Colinear Spherical Three Center Shell Model*

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Abstract. The work is dedicated to the development of a specialized shell model able to describe the transition of the level scheme from a parent nucleus through three partially overlapped schemes up to three totally separated fragment schemes. The model treats three intersected equal sphere configurations. For a given mass number, the only independent variable is the distance between centers. Spin-orbit and l-squared interaction terms are calculated as geometry dependent. The calculations are repeated for neutrons and protons separately. One obtains the levels which are used to compute the shell corrections. An application is presented for the symmetric splitting of ^{144}Nd into three ^{48}Ca fragments.

1 Introduction

This work addresses to such particular phenomena as the tripartition configuration and ternary fission, reprted 50 years ago [1]. In 1958 it was shown [2], on the basis of a macroscopic liquid drop model that for heavy nuclei it is possible to obtain an energetically more favourable division into three or even in four fragments than in the case of binary fission. The progress in understanding the connection between scission configuration and the binary fission mechanism and mass yield is still recent. The reaction energy must be positive [3], when calculated with experimental masses [4]. It is accepted that for ternary and multicluster fission the aligned configurations of fragments in touch, possesing an axial symmetry are more probable the non-axial compact configurations which lead to a larger potential energy. Alpha-accompanied fission remains up to now the most probbale mode of tripartition. Other configurations are possible however, and with recent, more performant detectors, like the GAMMASPHERE in United States, it is now possbile to verify these hypothesis. The ability to predict probable ternary configurations and the most favourable combinations between parent nucleus and the three fragment partition can be supported only using a very specialized model able to describe the microscopic transition from a unique energy level scheme, going through three partially overlapped schemes and ending to the totally separated three potential wells, corresponding to the separated fragments. Such a model has not been done before and is about to be described in this work. The model shall yield the necessary proton and neutron energy levels during the evolution of the nuclear shape from a single

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system towards three superposed fragment configuration. The proton and neurton level schemes are further used for the calculation of the shell corrections along the ternary phenomenon evolution.

2 Shapes and Parametrization

The shapes which are described by the present model are presented in Figure 1 and consist in three intersected spheres corresponding to three symmetrical fragments $A/3$, resulted from the fragmentation of an initial nucleus A. The fragments are colinear, hence one has axial symmetry. $-z_1, 0$ and, z_1 are the centers of the fragments. $-z_{01}$ and z_{01} are the matching points between the intersected fragments. Once the mass and atomic number are given, the only free parameter which is needed to describe a certain point in the ternary shape evolution is the distance between the centers of the side fragments, R. When R increases, the shape goes from one sphere to three.

A typical evolution of the tripartition configuration is obtained when the distance between centers varies from zero (initial nucleus) up to the sum of the radius values for three touching final fragments. The starting point is the initial, spherical parent nucleus. At this moment the three centers completely overlap. When R starts to increase, the three fragments begin to emerge. The nuclear volume is not equally distributed. At the beginning, for small R, most of the volume is divided between the side fragments, whereas the middle fragment has only a small part of it. As R increases, the three fragments shape themselves more clearly, the middle fragment increases in volume and the side ones decrease. Consequently the radii are evolving towards the final values of the separated fragments. This important feature influ-

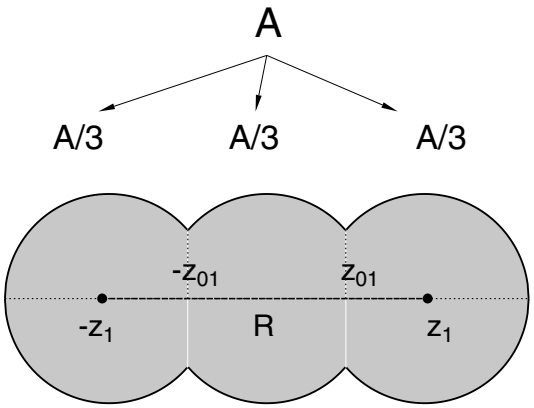

Figure **1.** Typical ternary colinear symmetric configuration for the splitting of an initial A-parent nucleus. The main independent variable, R, is the distance between the side centers. The pint $-z_1, 0, z_1$ are the centers of the fragments.

ences the value of the microscopic potential. At the end the three fragments become equal in volume when the touching point is reached.

