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Particle-in-cell Simulation of Processes in the Electron Gas

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Elementary interaction processes of charged particles in an electron beam with a current of about 1 A are studied numerically concerning the electron cooling problem. A one-dimensional particle-in-cell code is used to consider the following processes: expansion of the free electron gas, temperature equalization in the electron gas, natural oscillations in quasi electron-positron and electron-proton gases. In this method, the free electron gas expands due to electrostatic repulsion between electrons at a constant total energy. The model of a free electron gas represented by computational particles in the form of endless plates is also solved analytically. In this case, the velocity deviation as a function of time and the distance between the charge centers of the two halves of the electron gas are found analytically. And this is compared with the result of the numerical calculation. If the electron gas is represented as two subsystems with different temperatures, this leads to temperature equalization in the simulation. The paper considers several cases with different initial temperature conditions and finds the relaxation time. The simulation result of electron-positron and electron-proton gases shows that their oscillations are accompanied by Landau damping. The spectral frequency distribution of these oscillations shows the maxima that correspond to theoretical estimates.

Keywords: Particle-in-cell, Kinetics, Plasma, Natural oscillations, Simulation.

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1. INTRODUCTION

The method of electron cooling is widely used but it also remains a source of theoretical and experimental research [1-5]. In particular, at the future facility FAIR (Facility for Antiproton and Ion Research) it is planned to exploit a storage ring of antiprotons at the HESR machine using an electron cooler with relativistic electrons. In 1988, a significant difference was shown experimentally in the processes of electron cooling of negatively and positively charged particles [1]. However, there is not a complete theory of electron cooling for negatively charged ions.

The difficulties of analytical methods are determined by a rather complicated mathematical formulation. Support by numerical methods allows obtaining fairly complete information about the system.

It is advisable to choose the Particle-In-Cell (PIC) method as a numerical solution for the electron cooling problem [6-9]. In this method, individual particles in a Lagrangian frame are tracked in continuous phase space, whereas moments of the distribution such as densities and currents are calculated simultaneously on Eulerian mesh points.

The paper presents the results of simulation of the processes performed using the PIC code created manually: expansion of the free electron gas, temperature equalization in the electron gas, natural oscillations in quasi electron-positron and electron-proton gases. The paper analyzes the simulation results and compares them with known theoretical formulas.

2. METHOD DETAILS

Electron cooling uses magnetized gas, so the Larmor radius is considerably shorter than the distance between particles. On the one hand, this prevents transverse expansion due to Coulomb repulsion, and on the other hand, it leads to rapid cooling [1]. Under such conditions, the one-dimensional motion approximation is applicable that implies the suppression of transverse motion due to a strong magnetic field.

The model of a one-dimensional gas is governed by the Vlasov and Poisson equations [9]:

$$\frac{\partial f_s}{\partial t} + v\frac{\partial f_s}{\partial x} + \frac{q_s}{m_s}E\frac{\partial f_s}{\partial v} = I\,,$$

$$\nabla^2\varphi = -\frac{\rho}{\varepsilon_0}\,, \qquad (1)$$

where $f_s(t, x, v)$ is the phase space distribution function for a given species s; m_s and q_s are the charge and mass of the species, respectively; E is the electric field; φ is the electric potential; ρ is the electric charge density, and I is the Boltzmann collision integral. Pair collisions in the problems under consideration can be neglected, therefore $I = 0$.

The Vlasov equation is solved by the PIC method in which the distribution function $f_s(t, x, v)$ is given by the superposition of computational particles [8]:

$$f_s = \sum_p f_p = \sum_p N_p \delta\left(v - v_p\right)\frac{1}{\Delta_p} b_1\left(\frac{x - x_p}{\Delta_p}\right),$$

where f_p is the distribution function for the computational particles, N_p is the number of physical particles that are present in the computational particle, b_1 is the first-order B-spline function, Δ_p is the size of computational particles, x_p and v_p are the position and velocity of the computational particles, respectively.

