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Expansion of two-ion-species spherical plasmas as a source of mono-energetic ions

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The problem of collisionless expansion of two-species spherical plasma into vacuum is solved numerically by using of a spherical coordinate electrostatic particle code. A theoretical solution is also presented for the case of Coulomb explosion when light ions can be treated as an impurity. The expansion of the two-ion-species clusters is shown to be a source of high quality mono-energetic ions moving in the solid angle of 4π. Dependencies of the light ions parameters on the electron average energy and target composition are discussed. As example, two different target designs are compared.

Keywords: Mono-energetic ions, cluster expansion, Coulomb explosion, multi-flows.

1. Introduction

Interaction of a short laser pulse with spherical micro-targets is known to serve as a source of energetic ions [1, 2]. If the electric field in the laser pulse is much higher than the electrostatic Coulomb field of fully evacuated cluster ion core, this expansion can be described as a Coulomb explosion (CE) [3,4]. The condition for CE may be written as $I \gg (1/8\pi)cQ_0^2/R_0^4$, where I is the laser intensity, Q_0 is the full charge of the cluster, R_0 is its initial radius, and c is the speed of light. For smaller laser intensities, the finite charge of electrons must be accounted for. The best known model of plasma expansion in this case is the model of initially cold ions and hot electrons with thermal-like energy distribution. For quasi-neutral expansion of a plasma this problem was analytically solved in the kinetic approach for different initial plasma density profiles and electron distributions [5,6] whereas quasi-neutral self-similar hydrodynamic solutions have appeared a few decades ago [7, 8]. However, if the laser field is high enough to create an unbalanced charge inside the clusters, the quasi-neutral expansion model becomes inapplicable. In this case, more complicated hydrodynamic approaches [9, 10] or hybrid models [11, 12] for constructing approximate semi-analytical solutions were used.

Expansion of an inhomogeneous cluster can provide a spectrum of ions with monoenergetic peak [4, 13]. However, the number of such monoenergetic ions is small and the use of two-ion-species targets can considerably improve mono-energeticity [14, 15]. In such targets the light ions with the low charge accelerate in the field of the highly-charged heavy species, expand from the cluster as a shell and form quasi-monoenergetic spectrum under the Coulomb piston effect from the ion core. Although the heavy ions in the case of homogeneous cluster can be described hydrodynamically, the light ions appear to participate in multi-flows motion and thus have to be analyzed with a kinetic approach.

The exploding spherical target has maximum electric field on its boundary. For this reason, a good proposal for improving mono-energeticity is to form a double-layered target composed of the heavy core and a thin shell of light ions [16, 17]. We call such target design a heterogeneous cluster, and the target composed of uniformly mixed light and heavy ions is referred to as homogeneous.

An analysis of the two-species expansion with an impurity of the light species has been performed in the recently published paper [15]. In this work we present a simple analytical model for Coulomb explosion of a two-ion-species cluster having homogeneous impurity of light ions and results of numerical kinetic simulations of Coulomb explosion and non-neutral thermal-like expansion of spherical electron-ion target for an arbitrary light ions concentration. The fully kinetic particle simulations are done for both homogeneous and heterogeneous cases. We discuss dependencies of the light ions spectra on the electron temperature T_e, on the relative charge of light ions $\rho_0 = Q/Q_1$, where Q_1 and Q are, correspondingly, total charge of heavy and light ions in the target, and on the kinematic parameter $\mu = M_1 Z/M Z_1$, where M_1 and M are masses of heavy and light ions and Z_1 and Z are their charges. We also compare the energy spectra of light ions for the homogeneous and heterogeneous targets.

