Dynamics of the Coulomb explosion of composite clusters

E. Boella[1,2], B. Peiretti Paradisi[1], A. d'Angola[3], G. Coppa[1], L. O. Silva[2]

[1] *Dipartimento Energia, Politecnico di Torino, Torino, Italy*

[2] *GoLP/Instituto de Plasmas e Fusão Nuclear - Laboratório Associado, Instituto Superior Técnico, Lisboa, Portugal*

[3] *Scuola di Ingegneria, Università della Basilicata, Potenza, Italy*

Coulomb explosion of pure ion nanoplasmas is an important problem in the field of ultra intense laser-cluster interaction with relevance for plasma physics, fusion research [1, 2] and imaging by "diffraction before destruction" [3]. In the present paper, a study of Coulomb explosion in composite clusters consisting of two atomic species is presented. The work focuses on heavy-light systems made of hydride molecules composed by carbon and hydrogen, in order to collect valuable information for coherent diffractive imaging [4]. Numerical simulations have been performed by using the shell method [5] that, despite of its simplicity, allows one to capture all the relevant physics involved with a reduced computational time. Moreover, a theoretical model, which is useful for a deep comprehension of the explosion dynamics, has been developed; results have been compared with numerical simulations showing perfect agreement.

Numerical results

The explosion of a a pure ion sphere of initial radius $R_0 = 20\,\mathrm{nm}$ composed by $N_0 \simeq 4.5 \cdot 10^5$ ions for an initial density of $n_0 = 10^{22}\,\mathrm{cm}^{-3}$ has been modeled. The cluster is constituted by a mix of 30% carbon ions ionized once and 70% hydrogen ions, so that $m_C/m_H = 12$, $q_C/q_H = 1$ and $N_H/N_0 = 0.7$. At the initial time, ions are at rest and uniformly distributed in the sphere. The evolution of the electric field and the hydrogen density are shown in Fig. 1. At the initial time, hydrogen and carbon ions contribute to create a monotonic increasing electric field, which accelerates the H^+ ions more with respect to C^+ ions, because of their smaller mass to charge ratio. Consequently, the lighter particles can overtake the heavier ones and propagate ahead of them. The radial electric field, which has a linear behavior inside the bulk sphere of the C^+ ions, decreases approximately as $1/r^2$ outside. Therefore, faster light ions coming from the bulk tend to reach the ones initially on the periphery of the cluster, which are slower due to the decaying field, forming a thin hydrogen shell.

Analytical model

The species with a larger q/m moves faster with respect to the other, creating two concentric spherical regions, S_1 and S_2, with radius $R_1(t)$ and $R_2(t) \leq R_1(t)$. The sphere S_2 contains a mixture of light and heavy particles, R_2 representing the frontline of the heavy ions. Instead, the