Equation (1) can be discretized using the three-point formula:

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$$\varepsilon_0 \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{\Delta x^2} = -\rho_i ,$$

where Δx is the cell size, the densities ρ_i are defined as average over the cells:

$$\rho_i = \sum_p \frac{q_s N_p}{\Delta x} b_1\left(\frac{x_i - x_p}{\Delta_p}\right).$$

The evolution equations are obtained by taking the corresponding moments of the Vlasov equation [8]:

$$N_p m_s \frac{dv_p}{dt} = N_p q_s E_p , \quad \frac{dx_p}{dt} = v_p , \quad \frac{dN_p}{dt} = 0 , \quad (2)$$

where E_p is the average electric field acting on the computational particle.

To achieve the goal of solving equation (2), the so-called leap-frog algorithm is used:

$$\left(x_p^{n+1} - x_p^n\right) / \Delta t = v_p^{n+1/2},$$

$$\left(v_p^{n+3/2} - v_p^{n+1/2}\right) / \Delta t = \frac{q_s}{m_s} E_p\left(x_p^{n+1}\right),$$

where n is the time level.

3. SIMULATION

3.1 Expansion of the Electron Gas

The subsection considers an expansion of the free electron gas using the PIC simulation. We find changes in velocity variance, density, kinetic and potential energies of the gas over time and compare the expansion dynamics obtained by modeling with theory.

The electron gas is not in thermodynamic equilibrium, so the concept of temperature does not apply to it. The quantity T_e will be called the initial temperature (traditionally for beam physics), which implies velocity spread.

At the initial time, the electron concentration is n_e and the velocity deviation is

$$v_0 = \sqrt{k_B T_e / m_e} , \quad (3)$$

where k_B is the Boltzmann constant, m_e is the electron rest mass.

In the framework of the PIC method, the gas is represented by $N = 1000$ computational particles. Each computational particle consists of N_e electrons and has the shape of an infinite plate with width

$$x_0 = \sqrt{\varepsilon_0 k_B T_e / \mathrm{e}^2 n_e} , \quad (4)$$

where e is the electron charge.

The initial velocities of the computational particles are drawn from a Gaussian distribution using an algorithm based on the classical central limit theorem. The mean of the distribution is

$$\mu \approx 0 . \quad (5)$$

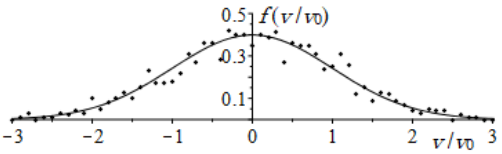

Fig. 1 – Typical velocity distribution function of the electron gas at the initial time

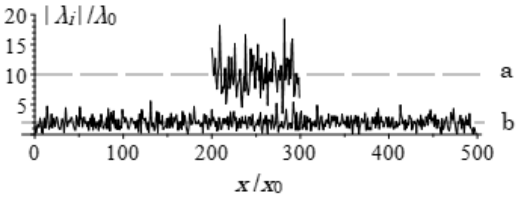

Fig. 2 – Absolute charge density of the electron gas at $t = 0$ (a) and $t = 2.8t_0$ (b)

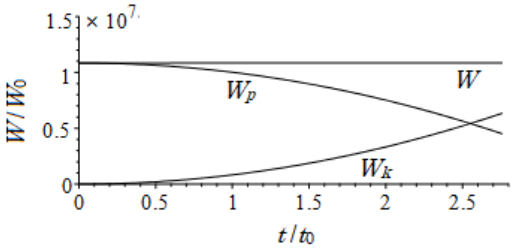

Fig. 3 – Change in kinetic, potential, total energy of the electron gas over time

Fig. 1 shows the initial velocity distribution of the gas (the dots) compared to the standard normal distribution (the solid line) with its deviation $\sigma = 1$ and expectation $\mu = 0$.