3 The Potential

The core of the potential consists of three oscillators, partially overlapping. It is an axial potential, hence it is written in cylindrical coordinates. It has a ρ-part, perpendicular on the symmetry axis, and a z-part, along the symmetry axis. The total oscillator potential reads:

$$V(\rho, z, \phi) = V(\rho) + V(z) \tag{1}$$

as the sum of the two direction potentials. The ρ-part depends on the perpendicular frequency ω_ρ and the ρ-coordinate:

$$V(\rho) = \frac{1}{2} m_0 \omega_\rho^2 \rho^2 \tag{2}$$

Since the three fragments are equal, the frequency is the same. The potential has to describe the nuclear surface, thus it has to be centered in the middle of each fragment. This request is fulfilled by the expression of the z-part of the potential $V(z)$, which reads:

$$V(z) = \begin{cases} \frac{1}{2} m_o \omega_z^2 (z - z_1)^2 \ , z > z_{01} \\ \frac{1}{2} m_o \omega_z^2 z^2 \qquad\quad , -z_{01} < z < z_{01} \\ \frac{1}{2} m_o \omega_z^2 (z + z_1)^2 \ , z < -z_{01} \end{cases} \tag{3}$$

$V(z)$ has three expressions, each of them being active within the corresponding fragment region, where $-z_1, 0$ and z_1 are the colinear centers. Since the volume of the nuclear shape depends on the mass number if incompressibility is assumed, the geometric parameters are directly related to the potential through the oscillator frequencies. Once the shape is given by the mass number and the distance between centers, the three center potential is determined.

4 The Three-Center Hamiltonian

The total Hamiltonian comprises the three oscillator Hamiltonian, to which one adds the spin-orbit and the usual l-squared term:

$$H = H_{3osc} + V_{\hat{l}\hat{s}} + V_{\hat{l}^2} \tag{4}$$

Such a Hamiltonian is obviously not separable. What one can do is to work on the oscillator part H_{3osc} In cylindrical coordinates, the oscillator part reads the following expression:

$$H_{3osc} = -\frac{\hbar^2}{2m_0}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z^2}\right] + V(\rho) + V(z) \qquad (5)$$

where one has to replace $V(\rho)$ and $V(z)$ with the appropriate terms, as one moves from the first fragment to the middle one and the last one. Due to the z-dependence of the ρ-potential, as one shifts from one fragment to another, the oscillator Hamiltonian is not separable. But imposing the condition of equal ρ-frequencies: $\omega_{\rho_1} = \omega_{\rho_2} = \omega_{\rho_3}$ one has the same form for $V(\rho)$. In this situation one can choose the total wave function as the solution of the oscillator Schroedinger equation to be a product of three one-dimensional functions:

$$\Psi(\rho, z, \phi) = \Phi_m(\phi) R_{n_\rho}^{|m|}(\rho) Z_\nu(z) \qquad (6)$$

In this case one obtains three one-dimensional eqautions. The Φ and ρ equations are imediately solved. The angular function and the weighted Laguerre polynomial equations produce the solutions along two out of three coordinates:

$$\begin{aligned}
\Phi_m(\phi) &= \frac{1}{\sqrt{2\pi}} \exp(im\phi) \\
R_{n_\rho}^{|m|}(\rho) &= \left(\frac{2\Gamma(n_\rho+1)\alpha_1^2}{\Gamma(n_\rho+|m|+1)}\right)^{\frac{1}{2}} \exp\left(-\tfrac{\alpha_1^2\rho^2}{2}\right)(\alpha_1^2\rho^2)^{\frac{|m|}{2}} L_{n_\rho}^{|m|}(\alpha_1^2\rho^2)
\end{aligned}$$

Here $L_{n_\rho}^{|m|}$ is the Laguerre polynomial and Γ is the Gamma function. A small part of the problem is solved, since one has two out of three necessary quantum numbers and two out of the three wave functions. The total three-oscillator energy levels have two parts:

$$E_{3osc} = E_{\rho,\phi} + E_z \qquad (7)$$

The (ρ, ϕ) part is already solved by the previous two equations. Once one has the n_ρ and m quantum numbers, the (ρ, ϕ) energy is determined. For the z-part of the energy, one has to solve the corresponding z-axis Schroedinger equation:

$$\left[\frac{\partial^2}{\partial z^2} + \frac{2m_0 E_z}{\hbar^2} - \frac{2m_0}{\hbar^2}V(z)\right] Z(z) = 0 \qquad (8)$$

After a series of simple calculations, one obtains the Hermite function typical equations, with two independent solutions:

$$Z_\nu(z) = \exp(-z^2/2)\mathcal{H}_\nu(\pm z) \qquad (9)$$

where $\mathcal{H}_\nu(\pm z)$ is the Hermite function of non-integer indices ν. One observes at this point that ν depends on the geometrical configuration through the potential $V(z)$.

