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Dedicated to Professor Marin Ivaşcu's 80^{th} Anniversary

FISSILITY OF NUCLEAR AND ATOMIC CLUSTER SYSTEMS

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Abstract. The liquid drop model deformation energy of a nuclear system is calculated in spherical coordinates with deformation parameters $\{\alpha_{\lambda\mu}\}$ as well as for shapes with cylindrical symmetry with deformations $\{a_n\}$ assuming small values of quadrupolar deformation parameter. The particularity of charged metallic clusters are stressed. Stable, unstable, and metastable states are defined using the fissility parameter, the released energy, and the fission barrier.

Key words: Nuclear fission, liquid drop model, Coulomb energy, surface energy, charged metallic atomic clusters, stability of clusters.

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1. INTRODUCTION

Fissility is a very useful concept first introduced by Lord Rayleigh [1] who studied in 1882 the "equilibrium of liquid conducting masses charged with electricity". His liquid drop model (LDM) [2] was adapted by Niels Bohr to atomic nuclei [3] and dominated the theory of nuclear fission since 1939 [4, 5] until 1967 [6]. It was used not only to explain [4] the discovery of the induced nuclear fission [7], but also to show [5] that induced fission was more likely to occur with ^{235}U than ^{238}U and to predict spontaneous fission which was discovered next year [8].

Atomic clusters (AC) are similar with atomic nuclei because both systems consists of fermions moving freely in a confined space. In this way we have the possibility of using the nuclear LDM [9] and the macroscopic-microscopic method (MMM) with shell and pairing corrections [6] to study neutral and charged atomic clusters [10–29].

We used the LDM [30] and the MMM [31] to study neutral hemispheroidal AC deposited on a surface. We derived analytical relationships for the deformation-

dependent LDM energies of oblate and prolate hemispheroidal AC as well as for the spheroidal cap shapes [32]. A superdeformed prolate hemispheroid was found to be the most stable shape within LDM when the interaction energy with the substrate is negligible low. It is also the shape with maximum degeneracy of quantum states of the new shell model based on the hemispheroidal harmonic oscillator [33–36] used to compute the shell and pairing corrections [37]. Oblate equilibrium shapes may be also obtained by simulating the interaction via a major change of the surface tension at the contact surface [38]. We had also studied the stable deformations and the singly charged trimer emission from charged metallic drops of different shapes under the influence of Coulomb energy [39, 40], providing a simple explanation of a well established experimental fact: the high yield observed in "Coulomb explosion" (fission) of charged metallic clusters for a singly charged trimer fragment (the analog of the α-decay, having a magic number of 2 delocalized electrons) is the consequence of having both the LDM and shell corrections minima at the fragmentation corresponding to the same number of two delocalized electrons.

Compared to nuclei, in which the electric charge of protons is assumed to be homogeneously distributed in the volume, in metallic atomic clusters the excess charge of electrons produced by ionization is concentrated on the surface, which makes the calculations of electrostatic energy of metallic clusters more complicated compared to that of nuclei.

In the present paper we are dealing with the nuclear (always charged drops) and charged (ionized) atomic cluster fissility. A high fissility is observed in heavy nuclei and in small size charged atomic clusters. Fissility is a parameter characterizing the stability of charged liquid drops. We shall start the study by deriving the deformation energy of a nuclear system within the LDM assuming small deformations around a spherical shape.

2. LDM DEFORMATION ENERGY OF A SPHERICAL NUCLEUS AND OF A SPHERICAL METALLIC CLUSTER

The charge density of a spherical nucleus with atomic number Z and a radius R_0 is given by:

$$\rho_e = \rho_0 = \frac{Ze}{4\pi R_0^3/3} \tag{1}$$

where e is the electron charge. In order to determine the potential V we use the spherical symmetry of the problem. We write the Poisson equation [41]:

$$\Delta V(\vec{r}) = -4\pi\rho_e \; ; \quad \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dV}{dr}\right) = -4\pi\rho_e \tag{2}$$

For $r > R_0$ the charge density is zero, hence the potential V_e obeys the differential equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dV_e}{dr}\right) = 0 \tag{3}$$

First integration gives

$$\frac{dV_e}{dr} = \frac{C_1}{r^2} \tag{4}$$

In order to determine C_1 we use Gauss theorem for a radius $R' \geq R_0$

$$E(R')\cdot 4\pi R'^2 = 4\pi Ze\,; \quad ER'^2 = Ze \tag{5}$$

$$\frac{dV_e}{dr} = -E = \frac{C_1}{r^2}\,; \quad C_1 = -ER'^2 = -Ze \tag{6}$$

$$\frac{dV_e}{dr} = -\frac{Ze}{r^2}\,; \quad V_e = \frac{Ze}{r} + C_2 \tag{7}$$

and $C_2 = 0$ because $V(\infty) = 0$.