2. Coulomb explosion of a cluster with an impurity of light ions

In this section we present a simple analytical model of CE of a cluster with an impurity of light ions. In this model we consider $Zn \ll Z_1 n_1$ where n_1 and n are, correspondingly, particles density of light and heavy ions. This allows one to neglect the self-electric

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field of light ions and investigate their motion in the background (given) field of the heavy ions. The only controlling parameter which determines the motion of the light impurity is the kinematic parameter μ. The distribution function of light ions in the given electric field E of the heavy ions can be written as [4, 17]:

$$F(t,r,v) = \frac{1}{r^2}\int_0^1 \mathrm{d}h\, n_0 h^2 \cdot \delta[r - R(t,h)]\delta[v - U(t,h)]\,, \tag{1}$$

where functions R and U are solutions to

$$\begin{aligned} &R_t = U\,, U_t = eZE(t,R)/M\,, \\ &R|_{t=0} = h\,, U|_{t=0} = 0\,. \end{aligned} \tag{2}$$

In Eq.(2), h is the initial location of a light ion, and $R(h,t)$ and $U(h,t)$ are Lagrangian coordinate and velocity of light ions, t and r are time and spatial coordinates. The v in Eq.(1) stands for the radial velocity of the particles.

We use dimensionless coordinates with the time, radial coordinate, electric field, velocity, density and energy (temperature) measured in ω_{L1}^{-1}, R_0, $4\pi e Z_1 n_1 R_0$, $\omega_{L1} R_0$, n_1^0, $M_1 \omega_{L1}^2 R_0^2/2$ correspondingly, where n_1^0 is the initial particle density of the heavy ions and ω_{L1} is their initial plasma frequency. In these units the electric field is given by:

$$E(r,t) = \begin{cases} r/3\,, & r < r_1(t) \\ 1/3r^2\,, & r > r_1(t)\,, \end{cases} \tag{3}$$

where $r_1(t)$ is the coordinate of heavy ion front and can be found as a solution to the equation $\ddot{r_1} = 1/(3\,r_1^2)$ with initial condition $r_1|_{t=0} = R_0$. Once the solution to the Eq.(2) with the field (3) is obtained one can find density distribution and energy spectrum of the light ions using the following expressions:

$$\begin{aligned} n(t,R) &= \frac{(h/R(h,t))^2}{|\ \partial h/\partial R(h,t)\ |}\,, \\ \frac{dN}{d\varepsilon} &= \frac{3}{2}\ \frac{R^2\, n(t,R)}{U\ |\partial U/\partial R|}\,, \end{aligned} \tag{4}$$

where $n(R,t)$ is the light ion density normalized to its initial value n_0. Energy spectrum is normalized to unity ($\int_0^\infty d\varepsilon (dN/d\varepsilon) = 1$). In the expression for $dN/d\varepsilon$, spatial coordinate $R(U)$ should be taken as a function of velocity $U = \sqrt{\varepsilon}$. In case of more than one flow motion, density and energy distributions should be calculated by summing over different branches of $R(U)$ and $U(R)$.

There are two different solutions in the regions $R < r_1(t)$ and $R > r_1(t)$. In the region $R < r_1(t)$ the light particles appear distributed homogeneously with linear $U(R)$. In the region $R > r_1$ functions $U(R)$ and $R(U)$ have maxima $\mathrm{d}U/\mathrm{d}R = 0$ and $\mathrm{d}R/\mathrm{d}U = 0$ at some surfaces. This is responsible for formation

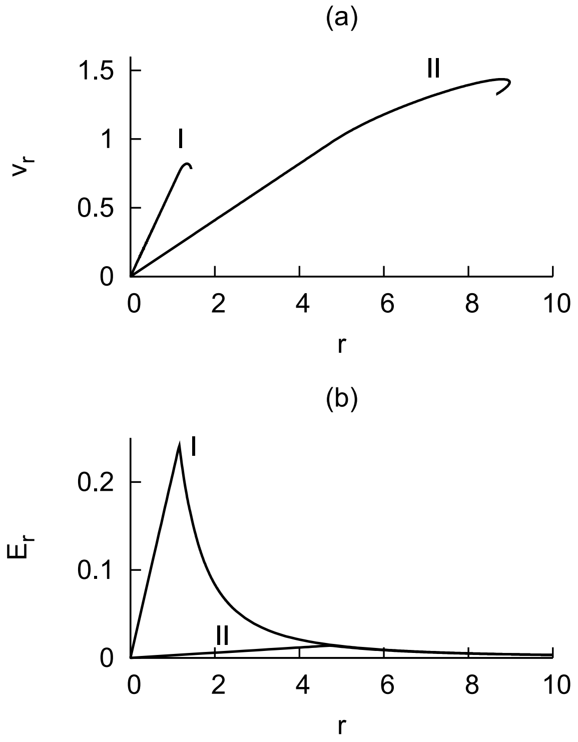

Fig. 1 Light ions in phase space (a) and electric field distribution (b) for $t = 1$ (lines I) and $t = 7$ (lines II).