If one replaces the z-potential with each of the three-center expressions, one obtains the solution along the symmetry axis:

$$Z_\nu(z) = \begin{cases}
C_{1n} \exp\left[-\frac{\alpha^2(z-z_1)^2}{2}\right]\mathcal{H}_\nu[\alpha(z-z_1)] & , \quad z \geq z_{01} \\
C_{0n} \exp\left(-\frac{\alpha^2 z^2}{2}\right)[\mathcal{H}_\nu(z) + (-1)^n\mathcal{H}_\nu(-z)] & , -z_{01} < z < z_{01} \\
(-1)^n C_{1n} \exp\left[-\frac{\alpha^2(z+z_1)^2}{2}\right]\mathcal{H}_\nu[-\alpha(z+z_1)] & , \quad z \leq -z_{01}
\end{cases}$$

In this expression α is the frequency-dependent parameter. There are three unknown quantities: two normalization constants, c_{1n} and c_{0n} (due to symmetry the wave function for the two side fragments have the same normalization constant, c_{1n}) and the z-quantum number, ν. From the continuity of the wave function Z_ν and its derivative Z'_ν:

$$Z'_\nu(z) =$$

$$\begin{cases} C_{1n}\exp\left[-\frac{\alpha^2(z-z_1)^2}{2}\right]\alpha\{-(z-z_1)\mathcal{H}_\nu[\alpha(z-z_1)]+2\nu\mathcal{H}_{\nu-1}[\alpha(z-z_1)]\} \\ z \geq z_{01} \\ C_{0n}\exp-\frac{\alpha^2 z^2}{2}\alpha\{-z[\mathcal{H}_\nu(z)+(-1)^n\mathcal{H}_\nu(-z)]2\nu[[\mathcal{H}_{\nu-1}(z)+(-1)^{n+1}\mathcal{H}_{\nu-1}(-z)]\} \\ -z_{01} < z < z_{01} \\ (-1)^n C_{1n}\exp\left[-\frac{\alpha^2(z+z_1)^2}{2}\right]\alpha\{(z+z_1)\mathcal{H}_\nu[-\alpha(z+z_1)]+2\nu\mathcal{H}_{\nu-1}[-\alpha(z+z_1)]\} \\ z \leq -z_{01} \end{cases}$$

at the matching points $\pm z_{01}$ of the z-potential, one obtains two equations. The third is acquired from the normalization condition:

$$C_{1n}^2 j(\nu,\nu;-z_{01},\infty)+C_{0n}^2[j(\nu,\nu;-z_{01},z_{01})+(-1)^n j(\bar{\nu},\nu;-z_{01},z_{01})]=\frac{\alpha}{2} \tag{10}$$

where $j(\nu,\nu;x_1,x_2)$ are the z-integrals along the symmetry axis between the limits x_1 and x_2. The integrals are performed numerically over the range of each corresponding fragment. The system is solved numerically and the solution of two constants and the z-quantum number is determined for each step of the ternary configuration. With solving this system, the complete function basis, specific to tripartition fragmentation, is obtained.

At this point the first ternary signature of the process evolution is obtained as the variation of the z-quantum numbers ν. The variation is displayed in Figure 2.

Calculations have been applied to the symmetric splitting of neodymium in three ^{48}Ca fragments. The starting points are the integers corresponding to a unique center. Then the z-quantum numbers decrease through non-integer values. At the end of the process, the numbers merge three by three into the final integers, specific for each ^{48}Ca totally separated fragment. The three oscillator part is solved. A first set of calculations has as a result the three-oscillator energy levels as a function of the distance between centers. The starting values are the usual one oscillator level sequence, which is obtained here by the total superposition of the three centers and is presented in Figure 3. As the distance R increases, the levels are mixing. Towards the end of the process, the levels converge in three identical oscillator schemes, particular for the three ^{48}Ca.