For $r \leq R_0$ the potential V_i may be found from the equation

$$\frac{d}{dr}\left(r^2\frac{dV_i}{dr}\right) = -4\pi\rho_0 r^2 \tag{8}$$

$$r^2\frac{dV_i}{dr} = -\frac{4\pi}{3}\rho_0 r^3 + k_1\,; \quad V_i = -\frac{4\pi}{6}\rho_0 r^2 - \frac{k_1}{r} + k_2 \tag{9}$$

The potential for $r = 0$ should be finite, hence $k_1 = 0$.

$$V_i = -\frac{Zer^2}{2R_0^3} + k_2\,; \quad \rho_0 = Ze/(4\pi R_0^3/3) \tag{10}$$

The continuity at $r = R_0$ gives us

$$V_i(R_0) = V_e(R_0) = \frac{Ze}{R_0}\,; \quad k_2 = \frac{3Ze}{2R_0} \tag{11}$$

hence

$$V_i(r) = \begin{cases} \frac{Ze}{R_0}\left(\frac{3}{2} - \frac{r^2}{2R_0^2}\right) & r \leq R_0 \\ \frac{Ze}{r} & r \geq R_0 \end{cases} \tag{12}$$

$$V_i(0) = \frac{3Ze}{2R_0} \tag{13}$$

In spherical coordinates the electrostatic energy

$$E_C^0 = \frac{\rho_e}{2}\int V(r)d^3r = \frac{\rho_e}{2}\int_0^{R_0}\frac{Ze}{R_0}\left(\frac{3}{2} - \frac{r^2}{2R_0^2}\right)4\pi r^2 dr \tag{14}$$

$$E_C^0 = \frac{3Z^2e^2}{4R_0^4}\int_0^{R_0}\left(3r^2 - \frac{r^4}{R_0^2}\right)dr = \frac{3Z^2e^2}{5R_0} \tag{15}$$

For a metallic sphere the potential is constant on the surface $V = Ze/R_0$

$$E^0_{C-met} = \frac{\rho_{e-surf}}{2}\int V dS = \frac{Ze}{4\pi R_0^2}\frac{1}{2}\frac{Ze}{R_0}4\pi R_0^2 = \frac{Z^2e^2}{2R_0} \tag{16}$$

Consequently the uniform distribution of charge in the nuclear volume gives a 0.6 numerical coefficient in front of $(Ze)^2/R_0$, while the surface distribution of the metallic cluster makes only 0.5.

Within LDM the radius of a nucleus with mass number A is expressed as $R_0 = r_0 A^{1/3}$, where the nuclear radius constant is of the order of $r_0 \simeq 1.2$ fm, and the radius of a metallic cluster (say Na) of a size n_e would be $R_0 = r_s n_e^{1/3}$ where the Wigner-Seitz radius $r_s = 2.08$ Å for Na. 1Å$= 10^{-1}$ nm$= 10^{-10}$ m$= 10^5$ fm.

3. SMALL DEFORMATIONS

In the general case of nonaxial shapes [41–44] one can use the spherical harmonics satisfying the differential equation:

$$\nabla^2 Y_{\lambda\mu}(\theta,\phi) = -\lambda(\lambda+1)Y_{\lambda\mu}(\theta,\phi) \tag{17}$$

where the angular spherical coordinates are $0 \le \phi \le 2\pi$ – azimuth, and $0 \le \theta \le \pi$ – colatitude; λ –degree, μ –order.

