N-body simulation of nanoplasmas

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Introduction

The interaction of ultraintense lasers with atomic or molecular clusters leads to the formation of approximately spherical nanoplasmas [1] composed by $10^2 \div 10^4$ ions and electrons. These plasmas expand into vacuum [2], ranging from quasi-neutral plasma expansion to pure Coulomb explosion [3]. In any case, Vlasov-Poisson kinetic model is considered the rigorous way of studying this phenomenon [4]. In fact, kinetic theory applies to systems with an extremely large set of particles, while nanoplasmas are composed by a number of particles that ranges from some hundreds to few thousands. Can the standard kinetic theory be adopted in this case? To answer this question, a particular physical problem is considered here: the charging transient that occurs at the beginning of the cluster expansion. More specifically, the dynamics of a spherical nanoplasma is studied, in which ions are immobile and uniformly distributed while the initial distribution of electrons is assumed to be Maxwellian. These nanoplasmas are weakly coupled and, consequently, collisions do not seriously interfere with phenomena occurring on a time scale of the order of the inverse of the plasma frequency. For the physical situations examined here, the ratio between the electron collision frequency and the electron plasma frequency is in the range $3 \cdot 10^{-2} \div 10^{-3}$ (for temperatures of the order of 10^2 - 10^3 eV). In the work, reference solutions for the Vlasov equation are compared with results obtained by solving the exact equations of motion for the real set of interacting particles, for which ensemble averages have been utilized in order to take into account the different initial positions and velocities.

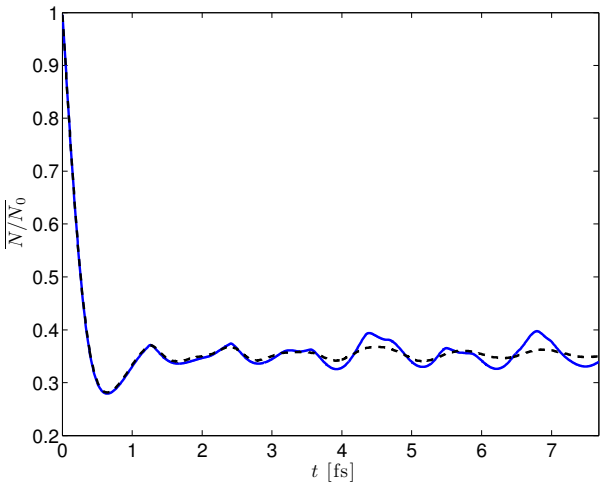

Figure 1: Time evolution of the fraction of electrons inside a cluster of radius $R = 2.28$ nm obtained with the Vlasov-Poisson model. In the calculations, $N_0 = 500$, $N_p = 100$ (dashed line), $5 \cdot 10^3$ and $5 \cdot 10^5$ (full lines) and $M = 10^3$.

Reference solution of the Vlasov-Poisson model

Reference solutions of the Vlasov-Poisson model are here obtained by using a particle-based, gridless algorithm, the shell model [5], developed by the Authors. By resorting to the spherical symmetry of the system, a purely radial electric field is calculated and the collisionality is strongly reduced with a reasonable number N_p of computational particles, so reducing considerably the computational time. In the calculations, initial positions and velocities $\mathbf{x}_{i0}, \mathbf{v}_{i0}$ of the computational particles are assigned by using pseudorandom numbers, considering that electrons are uniformly distributed in space inside a sphere of radius R and with a Gaussian distribution in the velocity space with a variance $v_{th} = (k_B T)^{1/2}$. The electron dynamics is simply described by the following equations

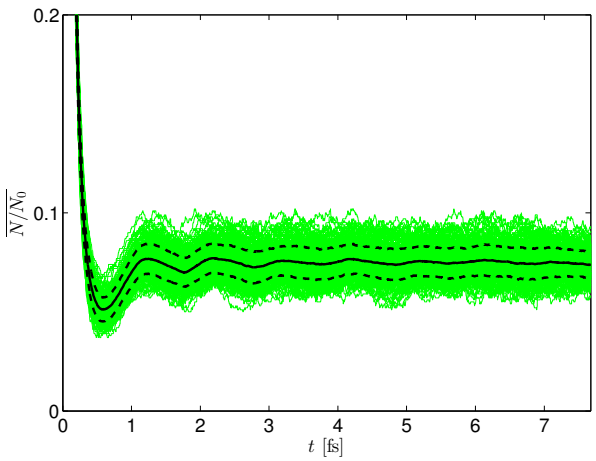

Figure 2: Time evolution of the fraction of electrons inside a cluster of radius $R = 2.29$ nm with the N-body simulations. In the calculations $N_0 = 10^3$, $n = 10^{28}$ m^{-3}, $T = 10^3$ eV and $M = 250$. Ensemble average (full line), single calculations (green) and standard deviation range (dashed lines) are reported.

