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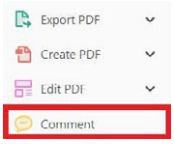

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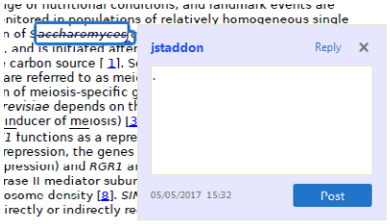

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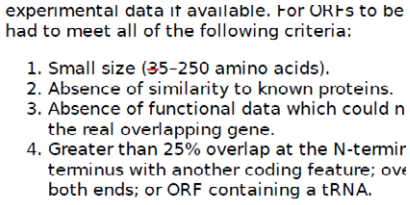

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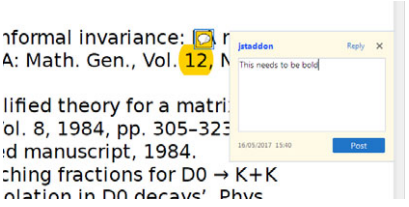

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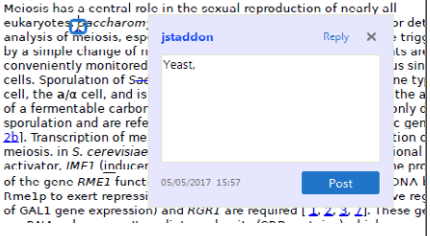

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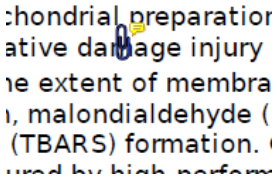

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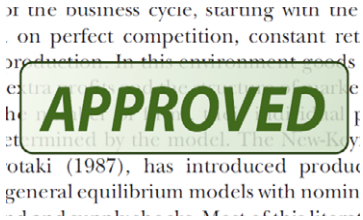

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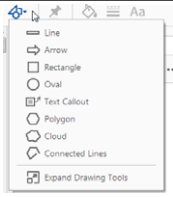

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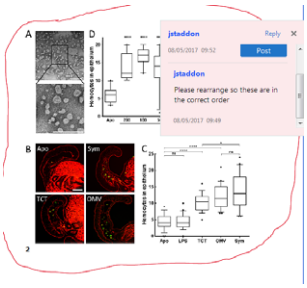

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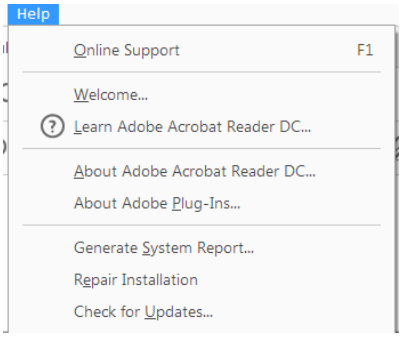

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ORIGINAL ARTICLE

Contributions to Plasma Physics

Simulation of positronium plasma by the molecular dynamics method

S.K. Kodanova[1] M.K. Issanova T.S. Ramazanov A.K. Khikmetov S.A. Maiorov[2,3]

[1]IETP, Al-Farabi Kazakh National University, Almaty, Kazakhstan

[2]Prokhorov General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

[3]Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia

Correspondence
S.K. Kodanova, IETP, Al-Farabi Kazakh National University, Al-Farabi 71, Almaty 050040, Kazakhstan.
Email: kodanova@physics.kz

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Abstract

In this paper, the relaxation properties of a fully ionized, hot, ideal plasma have been studied using the molecular dynamics method. As an example, the classical problem of equalization of the electron and ion temperatures for various mass ratios is considered, the relaxation times for temperatures is determined, and the influence of the number of particles and the type of boundary conditions on the simulation results is studied. The simulation results are compared with the available theoretical results.