Nuclear surface is parameterized by expressing the nuclear radius in the direction $(\theta,\phi) = \Omega$:

$$R(\theta,\phi) = R_0\left[1 + \sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda}\alpha^*_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right] \tag{18}$$

where $\alpha_{\lambda\mu}$ are deformation parameters. Complex conjugation leads to

$$Y^*_{\lambda\mu}(\theta,\phi) = (-1)^\mu Y_{\lambda-\mu}(\theta,\phi)\,; \quad \alpha^*_{\lambda\mu} = (-1)^\mu \alpha_{\lambda-\mu} \tag{19}$$

and orthogonality

$$\int d\Omega Y^*_{\lambda\mu}Y_{\lambda'\mu'} = \delta_{\lambda\lambda'}\delta_{\mu\mu'}. \tag{20}$$

In the lowest order $Y_{00} = 1/\sqrt{4\pi}$.

To calculate the Coulomb energy we also need the ratio $1/|\vec{r}-\vec{r'}|$ which may be [44] developed in a series of Legendre polynomials

$$\frac{1}{\left|\vec{r}-\vec{r'}\right|} = \sum_{i=0}^{\infty}\frac{r_<^\lambda}{r_>^{\lambda+1}}P_\lambda(\cos\gamma) \tag{21}$$

where $r_<$ ($r_>$) is the smaller (larger) of $|\vec{r}|$, $|\vec{r'}|$, and γ is the angle between $\vec{r}$ and $\vec{r'}$.

The addition theorem for spherical harmonics

$$P_\lambda(\cos\gamma) = \frac{4\pi}{2\lambda+1}\sum_{\mu=-\lambda}^{\lambda} Y^*_{\lambda\mu}(\theta',\phi')Y_{\lambda\mu}(\theta,\phi) \tag{22}$$

allows us to write

$$\frac{1}{\left|\vec{r}-\vec{r'}\right|} = 4\pi\sum_{\lambda=0}^{\infty}\sum_{\mu=-\lambda}^{\lambda}\frac{1}{2\lambda+1}\frac{r_<^\lambda}{r_>^{\lambda+1}}Y^*_{\lambda\mu}(\theta',\phi')Y_{\lambda\mu}(\theta,\phi) \tag{23}$$

3.1. VOLUME CONSERVATION

We can reduce the number of the independent deformation parameters by using the volume conservation:

$$\mathcal{V} = \int d\Omega\int_0^{R(\Omega)} r^2 dr = \frac{1}{3}R_0^3\int d\Omega\left(1+\sum_{\lambda\mu}\alpha^*_{\lambda\mu}Y_{\lambda\mu}(\Omega)\right)^3 \tag{24}$$

We keep terms up to the second order in deformation parameters. Using the identity $(a+b)^3 = a^3+3a^2b+3ab^2+b^3$, with $a=1$ and $b=\sum_{\lambda\mu}$ from the above equation, we have

$$\mathcal{V} \approx \frac{1}{3}R_0^3\int d\Omega\left(1+3\sum_{\lambda\mu}\alpha^*_{\lambda\mu}Y_{\lambda\mu}(\Omega)+3\sum_{\lambda\mu}\sum_{\lambda'\mu'}Y_{\lambda\mu}(\Omega)Y_{\lambda'\mu'}(\Omega)\right) \tag{25}$$

Now we use the fact that $Y_{00} = 1/\sqrt{4\pi}$ and the orthogonality relationship, so that

$$\int d\Omega Y_{\lambda\mu}(\Omega) = \sqrt{4\pi}\int d\Omega Y_{00}(\Omega)Y_{\lambda\mu}(\Omega) = \sqrt{4\pi}\delta_{\lambda 0}\delta_{\mu 0} \tag{26}$$

$$\mathcal{V} \approx \frac{1}{3}R_0^3\left(4\pi+3\sqrt{4\pi}\alpha_{00}+3\sum_{\lambda\mu}|\alpha_{\lambda\mu}|^2\right) \tag{27}$$

hence the volume conservation $\mathcal{V} = 4\pi R_0^3/3$ requires

$$\sqrt{4\pi}\alpha_{00}+\sum_{\lambda\mu}|\alpha_{\lambda\mu}|^2 = 0 \tag{28}$$

3.2. COULOMB AND SURFACE ENERGY

For a nucleus with a charge density ρ_e

$$E_C = \frac{1}{2}\int d^3r\int d^3r'\frac{\rho_e(\vec{r})\rho_e(\vec{r'})}{|\vec{r}-\vec{r'}|} \tag{29}$$