of singularities in the light ions energy spectrum and density distribution. The positions of the light ions in the phase space for $\mu = 3$ along with the radial electric field distribution for time moments $t = 1$ and $t = 7$ are given in Fig.1a,b. It demonstrates the formation of the multi-flows region. The energy spectrum of light ions for $\mu = 3$ at $t \to \infty$ is given in Fig.2a by the solid line. The spectrum has a cut-off at $\varepsilon = \varepsilon_{max}$ and in its near vicinity the spectrum behaves as $(\varepsilon_{max} - \varepsilon)^{-1/2}$. The low energy part of the spectrum has square a root dependence on energy: $dN/d\varepsilon \propto \sqrt{\varepsilon}$. The spectrum has a break at $\varepsilon = \varepsilon^*$ which indicates the multi-flows region. We have obtained a simple fitting formula for the dependence $\varepsilon_{max}(\mu)$:

$$\varepsilon_{max} = \big[\mu - 1/3\big](M/M_1). \tag{5}$$

The case of $\mu = 3$ illustrated in Fig.1 corresponds, for example, to a $C^{+4}H^{+1}$ cluster which may be achieved by irradiation of a carbohydrate target by $\sim 10^{18}\,\mathrm{W/cm^2}$ laser. The diameter of the target may be of order 20 nm in this case for the Coulomb explosion or a high-temperature expansion process ($T \gtrsim 1$) to occur.

3. Thermal-like expansion of plasma targets having finite ρ_0

If ρ_0 is finite and electrons present, the self field of the light ions and electrons has to be accounted

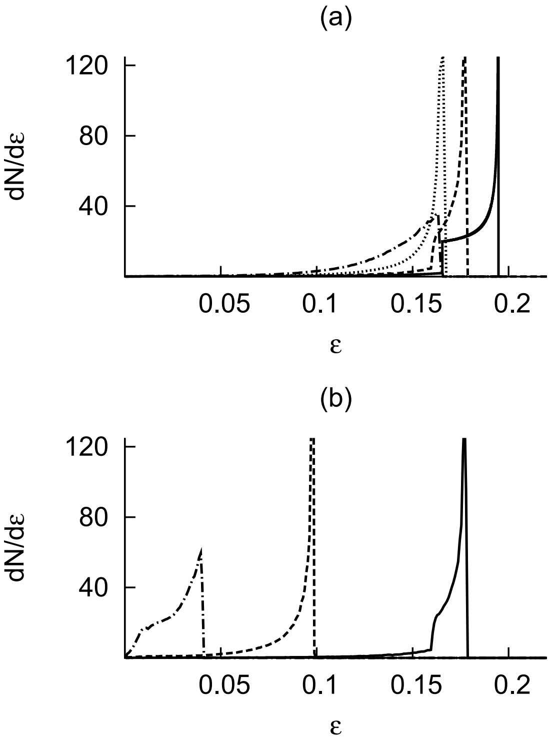

Fig. 2 Asymptotic energy spectra of light ions for $\mu = 3$. (a) Coulomb explosion with $\rho_0 \to 0$ (solid line), $\rho_0 = 0.33$ (dashed line), $\rho_0 = 0.5$ (dotted line) and $\rho_0 = 1$ (dash-dotted line). (b) $\rho_0 = 0.33$ and: Coulomb explosion (solid line), $T = 0.3$ (dashed line), $T = 0.05$ (dash-dotted line).