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \qquad \frac{d\mathbf{v}_i}{dt} = -\frac{e}{m}\mathbf{E}(r_i,t), \qquad i = 1,2,...,N_p \tag{1}$$

The electric field $\mathbf{E}(r_i,t)$ is calculated assuming that each computational particle behaves like a spherical shell of radius r_i. With this assumption, $\mathbf{E}(r_i,t)$ depends on the total charge due to the shells located at $r \leq r_i$

$$\mathbf{E}(r_i) = \mathbf{E}_{ion}(r_i) - q\frac{[N(r_i) - 1/2]}{r_i^2}\mathbf{e}_r, \qquad \mathbf{E}_{ion}(r) = eN_0 \min\left(\frac{r}{R^3}, \frac{1}{r^2},\right)\mathbf{e}_r \tag{2}$$

where q is the charge of each computational particle and $N(r_i)$ the number of computational particles located inside a sphere of radius r_i. The hypothesis of spherical symmetry of the electric field, which is exact in the limit of $N_p \to +\infty$, reduces considerably the collisionality, as point-like particle interactions are excluded. Moreover, the calculation of the electric field is extremely fast. The solution of the Vlasov equation is obtained as the limit for $N_p \to +\infty$. This is clearly shown in Fig. 1, in which the time evolution of the fraction of electrons inside

composed by $N_p = 100$, $5 \cdot 10^3$ and $5 \cdot 10^5$ computational particles is considered. The results obtained for $N_p = 5 \cdot 10^3$ and $5 \cdot 10^5$ are practically indistinguishable, showing the convergence of the method to the solution of the Vlasov equation. This convergence study on the number N_p of computational particles has been verified for each result here presented.

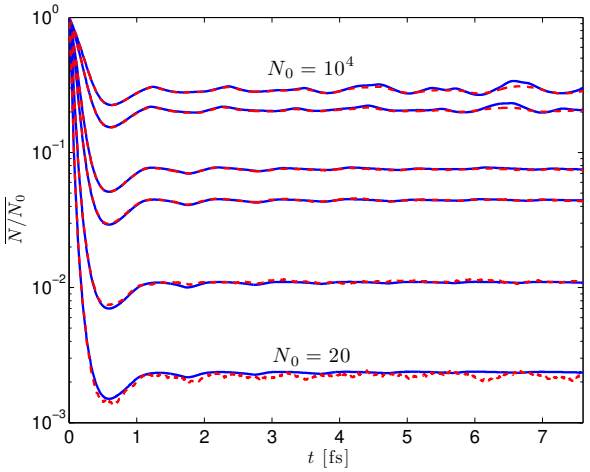

Figure 3: Time evolution of the fraction of electrons inside the clusters for N_0=20, 100, 500, 10^3, $5{\cdot}10^3$, 10^4, $n = 10^{28}$ m^{-3} and $T = 10^3$ eV. The exact solutions (dashed lines) are compared with the ones obtained with the Vlasov model (full lines).

N-body simulation of the electron dynamics

An accurate solution of the expansion of electrons is obtained solving numerically the system of equations of motion where the Coulomb force acting on each electron is due to the uniform positive charge of the immobile ions and to the exact contribution of the other electrons:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \qquad \frac{d\mathbf{v}_i}{dt} = \sum_{j \neq i} \frac{e^2}{m} \frac{\mathbf{x}_i - \mathbf{x}_j}{r_{ij}^3} - \frac{e}{m} \mathbf{E}_{ion}(r_i) \tag{3}$$

The electron velocities $\{\mathbf{v}_{i0}\}$ are initially distributed according to the Maxwell-Boltzmann distribution while the space distribution $\{\mathbf{x}_{i0}\}$ is uniform. Moreover, ensemble averages have been obtained considering M calculations in which initial conditions of electrons change by using pseudorandom numbers. Any macroscopic quantity of the system $\mathscr{P}^{(\alpha)}$ calculated at time t will be a function of the α-th set of initial conditions $\{\mathbf{x}_{i0}^{(\alpha)}\}, \{\mathbf{v}_{i0}^{(\alpha)}\}$, and ensemble averages and variances are estimated as

$$\overline{\mathscr{P}}(t) = \frac{1}{M} \sum_{\alpha=1}^{M} \mathscr{P}^{(\alpha)}, \qquad \sigma_{\mathscr{P}}^2(t) \simeq \frac{1}{M-1} \sum_{\alpha=1}^{M} \left[\mathscr{P}^{(\alpha)}(t) - \overline{\mathscr{P}}(t) \right]^2 \tag{4}$$