When ρ_e is constant inside nucleus and zero outside

$$E_C = \frac{\rho_e^2}{2}\int d^3r \int d^3r' \frac{1}{|\vec{r}-\vec{r'}|} \tag{30}$$

which is in spherical coordinates

$$E_C = \frac{\rho_e^2}{2}\int d\Omega \int d\Omega' \int_0^{R(\Omega)} r^2 dr \int_0^{R(\Omega')} r'^2 dr' \frac{1}{|\vec{r}-\vec{r'}|} \tag{31}$$

We can split the integrals over r in the following way

$$\int_0^{R(\Omega)} dr \int_0^{R(\Omega')} dr' = \left(\int_0^{R_0} dr + \int_{R_0}^{R(\Omega)} dr\right)\left(\int_0^{R_0} dr' + \int_{R_0}^{R(\Omega')} dr'\right) \tag{32}$$

$$\int_0^{R(\Omega)} dr \int_0^{R(\Omega')} dr' = \int_0^{R_0} dr \int_0^{R_0} dr' + 2\int_{R_0}^{R(\Omega)} dr \int_0^{R_0} dr' + \int_{R_0}^{R(\Omega)} dr \int_{R_0}^{R(\Omega')} dr' \tag{33}$$

so that [43]

$$E_C = E_C^0 + E_{C,m} + E_{C,\lambda} \tag{34}$$

E_C^0 was given above and the other two terms are

$$E_{C,m} = \rho_e^2 \int d\Omega \int d\Omega' \int_{R_0}^{R(\Omega)} r^2 dr \int_0^{R_0} r'^2 dr' \frac{1}{\left|\vec{r}-\vec{r'}\right|} \tag{35}$$

$$E_{C,\lambda} = \frac{\rho_e^2}{2} \int d\Omega \int d\Omega' \int_{R_0}^{R(\Omega)} r^2 dr \int_{R_0}^{R(\Omega')} r'^2 dr' \frac{1}{\left|\vec{r}-\vec{r'}\right|} \tag{36}$$

Now we use the addition theorem for spherical harmonics (22), allowing to make the expansion from (23) so that

$$E_{C,m} = 4\pi\rho_e^2 \sum_{\lambda\mu} \frac{1}{2\lambda+1} \int d\Omega' Y_{\lambda\mu}(\Omega') \int d\Omega Y_{\lambda\mu}^*(\Omega) \int_{R_0}^{R(\Omega)} r^2 dr \int_0^{R_0} r'^2 dr' \frac{1}{r_>} \tag{37}$$

The integration over Ω' can be done multiplying and dividing with $Y_{00} = 1/\sqrt{4\pi}$ and then using the orthonormalization of the spherical harmonics

$$\int d\Omega' Y_{\lambda\mu}(\Omega') = \sqrt{4\pi}\int d\Omega' Y_{00}^* Y_{\lambda\mu}(\Omega') = \sqrt{4\pi}\delta_{\lambda 0}\delta_{\mu 0} \tag{38}$$

so that the sum over λ and μ collapses to the term with $\lambda = 0$ and $\mu = 0$ leading to

$$E_{C,m} = 4\pi\rho_e^2 \int d\Omega \int_{R_0}^{R(\Omega)} r^2 dr \int_0^{R_0} r'^2 dr' \frac{1}{r_>} \tag{39}$$

The integral over r is performed after split into two parts because of the definition of $r_>$

$$\int_0^{R_0} r'^2 dr' \frac{1}{r_>} = \int_0^r r'^2 dr' \frac{1}{r} + \int_r^{R_0} r'^2 dr' \frac{1}{r'} = \frac{1}{2}\left(R_0^2 - \frac{1}{3}r^2\right) \tag{40}$$

so that

$$\int_{R_0}^{R(\Omega} r^2 dr \frac{1}{2}\left(R_0^2 - \frac{1}{3}r^2\right) = \frac{1}{6}\left[R_0^2 R^3(\Omega) - R_0^5 - \frac{1}{5}R^5(\Omega) + \frac{1}{5}R_0^5\right] \tag{41}$$