One observes the increment of the space between the shells, as the mass number decreases.

5 Spin-Orbit Interaction

In order to complete the energy of the ternary system, one has to add the spin-orbit and l^2 interactions. Due to the fact that spin-orbit intensities κ and μ are nuclear mass dependent these quantities can change when one passes from one fragment to another, within the tripartition shape. This fact makes the intensities z-dependent. Since the spin-orbit operators contain derivatives, the usual expression is not hermitian. For this reason, one shall replace the two potentials with anti-commutators between the strengths as (ρ, z) functions instead of constants, and the angular momentum dependent operators, as one can read:

$$V_{ls} = \begin{cases} -\left\{\dfrac{\hbar}{m_0\omega_{01}}\kappa_1(\rho,z), (\nabla V(z > z_{01}) \times p)s\right\} & , A_1 - region \\ -\left\{\dfrac{\hbar}{m_0\omega_{02}}\kappa_2(\rho,z), (\nabla V(-z_{01} < z < z_{01}) \times p)s\right\} & , A_2 - region \\ -\left\{\dfrac{\hbar}{m_0\omega_{03}}\kappa_3(\rho,z), (\nabla V(z < -z01) \times p)s\right\} & , A_3 - region \end{cases}$$

and the corresponding l^2 dependent potential has a similar expression.

Each of the operators has three expressions, as one moves from one fragment region A_1 to the next A_2 and so on. The potential is also replaced successively by one of the above three expressions.

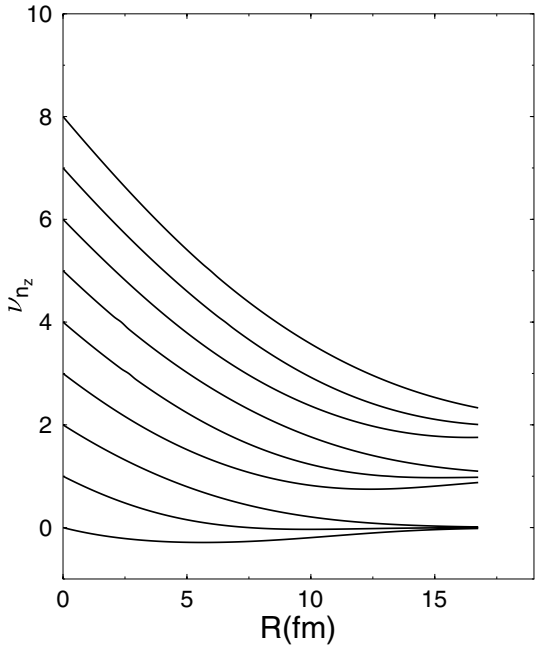

Figure **2.** Evolution of the z-quantum numbers ν with increasing distance between centers R.

The general expression of the spin-orbit operator is constructed using the creation and annihilation operators:

$$ls \rightarrow \tfrac{1}{2}(\mathbf{\Omega}^{+}\mathbf{s}^{-} + \mathbf{\Omega}^{-}\mathbf{s}^{+}) + \mathbf{\Omega}_{z}\mathbf{s}_{z} \tag{11}$$

With these new operators one can construct now the total spin-orbit operator from the creation and annihilation parts. To comply to the anti-commutator rule, three combinations of Heaviside functions are employed. Each of them ensures the action of the specific operator only within the region where the corresponding fragment is active. These regions are bordered by surfaces which pass through the matching points of the ternary configuration. The last step of the spin-orbit part is to obtain the dependence of the operators on the specific ternary configuration at a given geometry. This is fulfilled by the use of different corresponding potentials for each region. The final three expressions for the creation operator read:

$$\begin{aligned}
&\langle \prime|\mathbf{\Omega}^{+}|\rangle = \\
&\langle \prime|\{\mathbf{\Omega}^{+}(z > z_{01}), \Theta(z - z_{01}]\}|\rangle && \rightarrow A_1, \quad z > z_{01} \\
&\langle \prime|\{\mathbf{\Omega}^{+}(-z_{01} < z < z_{01}), [\Theta(z + z_{01}) - \Theta(z - z_{01})]\}|\rangle && \rightarrow A_2, -z_{01} \leq z \leq z_{01} \\
&\langle \prime|\{\mathbf{\Omega}^{+}(z < -z_{01}), [1 - \Theta(z + z_{01})]\}|\rangle && \rightarrow A_3, \quad z < -z_{01}
\end{aligned} \tag{12}$$

