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On the ternary fission of atomic clusters

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Abstract. – Comparison of ternary fission of the metallic cluster Na_{27}^{+++} into equal fragments with binary fission is made by use of the Shell Correction Method. We conclude that favourable fission barriers and energy releases of that tripartition along with some dynamical properties make ternary fission a very attractive process for further investigation.

Fission of atomic clusters is a modern problem where some concepts and methods originally developed for nuclear fission are adapted and applied. Tripartition is a special case of multi-fragmentation processes, which are energetically more favourable than binary fission [1], but which have never been observed in nuclei at low and intermediate energies [2].

Our purpose is to reflect this problem in the light of physics of fission of atomic clusters. Among several candidates for studying ternary fission, symmetric fission of Na_{27}^{+++} into three magic fragments looks very promissing, in view of its large energy release. For ternary fission we consider the decays:

$$Na_{27}^{+++} \to Na_{27-2\,p}^{+} + 2\,Na_{p}^{+} \ , \tag{1}$$

with $p = 9$ and 3, which we have compared with various binary processes,

$$Na_{27}^{+++} \to Na_{27-p}^{++} + Na_{p}^{+} \ . \tag{2}$$

It can be expected, therefore, that shell effects be very important in the case $p = 9$, playing a stabilizing role in the whole process.

Let us consider the energetics of the process as a first step towards understanding the physics involved. We may obtain a good estimate of the deformation energy using the Shell Correction Method (SCM). In this method, the total energy is the sum of an average energy, calculated in the Liquid Drop Model (LDM), and a shell correction term, given by Strutinsky's procedure. In the LDM, the energy consists of surface, curvature and Coulomb energies. We use the LDM parameters $\sigma = 2.94 \times 10^{-3}$ eV/bohr^2 for surface tension and $\gamma = 1.05 \times 10^{-2}$ eV/bohr for the curvature coefficient, obtained within the Stabilized Jellium Model. The latter is a simple modification of the Jellium Model which satisfies the condition of bulk stability [3]-[6].

TABLE I. – *Comparison of the binding energy per particle, E/N, cohesive energy, E_{coh}, and ionization energy, I, as calculated by the Shell Correction Method* (SCM), *and Kohn-Sham* (KS) *theory, in the Local Density Approximation, for spherical Stabilized Jellium clusters, compared to experiment. All energies are in* eV.

	Na_9			Na_9^+		
Method	E/N	E_{coh}	I	E/N	E_{coh}	I
SCM	−5.99	0.81	3.63	−5.59	0.40	8.10
KS	−5.91	0.75	3.44	−5.60	0.50	8.02
Exp.	—	0.67	4.01	—	—	—

For obtaining the shell correction we use a three-center harmonic-oscillator shell model. The value $\hbar\omega = 1.05$ eV is taken for the harmonic-oscillator parameter of the initial system. The method is known to work well for describing binding, cohesive and ionization energies of metal clusters. It gives results which are close to the results obtained by self-consistent quantal methods as the Kohn-Sham (KS) calculations for spherical jellium or stabilized jellium and to the experimental ones (*e.g.*, [4]-[7] and references therein). Some results for representative spherical sodium clusters —including products of our ternary fission— are presented in table I. The agreement of the SCM methods with KS results justifies the application of that method to the problem under consideration.

For the shape parameterization we choose three intersecting spheres with their centers along a straight line [8]. The collective coordinate is given by the distance between the centers of the outer fragments, d. We consider the outer fragments to be equal. Size asymmetry might be related to the number of atoms p in the outer fragments in the exit channel.

In nuclear physics, that configuration is preferable to the cloverleaf form [9]-[11]. This should also be true in our case because of the reduced Coulomb repulsion of the external fragments in

TABLE II. – *Calculated energy release, Q, and barrier heights, E_b, for some binary and ternary fission channels of* Na_{27}^{+++}. *Energies are in* eV.

Reaction	Q(LDM)	Q(SCM)	E_b(LDM)	E_b(SCM)
$3Na_9^+$	−3.12	−3.59	1.25	0.55
$Na_{21}^+ + 2\,Na_3^+$	−2.75	−1.79	0.80	
$Na_{24}^{++} + Na_3^+$	−2.38	−3.30	0.00	0.47
$Na_{22}^{++} + Na_5^+$	−2.41	−3.22	0.13	0.54
$Na_{18}^{++} + Na_9^+$	−2.19	−2.93	0.28	0.92