We expand the differences between R_0 and $R(\Omega)$ to second order in $\alpha_{\lambda\mu}$. By using the identity $(a+b)^3 = a^3 + 3a^2b + 3ab^2 + b^3$ we get

$$R^3 - R_0^3 \approx 3R_0^3\left((\sum)^2 + \sum\right) \tag{42}$$

and from $(a+b)^5 = a^5 + 5a^4b + 10a^3b^2 + 10a^2b^3 + 5ab^4 + b^5$ one is led to

$$\frac{1}{5}\left(R^5 - R_0^5\right) \approx R_0^5\left(2(\sum)^2 + \sum\right) \tag{43}$$

so that

$$E_{C,m} \approx \frac{2\pi}{3}R_0^5\rho_e^2 \int d\Omega \left(2\sum_{\lambda\mu}\alpha^*_{\lambda\mu}Y_{\lambda\mu}(\Omega) + \sum_{\lambda\mu}\sum_{\lambda'\mu'}\alpha^*_{\lambda\mu}Y_{\lambda\mu}(\Omega)\alpha_{\lambda'\mu'}Y^*_{\lambda'\mu'}(\Omega)\right) \tag{44}$$

$$E_{C,m} \approx \frac{2\pi}{3}R_0^5\rho_e^2\left(2\sqrt{4\pi}\alpha_{00} + \sum_{\lambda\mu}\alpha^*_{\lambda\mu}\alpha_{\lambda\mu}\right) = -\frac{2\pi}{3}R_0^5\rho_e^2\sum_{\lambda\mu}|\alpha_{\lambda\mu}|^2 \tag{45}$$

In the last integral

$$E_{C,\lambda} = \frac{\rho_e^2}{2}\int d\Omega \int d\Omega' \int_{R_0}^{R(\Omega)} r^2 dr \int_{R_0}^{R(\Omega')} r'^2 dr' \frac{1}{\left|\vec{r} - \vec{r'}\right|} \tag{46}$$

we use again (23) and assume that

$$\frac{r_<^\lambda}{r_>^{\lambda+1}} \approx 1/R_0 \tag{47}$$

for $r, r' \in [R_0, R(\Omega)]$ (on the surface). In this way

$$E_{C,\lambda} = \frac{2\pi\rho_e^2}{R_0}\sum_{\lambda\mu}\frac{1}{2\lambda+1}\int d\Omega Y^*_{\lambda\mu}(\Omega)\int d\Omega' Y_{\lambda\mu}(\Omega')\int_{R_0}^{R(\Omega)} r^2 dr \int_{R_0}^{R(\Omega')} r'^2 dr' \tag{48}$$

The integral over r gives the result $[R^3(\Omega) - R_0^3)]/3$ and that over r' is $[R^3(\Omega') - R_0^3)]/3$.

$$E_{C,\lambda} = \frac{2\pi\rho_e^2}{9R_0}\sum_{\lambda\mu}\frac{1}{2\lambda+1}\int d\Omega Y^*_{\lambda\mu}(\Omega)[R^3(\Omega) - R_0^3)]\int d\Omega' Y_{\lambda\mu}(\Omega')[R^3(\Omega') - R_0^3)] \tag{49}$$

Again, as in (42), we expand the differences between R_0 and $R(\Omega)$ to second order in $\alpha_{\lambda\mu}$, by using the identity $(a+b)^3 = a^3+3a^2b+3ab^2+b^3$ so that $R^3(\Omega)-R_0^3 \approx 3R_0^3((\sum)^2+\sum)$ and $R^3(\Omega')-R_0^3 \approx 3R_0^3((\sum)^2+\sum)$. From the product of integrals over Ω and Ω' we should also keep the lowest order in $\alpha_{\lambda\mu}$, that is

$$E_{C,\lambda} \approx 2\pi\rho_e^2 R_0^5 \sum_{\lambda\mu} \frac{1}{2\lambda+1} \int d\Omega Y^*_{\lambda\mu}(\Omega) \sum \alpha_{\lambda'\mu'} Y_{\lambda'\mu'} \int d\Omega' Y_{\lambda\mu}(\Omega') \sum \alpha_{\lambda'\mu'} Y_{\lambda'\mu'} \quad (50)$$

Now the orthonormality, eq. (20), of spherical harmonics allows to get the result

$$E_{C,\lambda} = \frac{\rho_e^2}{2} \int d\Omega \int d\Omega' \int_{R_0}^{R(\Omega)} r^2 dr \int_{R_0}^{R(\Omega')} r'^2 dr' \frac{1}{\left|\vec{r}-\vec{r'}\right|} \quad (51)$$

so that

$$E_{C,\lambda} \approx 2\pi R_0^5 \rho_e^2 \sum_{\lambda\mu} \frac{1}{2\lambda+1} |\alpha_{\lambda\mu}|^2 \quad (52)$$