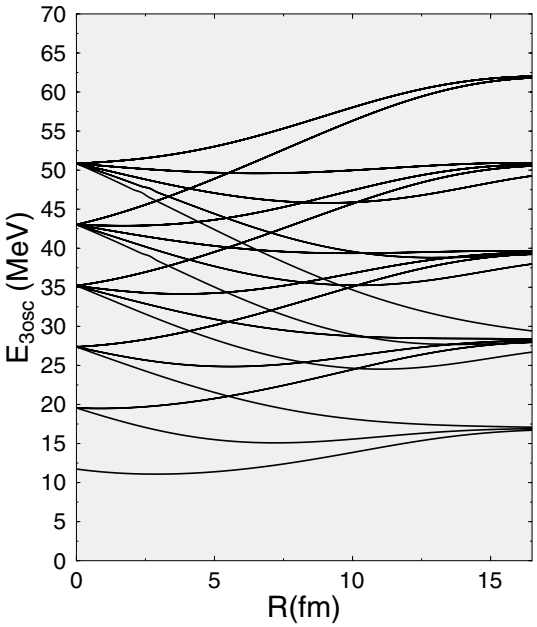

Figure **3.** Three center oscillator level scheme against the distance between centers for the symmetric splitting of ^{144}Nd into three ^{48}Ca fragments.

and the same is available for Ω^- and $\mathbf{\Omega}_z$.

The final expressions for the creation operators are frequency and geometry dependent:

$$\mathbf{\Omega}^+(z > z_{01}) = -e^{i\varphi}\left[\frac{\partial V(\rho,z>z_{01})(\rho,z)}{\partial\rho}\frac{\partial}{\partial z} - \frac{\partial V(\rho,z>z_{01}))}{\partial z}\frac{\partial}{\partial\rho} - \frac{i}{\rho}\frac{\partial V(\rho,z>z_{01})}{\partial z}\frac{\partial}{\partial\varphi}\right]$$

$$= -e^{i\varphi}\left[m_0\omega_\rho^2\rho\frac{\partial}{\partial z} - m_0\omega_z^2(z-z_1)\frac{\partial}{\partial\rho} - \frac{i}{\rho}m_0\omega_z^2(z-z_1)\frac{\partial}{\partial\varphi}\right]$$

$$\mathbf{\Omega}^+(-z_{01} < z < z_{01}) =$$
$$= -e^{i\varphi}\left[\frac{\partial V(\rho,-z_{01}<z<z_{01})}{\partial\rho}\frac{\partial}{\partial z} - \frac{\partial V(\rho,-z_{01}<z<z_{01})}{\partial z}\frac{\partial}{\partial\rho} + \frac{i}{\rho}\frac{\partial V(\rho,-z_{01}<z<z_{01})}{\partial z}\frac{\partial}{\partial\varphi}\right]$$

$$= -e^{i\varphi}\left[m_0\omega_\rho^2\rho\frac{\partial}{\partial z} - m_0\omega_z^2 z\frac{\partial}{\partial\rho} + \frac{i}{\rho}m_0\omega_z^2 z\frac{\partial}{\partial\varphi}\right]$$

$$\mathbf{\Omega}^+(z < -z_{01}) =$$
$$= -e^{i\varphi}\left[\frac{\partial V(\rho,z<-z_{01})(\rho,z)}{\partial\rho}\frac{\partial}{\partial z} - \frac{\partial V(\rho,z<-z_{01}))}{\partial z}\frac{\partial}{\partial\rho} - \frac{i}{\rho}\frac{\partial V(\rho,z<-z_{01})}{\partial z}\frac{\partial}{\partial\varphi}\right]$$

$$= -e^{i\varphi}\left[m_0\omega_\rho^2\rho\frac{\partial}{\partial z} - m_0\omega_z^2(z+z_1)\frac{\partial}{\partial\rho} - \frac{i}{\rho}m_0\omega_z^2(z+z_1)\frac{\partial}{\partial\varphi}\right]$$