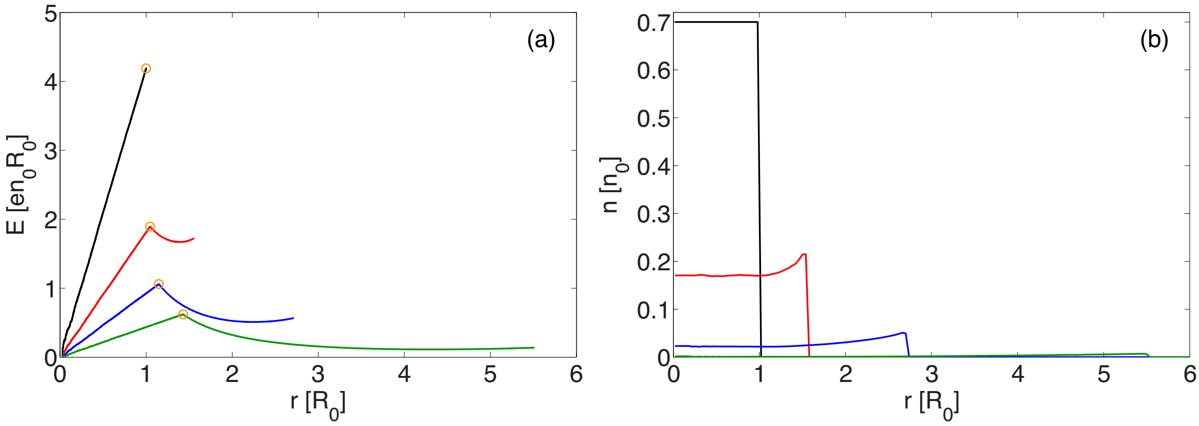

Figure 1: Coulomb explosion of a pure H^+ - C^+ (70-30%) cluster with $R_0 = 20\,\text{nm}$ and $n_0 = 10^{22}\,\text{cm}^{-3}$: electric field (a), hydrogen density (b) at $t = 0$ (black), 24 (red), 48 (blue), $96t_0$ (green) where $t_0 = \sqrt{m_e/e^2 n_0}$. The orange circles in (a) indicate the carbon ion front.

spherical shell outside S_2 contains only light particles and therefore R_1 is the frontline of the light ions. Simulations also indicate that the electric field is linear inside S_2 (Fig. 1a):

$$E(r,t) = A(t)r. \tag{1}$$

Using this assumption, the equation of motion for the light and the heavy ions inside S_2 can be written in a simple way. Starting with the light ions, until they do not cross the frontline of the heavy ions (i.e., when they are still in S_2), their motion is governed by the equation:

$$m_1 \frac{\partial^2 r_1}{\partial t^2} = q_1 A(t) r_1, \tag{2}$$

where $r_1(t,r_0)$ is the radial position at time t of a light ion with initial position r_0 and initial zero velocity. Introducing the dimensionless quantity $\xi(t) = r_1(t,r_0)/r_0$, the dependency on r_0 drops and Eq. (2) becomes

$$\frac{\mathrm{d}^2\xi}{\mathrm{d}t^2} = \frac{q_1}{m_1} A(t)\xi, \quad \xi(0) = 1, \quad \frac{\mathrm{d}\xi}{\mathrm{d}t}(0) = 0. \tag{3}$$

Similarly, the radial position, $r_2(t,r_0)$ of heavy ions (with initial position r_0 and initial zero velocity) can be written as $r_2(t,r_0) = r_0\eta(t)$, where $\eta(t)$ satisfies the equation:

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2} = \frac{q_2}{m_2} A(t)\eta, \quad \eta(0) = 1, \quad \frac{\mathrm{d}\eta}{\mathrm{d}t}(0) = 0. \tag{4}$$

The term $A(t)$ is computed considering that the electric field at $r = R_2$, according to the Gauss law, is given by

$$E(R_2(t),t) = \frac{Q(t)}{[R_2(t)]^2}, \tag{5}$$

where $Q(t) = Q_2 + Q_1(t)$ is the total charge in S_2 at time t, being Q_2 the charge of the heavy ions that at $t = 0$ were contained in the sphere of radius R_0 and $Q_1(t)$ the charge due to the light ions that at time t are in S_2

$$Q_2 = q_2 \frac{4\pi}{3} R_0^3 n_2(0), \tag{6}$$

$$Q_1(t) = q_1 \frac{4\pi}{3} [r_0(t)]^3 n_1(0), \tag{7}$$

with $r_0(t)$ defined as $r_0(t) = R_0\eta(t)/\xi(t)$, which ensures $r_1(t, r_0) = R_2(t)$. Making use of Eqs. (1,5-7), $A(t)$ can be written as

$$A(t) = \frac{4\pi}{3} \left(\frac{q_1 n_1(0)}{\xi^3(t)} + \frac{q_2 n_2(0)}{\eta^3(t)} \right). \tag{8}$$

Thus, the trajectories of the light and heavy ions inside S_2 are determined by solving the following system of equations

$$\begin{cases} \dfrac{d^2\xi}{dt^2} = \dfrac{4\pi}{3} \dfrac{q_1}{m_1} \left(\dfrac{q_1 n_1(0)}{\xi^3} + \dfrac{q_2 n_2(0)}{\eta^3} \right) \xi \\ \\ \dfrac{d^2\eta}{dt^2} = \dfrac{4\pi}{3} \dfrac{q_2}{m_2} \left(\dfrac{q_1 n_1(0)}{\xi^3} + \dfrac{q_2 n_2(0)}{\eta^3} \right) \eta. \end{cases} \tag{9}$$