The particles are initially distributed randomly in the space area:

$$x_{t=0} \in \left[200x_0, 300x_0\right]. \quad (6)$$

Fig. 2a shows the dimensionless average absolute value of the linear charge density of the grid cells $|\lambda_i|/\lambda_0$ at the initial time. The density is measured in $\lambda_0 = N_e |e| / \Delta x$, where $\Delta x = x_0$ is the cell size. During the simulation, the gas expands symmetrically into the area $x_{\text{end}} \in [0, 500x_0]$ in time $t = 2.8t_0$ (Fig. 2b), where

$$t_0 = \sqrt{\varepsilon_0 m_e / e^2 n_e} . \quad (7)$$

The time level is $\Delta t = 0.001t_0$. The dashed line in Fig. 2 denotes the average absolute density of the gas.

As can be seen from Fig. 2, the free electron gas expands due to electrostatic repulsion between electrons. A 5-fold expansion along the axis is accompanied by a 2.5-fold decrease in the charge density.

For a more detailed understanding of the expansion dynamics, we determine the kinetic energy W_k, potential energy W_p, and total energy W at each time step in the simulation. The functions W_k, W_p, W, as functions of time, are shown in Fig. 3. Time is measured in t_0 (7). Energy is measured in $W_0 = N_e m_e v_0^2/2$.

From Fig. 3, over time, the kinetic energy of electrons increases, and the potential energy decreases at a constant total energy, i.e., expansion of the electron gas is a thermodynamically non-equilibrium process.

The gas model represented by computational particles in the form of endless plates can be described analytically. In this case, we find a change in velocity deviation over time and compare it with the result of numerical calculation.

Let r_{i0} be the initial position of the plates (computational particles), where $i = 1, 2, ..., N$. We assume that half of the plates is on the left side relative to the center of the area (6): $r_{i0} < 250x_0$, $i = 1, 2, ..., N/2$. So, the other half is on the right side: $r_{i0} > 250x_0$, $i = N/2$, and $N/2 + 1, ..., N$. Then the equations of motion for the i^{th} particle are

$$\begin{cases} (N+1-2i)F = -ma_i \left(i = 1,2,...,\dfrac{N}{2} \right), \\ (2N+1-2i)F = ma_i \left(i = \dfrac{N}{2}, \dfrac{N}{2}+1,...,N \right), \\ a_i = -a_{i+N/2} \left(i = 1,2,...,\dfrac{N}{2} \right), F = \dfrac{q^2}{2\varepsilon_0 S}, \end{cases} \quad (8)$$

where m, q, S are the mass, charge, and area of the plate, respectively; a_i is the acceleration.

The velocity of the particle is $v_i = v_{i0} + a_i t$, where v_{i0} is the initial velocity. So,

$$\begin{cases} v_i = v_{i0} - \dfrac{(N+1-2i)q^2 t}{2\varepsilon_0 Sm} \left(i = 1,...,\dfrac{N}{2} \right), \\ v_i = v_{i0} - \dfrac{(2N+1-2i)q^2 t}{2\varepsilon_0 Sm} \left(i = \dfrac{N}{2},...,N \right). \end{cases}$$

Taking into account the symmetry of the acceleration a_i and the fact that the average initial velocity $\langle v_{i0} \rangle \equiv \mu \approx 0$ (5), the average particle velocity $\langle v_i \rangle = 0$. Based on this and the equality $\langle v_{i0}^2 \rangle = \langle v_0^2 \rangle$, the velocity variance is:

$$\sigma^2 = v_0^2 + \frac{N^2 - 1}{3} \left(\frac{q^2}{2\varepsilon_0 Sm} t \right)^2. \quad (9)$$

The dimensionless version of Eq. (9):

$$\sigma^2 / v_0^2 = 1 + \frac{2500}{3} (t / t_0)^2, \quad (10)$$

where time is measured in t_0 (7), velocity is measured in v_0 (3).

The change in time of the distance between charge centers of two halves of the electron gas can also be described analytically.