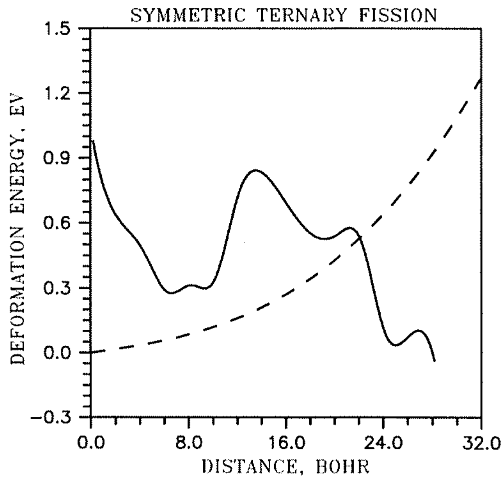

Fig. 1. – Deformation energy for the symmetric tripartition of Na_{27}^{+++} calculated within the Liquid Drop Model (LDM, broken line) and the Shell Correction Method (SCM, full line).

the linear configuration. Another reason comes from the dynamics, being noted below. Results of our calculations for the energy release Q and the barrier height E_b are presented in table II. The ternary processes are compared with some competing binary processes (channels $p = 3$, 5 and 9, where at least one fragment is magic). The values for binary fission are obtained using the asymmetric two-center shell model [5]. Symmetric tripartition has, as expected, the largest Q value, and a comparatively low barrier E_b. The strongly asymmetric exit channel with $p = 3$ has close values. Note the relevance of the shell correction. Binary channels have barriers similar to that of the most favourable ternary channel but lower energy releases. The former fact is in contrast to nuclear fission, where symmetric tripartition is characterized by essentially higher barriers [8], [9], [11]. It is a consequence of the strong stabilizing effect produced by the three closed shells. Account of the shell effect leads to an enhancement of the symmetric ternary fission in comparison with the binary one. The quantal correction lowers the fission barrier by a factor of two in the ternary case, while increasing it by 0.4–0.6 eV in the binary-fission processes.

In fig. 1 we plot the LDM and the total SCM energy as a function of the distance d for symmetric ternary fission up to the scission point. Due to the emergence of the final magic fragments, shell effects start to play a decisive role at the early stage of deformation, pushing the barrier downwards. As a result, the deformation energy has a maximum at $d \approx 14$ bohr, well before the separation point (32 bohr).

Regarding the dynamics of the problem, we note that nuclear binary fission occurs due to low-lying, pre-fission quadruple vibrations of the nuclear surface (*e.g.*, [12] and references therein). The ratio of the vibration energy to the barrier is around 1/8, so that the excitation of about 8–10 phonons is needed to overcome the barrier. For symmetric tripartition, our shape parameterization at the primary stage of fission is similar to hexadecapole deformations, within the applicability limits of spherical multipoles decomposition. It is worth noting that the cloverleaf form cannot be induced by pre-fission hexadecapole vibrations. In the case of the Na_{27}^{+++} cluster, the energies of pre-fission shape vibrations may be estimated in the LDM, assuming irrotational flow of an incompressible fluid [13]. This calculation gives $\hbar\omega_2 \approx 1.6 \times 10^{-3}$ eV and $\hbar\omega_4 \approx 10^{-2}$ eV, for the quadruple and hexadecupole oscillations, respectively. Therefore, the barrier-to-vibration-energy ratio is around 10^2–10^3. Large-amplitude collective motion of the ionic core towards fission involves a great number of vibration states, and thus can be described classically.

It is interesting to investigate cluster fission occurring as a result of exciting the plasma-type vibrations (*e.g.*, by laser radiation), in analogy with the photofission of nuclei from the giant dipole resonance. Note that, in the case of resonance between the plasmon mode and the laser frequency, the action of the externally applied radiation on the ionic core may be considerably enhanced. A similar effect takes place in atoms where the electron shell can play a resonator role (*e.g.*, [14] and references therein). We can consider a hydrodynamic description [15], allowing for both volume and surface electronic modes in metal clusters. This approach gives the well-known Mie modes, with energies $\hbar\omega_\ell^{\mathrm{Mie}} = \hbar\omega_{\mathrm{p}}\sqrt{\frac{\ell}{2\ell+1}}$ independent of the size of the spherical metal cluster, with ω_{p} the bulk plasmon frequency. For neutral sodium, the 2^+ plasmon energy is 3.75 eV, a value well above the barrier for both binary and ternary fission. The same applies to the 1^-, 3^- and the 4^+ plasmons, which have energies 3.42, 3.88, and 3.95 eV, respectively, also well above the barriers for both binary and ternary fission. This fact may affect the probability of multifragmentation, and increase the ternary-to-binary-fission probability ratio, in comparison with the nuclear case. A significant contribution to the ternary fission may be expected from the consecutive mechanism of multifragmentation [16]. Observation of fission from plasmon excitations in clusters would provide valuable information on how the excitation energy is transferred from the electronic vibration to the collective motion of the ionic core.

In conclusion, ternary fission of atomic clusters into comparable fragments is a new process of great interest. As in the nuclear case, the energy release for ternary fission turns out to be higher than for the binary case, but the barrier may be only lightly higher. Its further study shall help us to better understand the role of quantal effects in the fragmentation of finite Fermi systems.

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