The standard deviation $\sigma_{\mathscr{P}}$ shows dispersion of $\mathscr{P}^{(\alpha)}$ values from the average and one can say that a significative number of $\mathscr{P}^{(\alpha)}$ lies in the interval $\left[\overline{\mathscr{P}} - 2\sigma_{\mathscr{P}}, \overline{\mathscr{P}} + 2\sigma_{\mathscr{P}}\right]$. The ensemble average $\overline{\mathscr{P}}$ converges to the expected value $\langle \mathscr{P} \rangle$ as $M^{-1/2}$, being $\hat{\sigma}_M = \sigma_{\mathscr{P}}/\sqrt{M}$ an estimator of the statistical error of $\overline{\mathscr{P}}$ which lies in the interval $[\langle \mathscr{P} \rangle - 2\hat{\sigma}_M, \langle \mathscr{P} \rangle + 2\hat{\sigma}_M]$ with probability 0.95. Figure 2 shows the time evolution of the ensemble average of the fraction of electrons inside the cluster of radius $R = 2.88$ nm ($N_0 = 10^3$, $n = 10^{28}$ m^{-3}, $T = 10^3$ eV, $\varepsilon_p = 3 \cdot 10^{-3}$),

obtained solving the equations of motion with $M = 250$ different initial conditions; in the figure, the interval $[\overline{\mathscr{P}} - \sigma_{\mathscr{P}}, \overline{\mathscr{P}} + \sigma_{\mathscr{P}}]$ is also reported along with all the corresponding results of the M calculations obtained with different initial conditions.

Comparison between Vlasov-Poisson model and N-body simulation

Examples of the expansion of nanoplasma in the initial stage, in which only electrons are involved, are presented and discussed, comparing results obtained with a N-body simulation with the corresponding reference solutions of the Vlasov-Poisson model. Clusters with $n = 10^{28}$ m^{-3}, N_0= 20, 100, 500, 10^3, $2{\cdot}10^3$, $5{\cdot}10^3$, 10^4 electrons and temperatures $T = 10^2, 10^3$ eV have been considered (the radius of clusters R varies from 0.78 and 6.2 nm and the plasma parameter between $3{\cdot}10^{-2}$ (10^2 eV) - $3\cdot10^{-3}$ (10^3 eV). In Figs. 3 and 4 the time evolution of the ensemble averages of the fraction of electrons inside clusters of radius R are represented for $T = 10^2$ and 10^3 eV for different initial number of electrons N_0. From the comparison, one can observe that, in the collisionless case, the charge transient exhibits small-amplitude oscillations while in the "exact" model the oscillations are damped and the system reaches an equilibrium configuration.

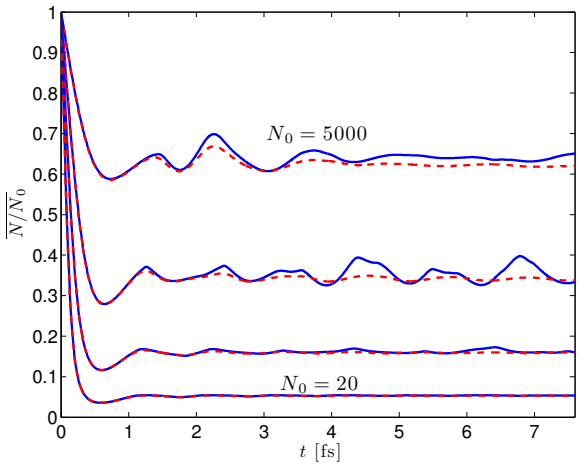

Figure 4: Same as Fig. 3 , with N_0=20, 100, 500, $5{\cdot}10^3$, $T = 100$ eV.

The results of the present work indicate that nanoplasma dynamics should not be uniquely analyzed by means of the collisionless kinetic theory. In fact the collisionless kinetic model is in good agreement with the exact solutions of the equation of motion, as far as mean values are considered; however, in a single experiment the calculated value may differ significantly from the average.

References

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