If R_1 is the center of charge of the left half and R_2 is the center of charge of the right half, then

$$\frac{N}{2} R_1 = \sum_{i=1}^{N/2} r_i \,, \quad \frac{N}{2} R_2 = \sum_{i=N/2}^{N} r_i \,, \quad (11)$$

where r_i are the positions of computational particles at time t, which are described by the equations

$$\begin{cases} r_i = r_{i0} - \dfrac{a_i t^2}{2} \left(i = 1,2,...,\dfrac{N}{2} \right), \\ r_i = r_{i0} + \dfrac{a_i t^2}{2} \left(i = \dfrac{N}{2}, \dfrac{N}{2}+1,...,N \right). \end{cases} \quad (12)$$

Based on (8), (11) and (12), the distance between the centers R is represented as:

$$R = R_2 - R_1 = R_0 + \frac{q^2 N}{4\varepsilon_0 Sm} t^2, \quad (13)$$

where $R_0 = R_{20} - R_{10}$ is the distance between the centers at the initial time. From (6), $R_0 = 50x_0$.

The dimensionless version of Eq. (13) is

$$\frac{R}{x_0} = 50 + 25 \left(\frac{t}{t_0} \right), \quad (14)$$

where time is measured in t_0 (7), distance is measured in x_0 (4).

The theoretical deviation curve of the gas velocity (10) and the distance between the centers of charge (14) coincides with the simulated one. The difference is no more than 3 %.

3.2 Temperature Equalization in Electron Gas

The electron gas is in the form of two subsystems. Subsystem A is defined by $N_a = 500$ computational particles with temperature T_a, subsystem B is defined by $N_b = 500$ computational particles with temperature T_b. The simulation leads to temperature equalization for the time τ.

Consider several cases when the initial temperature ratio $(T_a/T_b)|_{t=0}$ equals 10^4, 10^3, 10^2, 10. The calculation of the T_a/T_b ratio at each time step for the given initial conditions is shown in Fig. 4.

Fig. 4 shows that temperatures T_a and T_b equalize. The equalization time for cases with initial conditions $(T_a/T_b)|_{t=0} = 10^4$, 10^3, 10^2, 10 is the same. The ratio $T_a/T_b = 1.06 \pm 0.01$ is reached at time $\tau = 0.07t_0$, where t_0 is the unit of time (7).

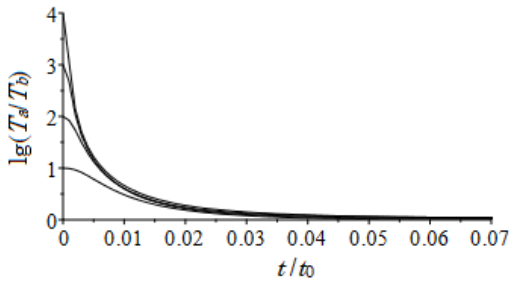

Fig. 4 – Temperature equalization of two subsystems in the electron gas

3.3 Natural Oscillations of Model Positron-electron and Proton-electron Gases

The subsection considers neutral electron-positron and proton-electron gases using the PIC simulation. It considers changes in kinetic and potential energy, the spatial distribution of particles over time, compares the

obtained frequency of natural oscillations with the theoretical value.

At the initial time, the gas consists of electrons and positrons of the same concentration n_e with the same velocity deviation v_0 (3). The particles are distributed normally in velocity and randomly in the space area: $x \in [200x_0, 500x_0]$, where x_0 is the unit of distance (4). The number of electron and positron computational particles is the same: $N_e = N_{e+} = 500$.

During the period $t = 10t_0$ of the simulation, the gas does not expand, the average linear charge density of the grid cells does not change.

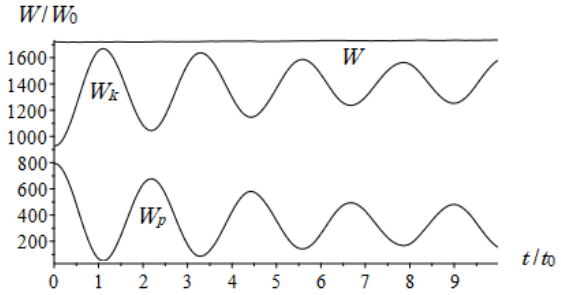

Fig. 5 – Change in kinetic, potential, total energy of the electron-positron gas over time