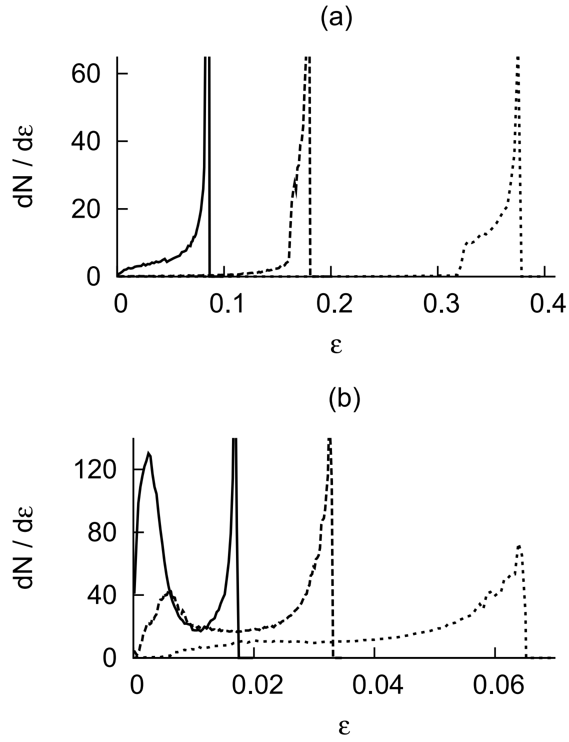

Fig. 3 Asymptotic energy spectra of light ions for $\rho = 1/6$ and CE (a) and $T = 0.05$ (b). $\mu = 1.5$ (solid lines), $\mu = 3$ (dashed lines), $\mu = 6$ (dotted lines).

for. For this purpose, we have employed a 1D electrostatic spherical gridless particle code in which the ions and electrons move in a self-consistent field. The electrons in our model have an initial 3D Maxwellian distribution characterized by a dimensionless temperature T. The case of Coulomb explosion corresponds to $T \to \infty$. The code has been tested on the known analytical and semi-analytical solutions for expansion of one-species plasma in different temperature regimes [4, 6, 12] and the analytical solution for the two-ion-species Coulomb explosion presented in Sec. 2.

The resulting spectra of light ions for Coulomb explosion of the cluster having finite ρ_0 are given in Fig.2a. The spectrum improves for modest values of ρ_0. This is caused by the fact that for small ρ_0, when the light ions can be considered as impurity, the light particles from the inside of the cluster acquire higher energy than those from its boundary. This results in a somewhat broader spectrum (solid line in Fig.2a). For larger ρ_0 the self field of the light ions partially compensates this difference providing a better monoenergeticity. If ρ_0 further increases, the light particles from the inside cannot overtake the ions from the near boundary domain that results in a single flow motion and broadening of the spectrum. This is accompanied by the disappearance of the singularity in the spectrum. Defining the spectrum width $\Delta\varepsilon = \varepsilon_{max} - \varepsilon_{min}$ in such a way that $dN/d\varepsilon(\varepsilon_{min}) = 2N/\overline{\varepsilon}$, where N is the total number of particles and $\overline{\varepsilon}$ is the average energy, we have found that the for CE case with $\rho \approx 0.4$, the value of $\Delta\varepsilon$ is less than 8%, with 90% of the light particles being inside this width.

The monoenergeticity also holds for finite temperatures. As the temperature drops, the charge of electrons partially balances the positive charge of ions. This leads to a smaller value of ε_{max}. If the electron Debye radius is λ_D, an estimation for the number of electrons inside the ion core is $Q_e \propto Q_1(R/(R+\lambda_D))^3$. In this way, a generalization of formula (5) to a case of finite (but not too low) temperature is

$$\varepsilon_{max} = \big(1 - (\frac{1}{1+\sqrt{T/2}})^3\big)\,[\mu - 1/3]\,\frac{M}{M_1}. \quad (6)$$

This estimation matches the results of simulations with 20% accuracy for electron temperatures $T \gtrsim 1/5$. For smaller temperatures one has to use the results of the numerical simulations.