We can add the three contributions E_C^0, $E_{C,m}$ — eq.(45), and $E_{C,\lambda}$ — eq.(52)

$$E_C = E_C^0 \left[1 - \frac{5}{8\pi} \sum \frac{|\alpha_{\lambda\mu}|^2}{2\lambda+1}(2\lambda+1) + \frac{15}{8\pi} \sum \frac{|\alpha_{\lambda\mu}|^2}{2\lambda+1}\right] \quad (53)$$

$$B_c = \frac{E_C}{E_C^0} = 1 - \frac{5}{4\pi} \sum \frac{\lambda-1}{2\lambda+1} |\alpha_{\lambda\mu}|^2. \quad (54)$$

$E_{C,m}$ receives contributions only from monopole redistribution of the charge, and $E_{C,\lambda}$ arises from the interaction of the multipole part of the potential field with the multipole charge distribution.

The main contributions to the LDM deformation energy are coming from the surface and electrostatic (Coulomb) energies

$$E_{LDM} = (E_s - E_s^0) + (E_C - E_C^0) = E_s^0(B_s - 1) + E_C^0(B_C - 1). \quad (55)$$

The surface energy [42] is proportional with the surface tension σ and surface area:

$$E_s = \sigma \int_{Surf} dS \quad (56)$$

The surface element in spherical coordinates

$$dS = \sqrt{1 + \frac{1}{R^2}\left(\frac{\partial R}{\partial \theta}\right)^2 + \frac{1}{R^2 \sin^2\theta}\left(\frac{\partial R}{\partial \phi}\right)^2} R^2 \sin\theta d\theta d\phi \quad (57)$$

which gives in the first order

$$dS \simeq \left[R^2 + \frac{1}{2}\left(\frac{\partial R}{\partial \theta}\right)^2 + \frac{1}{2\sin^2\theta}\left(\frac{\partial R}{\partial \phi}\right)^2\right] \sin\theta d\theta d\phi \quad (58)$$

Finally, in the first order, the ratio E_s/E_s^0 may be written [42] as

$$B_s = 1 + \frac{1}{8\pi}\sum_{\lambda\mu}(\lambda-1)(\lambda+2)|\alpha_{\lambda\mu}|^2 \tag{59}$$

and for a spherical atomic cluster we have $E_s^0 = 4\pi R_0^2\sigma = a_s n_e^{2/3} = 4\pi r_s^2 n_e^{2/3}\sigma$.

The stiffness constant $C_{\lambda\mu}$, defined by the following expression of the deformation energy

$$E_s + E_C - (E_s^0 + E_C^0) = \frac{1}{2}\sum_{\lambda,\mu} C_{\lambda\mu}|\alpha_{\lambda\mu}|^2 \tag{60}$$

is given by

$$C_\lambda = (\lambda-1)(\lambda+2)R_0^2\sigma - \frac{3e^2Z^2(\lambda-1)}{2\pi R_0(2\lambda+1)} \tag{61}$$

where $\sigma = a_2/(4\pi r_0^2)$ is the surface tension constant. One can see that $\lambda = 1$ leads to $B_c = B_s = 1$ and $C_1 = 1$, meaning that only quadrupole and higher order multipolarities contribute to the deformation energy. We saw above that $\lambda = 0$ takes care of the volume conservation.

The dimensionless deformation energy

$$\xi = \frac{E_s + E_C - E_s^0 - E_C^0}{E_s^0} = \frac{1}{2\pi}\sum_{\lambda\mu}\left[\frac{(\lambda-1)(\lambda+2)}{4} - X\frac{5(\lambda-1)}{2\lambda+1}\right]|\alpha_{\lambda\mu}|^2 \tag{62}$$

$$\xi = \frac{1}{2E_s^0}\sum_{\lambda\mu} C_\lambda|\alpha_{\lambda\mu}|^2 \tag{63}$$

The fissility is defined as

$$X = \frac{E_c^0}{2E_s^0} = \frac{(Z^2/A)}{(Z^2/A)_c} \tag{64}$$

with $(Z^2/A)_c = 40\pi r_0^3\sigma/(3e^2) \simeq 50$ [9]. The ratio Z^2/A, and consequently the fissility parameter X, becomes larger for heavier nuclei.