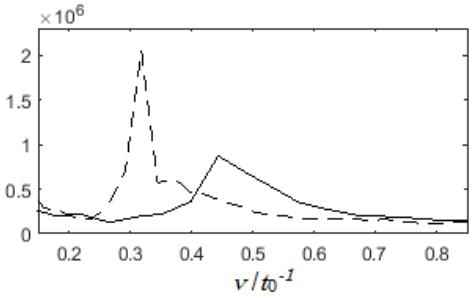

Fig. 6 – Frequency spectra of oscillations of electron-positron and electron-proton gases

At each time step of the simulation, we calculate the kinetic energy W_k, potential energy W_p, total energy W. The functions W_k, W_p, W as functions of time are shown in Fig. 5. Energy is measured in $W_0 = N_e m_e v_0^2/2$.

Fig. 5 shows that the total energy is conserved, but the potential and kinetic energies are oscillatory, accompanied by Landau damping. The spectrum of kinetic oscillations is shown in Fig. 6 as a solid line.

The theoretical frequency of natural oscillations of the electron-positron gas is $\nu_{th} / t_0^{-1} = \sqrt{2} / \pi$. The frequency obtained as a result of the computer experiment is $\nu_{\text{mod}} = 0.4439 \pm 0.04$, which coincides with the theoretical value with an error of 2 %.

If, in the model of the electron-positron gas, positrons are replaced by protons, that is, the electron-proton gas is considered, then the frequency of natural oscillations decreases. The frequency spectrum of the electron-proton gas is shown in Fig. 6 as a dotted line.

The theoretical frequency of natural oscillations of the electron-proton gas is $\nu_{th}/t_0{}^{-1} = 1/\pi$. The frequency $\nu_{mod}/t_0{}^{-1} = 0.3186 \pm 0.03$ obtained as a result of the computer experiment coincides with the theoretical value with an error of 0.2 %.

4. CONCLUSIONS

The simulation shows that the free electron gas expands due to electrostatic repulsion between electrons. A 5-fold expansion along the axis is accompanied by a 2.5-fold decrease in the charge density. In this case, the kinetic energy of electrons increases, and the potential energy decreases at a constant total energy, i.e., the expansion of the electron gas is a thermodynamically non-equilibrium process.

If the electron gas is represented as two subsystems with temperatures T_a and T_b with the initial conditions $(T_a/T_b)|_{t=0} = 10^4$, 10^3, 10^2, 10, then the temperature ratio $T_a/T_b = 1.06 \pm 0.01$ is reached in time $\tau = 0.07t_0$, where t_0 is the unit of time (7).

The simulation result of electron-positron and electron-proton gases shows that the gases have their oscillations accompanied by Landau damping. The obtained frequencies of these oscillations are in satisfactory agreement with analytical estimates.

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Моделювання процесів в електронному газі методом Particle-in-cell

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Елементарні процеси взаємодії заряджених частинок в електронному пучку струмом близько 1 А вивчаються чисельно щодо проблеми електронного охолодження. Приведені результати чисельного моделювання одновимірним методом Particle-In-Cell таких процесів як розширення електронного газу, вирівнювання температур двох підсистем електронного газу, власні коливання модельного електрон-позитронного та електрон-протонного газів. У рамках методу вільний електронний газ розширюється за рахунок електростатичного відштовхування між електронами при постійний повній енергії. Модель вільного електронного газу, яка представлена модельними частинками у вигляді нескінченних пластин, також вирішується аналітично. У цьому випадку аналітично знайдені відхилення швидкості як функція часу та відстань між центрами заряду двох половин електронного газу. І це порівнюється з результатом чисельного обчислення. Якщо електронний газ представити як дві підсистеми з різною температурою, це призводить до вирівнювання температури при моделюванні. У статті розглянуто кілька випадків з різними початковими умовами та знайдено час релаксації. Результат моделювання електрон-позитронного та електрон-протонного газів показує, що їх коливання супроводжуються затуханням Ландау. Спектральний розподіл частот цих коливань показує максимуми, які відповідають теоретичним значенням.

Ключові слова: Particle-in-cell, Кінетика, Плазма, Власні коливання, Моделювання.