The less the T the less the ρ_0 at which the multi-flows regime disappears. For example, for $T = 0.05$ this happens at $\rho \approx 0.15$ while for CE case the motion becomes a single-flow at $\rho_0 \approx 0.6$. The spectra of the light ions for finite temperatures and $\rho_0 = 0.33$, $\mu = 3$ are given in Fig.2b. The spectrum for $T = 0.05$ does

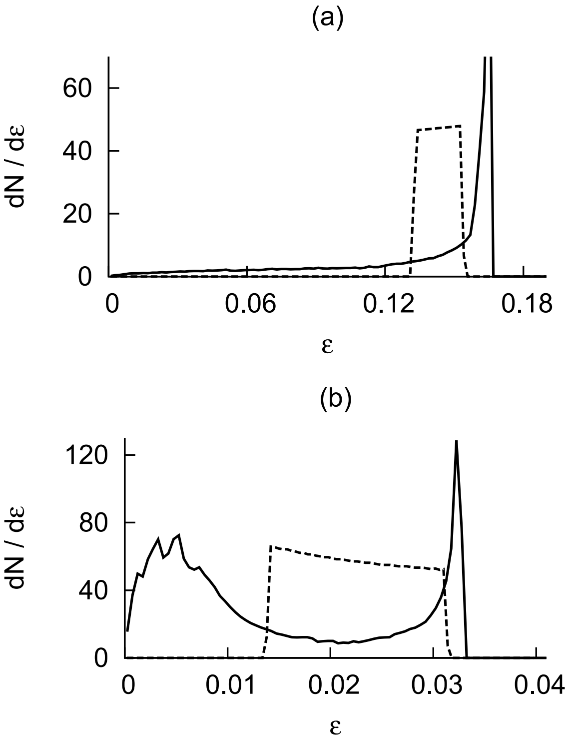

Fig. 4 Spectra of homogeneous (solid lines) and heterogeneous (dashed lines) compositions of the targets. $\mu = 3$, $\rho_0 = 0.33$, $t = 10$. (a) Coulomb explosion regime; (b) $T = 0.05$.

not have a singularity for such high ρ_0 but still can be considered as quasi-monoenergetic. A quantitative estimation shows that almost 1/4 of the light ions are concentrated within 10% energy spread for this case.

The dependence of the asymptotic spectra on μ for CE and a finite temperature and $\rho_0 = 1/6$ is illustrated in Fig.3. For both cases of finite and infinite temperatures the value of ε_{max} increases with increasing of μ (cf. Eqs.(5), (6) for $\rho \to 0$). As μ increases, the number of monoenergetic particles raises for both CE and $T > 0.05$ cases whereas the monoenergetic part of the spectrum broadens. This can be easily understood if one consider $\rho \to 0$: for both $\mu = 1$ and $\mu \to \infty$ the spectrum is broad. In this way, a moderate $\mu \approx 2 - 3$ is most appropriate for obtaining a high number of monoenergetic ions. The physical reason for this effect is the Coulomb piston acting on the light ions.

Let us now consider different target structuring. As was mentioned above, a heterogeneous target ([16,17]) should provide a high energy of the light ions because the light particles are initially located in the narrow domain near the maximum electric field. The small thickness of the layer is a factor of good monoenergeticity. For example, if $\rho_0 = 1/3$, $\mu = 3$ and mass densities of the species are approximately equal to each other, the thickness of the light ions layer is only 3-4% of the cluster radius. However, as follows from Fig.4, a homogeneous target with the same ρ_0 does not worsen the particle monoenergeticity and provides an even higher maximum energy for both CE and thermal-like regimes. It is obvious that the manufacture of homogeneous micro-targets is simpler that offers an advantage of their practical use.

4. Conclusion

In this paper, we have presented a theoretical description of Coulomb explosion for a two-ion-species spherical target with an impurity of light ions. A more general case of thermal-like expansion into vacuum of two-ion-species spherical targets with finite light ion concentration is described numerically from a unified approach. We have generally found that for a broad range of electron temperatures $0.05 < T \leq \infty$ and relative light ion charge the ion spectrum is narrow, with up to $70 - 90\%$ of the light ion particles being monoenergetic. We have also compared two different types of the targets and demonstrated the effectiveness of the simple homogeneous composition.

The analysis has shown that the two-ion-species clusters can serve as a source of mono-energetic ions. This can be employed, for instance, in optimization of laser triggered nuclear reactions in a cluster gas [18].

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