For *axially symmetric* shapes, the deformations parameters $\{a_n\}$ are defined by expanding in a series of Legendre polynomials

$$R(\theta,\phi) = R(\theta,0) = \frac{R_0}{a}\left[1 + \sum_{l=2}^{\infty} a_l P_l(\cos(\theta)\right] \tag{65}$$

For small quadrupolar deformations the above equations became

$$B_c \simeq 1 - 5\sum_n \frac{(n-1)}{(2n+1)^2}a_n^2 \simeq 1 - \frac{a_2^2}{5} \tag{66}$$

$$B_s \simeq 1 + \frac{1}{2}\sum_n \frac{(n-1)(n+2)}{2n+1}a_n^2 \simeq 1 + \frac{2a_2^2}{5} \tag{67}$$

The stability of nuclear shape relative to small quadrupolar deformations, a_2, can be studied by developing the relative deformation energy in terms of a_2 around $a_2 = 0$. To a very good approximation, one has

$$\xi = B_s - 1 + 2X(B_c - 1) \simeq \frac{2}{5} a_2^2 (1 - X) \tag{68}$$

It is clear that for $X < 1$ the deformation energy increases with the deformation parameter a_2 and there is a driving force toward the potential minimum at $a_2 = 0$ - the equilibrium shape. On the contrary, according to this result of a LDM, any nucleus with $X > X_{cr} = 1$, corresponding to $Z \geq 125$, has no chance to survive because its energy is decreasing continuously with increasing deformation parameter. For a long period of time the vanishing fission barrier was considered to be a reasonable explanation for the absence in nature of the very heavy elements. By including the shell effects, a nonzero fission barrier appears, showing that superheavy nuclei could exist.

4. CHARGED METALLIC CLUSTERS

The energy of a charge distribution with a surface density σ_e [14, 45, 46] is

$$E_C[\sigma_e] = \frac{1}{2} \int \int \frac{\sigma_e(\mathbf{r}) \sigma_e(\mathbf{r}_1) d^2\mathbf{S} d^2\mathbf{S_1}}{|\mathbf{r} - \mathbf{r}_1|} \tag{69}$$

The distribution σ_e on the surface is obtained by minimizing the energy under the constraint

$$q = ze = \int \sigma_e(\mathbf{r}) d^2\mathbf{S} \tag{70}$$

i.e. the functional derivative

$$\frac{\delta(E - \lambda q)}{\delta \sigma_e} = \frac{1}{2} \int \frac{\sigma_e(\mathbf{r}_1) d^2\mathbf{S_1}}{|\mathbf{r} - \mathbf{r}_1|} - \lambda = 0 \tag{71}$$

The LDM Q-value, called also dissociation energy, may be calculated by adding a surface, Coulomb and ionization term

$$Q = Q_s + Q_C + Q_{IP}; \quad Q_{IP} = \frac{e^2}{8} \left(\frac{z_1}{R_1} + \frac{z_2}{R_2} - \frac{z}{R_0} \right) \tag{72}$$

$$Q_s = E_s^p - (E_s^1 + E_s^2); \quad Q_C = E_C^p - (E_C^1 + E_C^2) \tag{73}$$

where E_s^p, E_C^p are the surface and Coulomb energies of the (charged) parent (LDM + shell and pairing corrections) at the equilibrium deformation, and $E_s^i, E_C^i (i = 1, 2)$ are the similar quantities for the fragments.

In order to compute the Coulomb barrier one has to take into account the image

charge induced by a point charge outside a metallic sphere

$$E_{C-im} = \frac{z_1 z_2 e^2}{R} - \frac{z_2 e^2 R_1^3}{2R^2(R^2 - R_1^2)} \tag{74}$$

which differs from $E_C = z_1 z_2 e^2/R$. One assumes that $R_1 > R_2$.

In the classical image charge model [14, 41] a point charge q_2 at the distance R from the center of the conducting sphere with a radius R_1 and the charge q_1 will produce two image charges: one at the center of the sphere ($q_2 R_1/R$) and the other ($-q_2 R_1/R$) at the distance R_1^2/R, so that the total energy is expressed by the above equation. The maximum of the interaction energy is placed at the distance $R = R_m \simeq R_t + 2$ Å.