The system (9) describes the trajectory of a light ion until the time $t_c(r_0)$, at which it reaches the front line of the heavy ions, i.e., $r_1(r_0, t_c) = R_2(t_c)$. Therefore, t_c can be calculated by solving the equation:

$$\frac{\eta(t_c)}{\xi(t_c)} = \frac{r_0}{R_0}. \tag{10}$$

The electric field for $r = r_1 \geq R_2$ can be computed as Q/r^2 where the quantity Q depends only on r_0 and is given by

$$Q(r_0) = \frac{4\pi}{3} \left(q_2 n_2(0) R_0^3 + q_1 n_1(0) r_0^3 \right). \tag{11}$$

The equation of motion for a light ion outside S_2 (i.e., for $t > t_c$) is

$$\frac{\partial^2 r}{\partial t^2} = \frac{q_1}{m_1} \frac{Q(r_0)}{r^2}, \quad r(t_c) = \eta(t_c) R_0, \quad \frac{\partial r}{\partial t}(t_c) = r_0 \frac{d\xi}{dt}(t_c). \tag{12}$$

Figure 2a shows the evolution of the frontline of the heavy and light ions for the same cluster considered in Fig. 1. Theoretical results have been compared with the ones obtained with the shell code, showing perfect agreement.

Equation (12) can be rewritten as

$$m_1 \frac{\partial^2 r}{\partial t^2} = -\frac{\partial}{\partial r} \left(\frac{q_1 Q(r_0)}{r} \right), \tag{13}$$

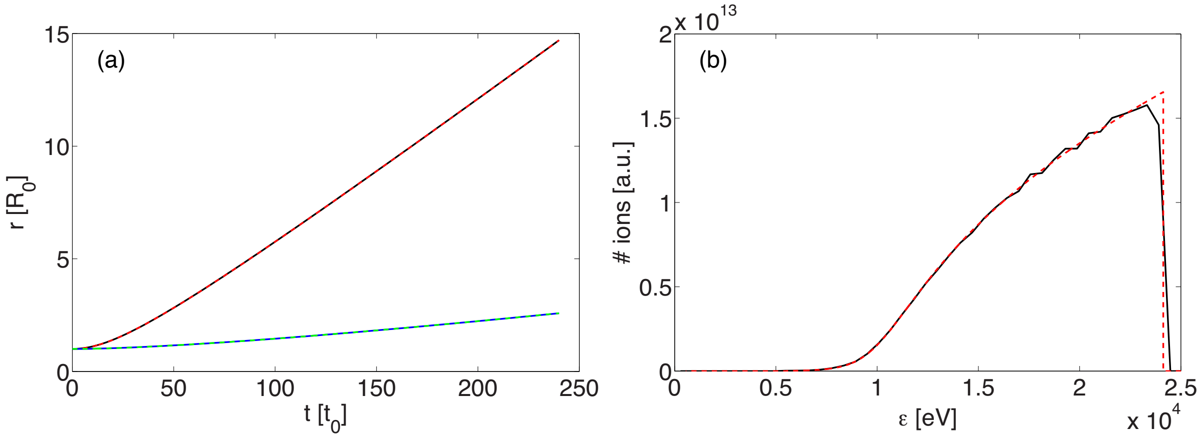

Figure 2: Frontline of the light (red dashed line) and heavy ions (green dashed line) versus time (a) and asymptotic energy spectrum (b) for the same cluster of Fig. 1. Theoretical results have been compared with numerical ones (solid black line and solid blue line).

and then integrated respect to t to compute the asymptotic kinetic energy (ε_∞) of the light ions

$$\varepsilon_\infty = \frac{1}{2} m_1 \left[\frac{\partial r}{\partial t}(t_c) \right]^2 + \frac{q_1 Q(r_0)}{r(t_c)}. \tag{14}$$

Figure 2b shows the asymptotic energy spectrum obtained with Eq. (14). Numerical results are also reported for comparison.

Conclusions

The Coulomb explosion of a sphere composed by two ion species has been studied with both a numerical and an analytical approach. The expansion dynamics shows peculiar differences with respect to the case of a homo-nuclear cluster composed by one ion species only. In particular, the non-monotonic electric field, in principle, could accelerate the light ions in a quasi-monoenergetic way. Preliminary result, if confirmed by future investigations, would represent a novelty, in contrast with the well known properties of Coulomb explosion of clusters composed by a single ion species, where the energy spectrum is much wider.

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