In this final form one can observe that each operator is centered in the middle of the fragment it represents. The total spin-orbit interaction is the sum of the the three regions:

$$\begin{aligned} V_{\mathbf{\Omega s}} = &-\frac{\hbar}{m_0\omega_{01}}\kappa_1\{\mathbf{\Omega s}(A_1),(A_1)\} \\ &-\frac{\hbar}{m_0\omega_{02}}\kappa_2\{\mathbf{\Omega s}(A_2),(A_2)\} \\ &-\frac{\hbar}{m_0\omega_{01}}\kappa_3\{\mathbf{\Omega s}(A_3),(A_3)\} \end{aligned} \tag{13}$$

Finally the matrix of the total Hamiltonian for the three center shell model can be constructed as the sum of the three superposed oscillators and the angular momentum dependent terms:

$$\langle i|3CSM|j\rangle = E_{3osc}(n_\rho,|m|,\nu) + \langle i|V_{\mathbf{\Omega s}}|j\rangle + \langle i|V_{\mathbf{\Omega}^2}|j\rangle \tag{14}$$

6 Results and Discussion

As the result of diagonalization of the total matrix one obtains the level scheme for colinear ternary fragmentation of a given system. Calculations have been applied to the symmetric splitting of ^{144}Nd into three ^{48}Ca. For zero distance between centers the three fragments completely overlap and one obtains the initial level scheme of

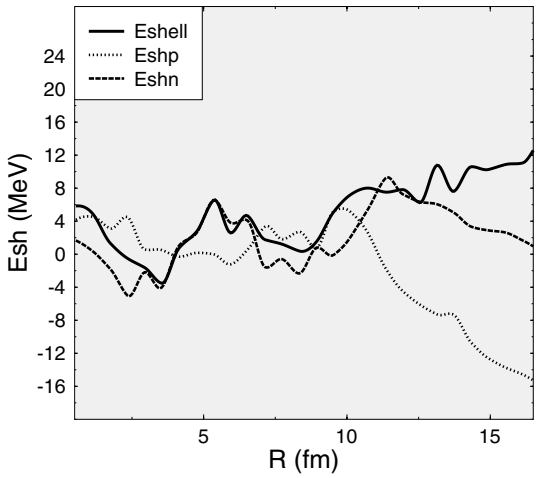

Figure **4.** Calculated shell corrections for protons, neutrons and total value for the symmetric splitting of ^{144}Nd into three ^{48}Ca.

the parent nucleus. Then, with increasing R the shape becomes more elongated and the three fragments begin to form. The levels are mixing now and one can observe the existence of energy gaps for certain geometries. At the end, the levels converge towards the typical shells of three separated ^{48}Ca.

Calculations are performed separately for neutrons and protons, since the the spin-orbit strength is different. The final level scheme is used as an input data for computing the shell corrections E_{sh}. This part has been fulfilled by using the Strutinsky method. In Figure 4 the results for ^{144}Nd are presented.

A first minimum is observable for a small distance between centers, at the beginning of the process. The shell corrections are added to the macroscopic liquid drop part of the energy. This first minimum in shell corections can produce a small potential pocket, which is in fact due to the initial deformation of neodymium. A maximum is followed by a second minimum in the very deformed, elongated region. At this point the fragments are only partially overlapped so that now one has a ternary effect. At the end of the process, when the three fragments reach the touching point, the individuality of ^{48}Ca is manifested. The magicity of the already formed proton and neutron level schemes produce the deep minimum in the shell corrections. Here one has three times the neutron and proton negative shell corrections, which correspond to 28 neutron and 20 proton magic numbers closures.

7 Conclusions

The three center shell model which has been constructed describes the transition of the parent neutron and proton level scheme to the three partially overlapped and finally separated fragment level schemes. Spin-orbit interaction operators are geome-

try dependent and generate the appropiate matrix elements influenced by the ternary character of the process. The minima calculated in the shell corrections along the tripartition splitting can lower the macroscopic barrier and decide which parent nucleus can be chosen as favourable for ternary fission studies. Also minima in the shell corrections obtained with the three center shell model level scheme could influence the stability of an elongated, linear three-body type system.

Acknowledgments

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