When an atomic cluster, M_N^{z+}, with N atoms is z times ionized, the number of its delocalized electrons left after ionization is $n_e = N - z$, where z is called the excess charge and N the size of the cluster. In the most frequently studied fission ("Coulomb explosion") process

$$M_N^{z+} \rightarrow M_{N_1}^{z_1+} + M_{N_2}^{z_2+} ; \quad n_e = n_{e1} + n_{e2} ; \quad z = z_1 + z_2$$

the parent is doubly charged ($z = +2$) hence the fragments are singly ionized: $z_1 = z_2 = 1$. The numbers of electrons are conserved: $N = N_1 + N_2$; $z = z_1 + z_2$; $n_e = N - z = n_{e1} + n_{e2}$; $n_{ei} = N_i - z_i$

For spherical shapes:

$$E_s^0 = 4\pi R_0^2 \sigma = a_s n_e^{2/3} = 4\pi r_s^2 n_e^{2/3} \sigma; \; E_{C-metal}^0 = z^2 e^2/(2R_0) = z^2 e^2/(2 r_s n_e^{1/3})$$

for a surface distribution of charge. The ratio to $E_C^0 = 3z^2 e^2/(5R_0)$ for bulk charge distribution is 5/6, *i.e.* 17 % smaller. σ is the surface tension and r_s is the Wigner-Seitz radius. Such material properties are tabulated [14, 19].

The fissility parameter

$$X = \frac{E_c^0}{2E_s^0} = \frac{e^2}{16\pi r_s^3 \sigma} \frac{z^2}{n_e} = \frac{n_c}{n_e} \tag{75}$$

for stability should be smaller than unity, *i.e.*

$$n_e > n_c = \frac{e^2 z^2}{16\pi r_s^3 \sigma} \tag{76}$$

Unlike in the nuclear case, where the stability of heavier nuclei is reduced, for charged atomic clusters with a given charge the unstable clusters are those with small number of delocalized electrons $n_e < n_c$.

In figure 1 we present the following possibilities: (*i*) $X < 1$; $Q < 0$; $B_f > 0$ – stable states; (*ii*) $X < 1$; $Q > 0$; $B_f > 0$ – metastable states; (*iii*) $X \geq 1$; $B_f \leq 0$ – unstable states. The released (dissociation) energy $Q = E^0 - (E_1 + E_2)$. When $Q > 0$ (exothermic reaction) the spontaneous fission is possible. For $Q < 0$ (endothermic re-

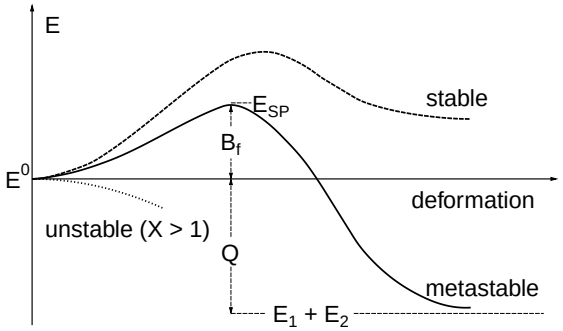

Fig. 1 – LDM deformation energy for stable, metastable, and unstable systems.

action) – induced fission: one has to excite the charged cluster to surpass the barrier. Fission barrier $B_f = E_{SP} - Q$; SP – saddle point. Fusion barrier may be approximated by $B_f + Q$.

In a metastable state the two fragments are temporarily held together by the potential barrier. There is a finite probability for the penetration of the barrier by the quantum-mechanical tunneling effect.

In conclusion the electrostatic energy of a spherical nucleus with a charge uniformly distributed in the volume is equal to $(Ze)^2/R_0$ times $3/5$ while the numerical coefficient is only $1/2$ for a metallic atomic cluster (with surface distribution of electric charge). The radius of a light spherical nucleus is of the order of few fm; the same quantity for a Na atomic cluster with few atoms is five orders of magnitude higher. Unlike in the nuclear case, where the fissility is proportional with Z^2/A and increases for heavier nuclei (hence superheavies are usually unstable within LDM), for charged atomic clusters fissility is expressed as n_c/n_e so it becomes larger for small number of delocalized electrons n_e.

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