and $\gamma = 0$, cf. eqs. 10–12. The cut of the multidimensional potential-energy surface that is plotted corresponds to $x = 0$, that is the ρ axis in this case is the y axis.

Fig. 11 Potential-energy surface for the reaction $^{24}\text{Mg}+^{24}\text{Mg}$ for ground-state nuclear shapes. The symmetry axes of the two nuclei are parallel and in the same plane, that is the Eulerian angles (α, β, γ) are $\alpha = 0$, $\beta = 0$, and $\gamma = 0$, cf. eqs. 10–12.

Fig. 12 Potential-energy surface for the reaction $^{24}\text{Mg}+^{24}\text{Mg}$ for ground-state nuclear shapes. The symmetry axes of the two nuclei are at right angles and in the same plane, that is the Eulerian angles (α, β, γ) are $\alpha = 0$, $\beta = 90^\circ$, and $\gamma = 0$, cf. eqs. 10–12. The cut of the multidimensional potential-energy surface that is plotted corresponds to $y = 0$, that is the ρ axis in this case is the x axis.

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