KEYWORDS

autocorrelation flow function, classical Coulomb system, Coulomb logarithm, mass ratio, mirror boundary conditions, molecular dynamics method, periodic boundary conditions, plasma, temperature relaxation

1 | INTRODUCTION

When different plasma components have distinct temperatures, the process through which those that have higher temperatures transfer energy to those with lower temperatures, which occurs through Coulomb collisions and the coupling of collective modes, until all the components reach the same equilibrium temperature is known as temperature relaxation. Temperature relaxation between electrons and ions in dense plasma is a key problem in understanding the interactions in high energy density physics.[1,2] Particularly for inertial confinement fusion (ICF),[3,4] the values of energy transfer rates are necessary to simulate energy depositions.[5,6] The experiments for diagnosing the process of temperature relaxation are currently advancing rapidly[7–9] due to powerful lasers such as the OMEGA, X-ray free electron lasers, and the National Ignition Facility.[10–12] To design and analyse the experiments, a simple computing simulation is required by applying classical and semi-classical approximations to deal with the Coulomb collisions in the regime of interest. Various approaches are used to study the relaxation processes in plasma,[13–15] and one of the most accurate methods is the molecular dynamics (MD) method.[16–20]

Starting from the first kinetic models, many authors have considered the problem of temperature relaxation using a computational experiment.[21–23] Theoretical models are typically limited by small deviations of the system from the equilibrium state. It is possible to calculate the processes of energy relaxation between two subsystems far from equilibrium only using the methods of numerical simulation.

In this work, the MD method is used to simulate temperature equalization in a fully ionized, hot, ideal plasma. As an example, a positronium plasma, that is, a system with equal masses and equal but opposite charges, is considered. To

Abbreviations: ACF, autocorrelation function; BPS, Brown, Preston and Singleton; GMS, Gericke, Murillo, and Schlanges; ICF, inertial confinement fusion; LS, Landau-Spitzer; MD, molecular dynamics.

describe the interaction of particles in the MD simulation, we have chosen the Coulomb potential. The Coulomb potential is a good model for ICF as an interaction potential. The bound electron–positron pairs in the calculations were observed at close distances, and the Coulomb potential was smoothed by a spline of the third order.[24] The system of equations of motion of charged particles must have initial and boundary conditions. Mirror or periodic boundary conditions are usually used as the boundary conditions; the Ewald summation procedure is sometimes applied for boundary conditions as well.

In our calculations, the initial state was chosen to be strongly non-equilibrium, and the distribution function of electrons and positrons at the initial moment was assumed to be the Maxwell function with very different temperatures. During relaxation of the initial state, the temperatures are equalized. It should be noted that the plasma can be either in a trap or fly into a vacuum; in any case, the interaction of the electron and positron subsystems leads to equalization of temperatures.

2 | FORMULATION OF THE PROBLEM

Let us consider a volume in which, at the initial moment of time, there are two components with different temperatures: a certain number of electrons with positrons for a positronium plasma. The systems with different numbers of particles $2N = 128,\ 512,\ 2,048,\ 4,096$ distributed inside the counting cell—a cube with an edge L—were considered. The dimensions of the cube were chosen from the condition $nL^3 = N$, where n is a numerical density of ions, which was set to be equal to 10^{12} cm^{-3}.

The two types of initial conditions were considered. The first type corresponds to the state when, at the initial moment of time, all the particles are fixed and distributed equiprobably inside the counting cell. This type of initial condition corresponds to experiments with ultracold plasma created by selective ionization of a cold gas. It is discussed in detail in ref. 25. The second type is the initial state when the particles at the initial moment of time are distributed equiprobably in the counting cell, and their speeds have a Maxwell distribution with different temperatures for positively and negatively charged particles.

Two types of boundary conditions were considered: mirror walls and periodic boundary conditions. In the case of periodic boundary conditions, the interaction of particles in only one cell was taken into account, that is, the Ewald summation procedure was not used.

2.1.1 | The numerical solution technique

We have tried a variety of standard numerical methods of solving dynamic equations: the over-stepping schemes and the Euler, Verlet, and Runge–Kutta methods. Substantial progress in the assessment of an enormous calculation size was achieved due to the creation of an original method. Assume that at a certain time moment, t_0, all the particles' coordinates $r_k(t_0)$ and velocities $v_k(t_0)$ are known. The procedure to determine the $r_k(t_0 + \Delta t)$ and $v_k(t_0 + \Delta t)$ values, for the external (large) time step Δt, is as follows.

One calculates the $r_k^{(0)}(t_0 + \Delta t/2)$ coordinate values corresponding to a rectilinear particle motion:

$$r_k^{(0)}(t_0 + \Delta t/2) = r_k(t_0) + v_k(t_0) \cdot \Delta t/2.$$

Then, the values of the forces acting upon the particles are calculated:

$$F_k^{(0)}(t_0 + \Delta t/2) = \sum_{l \neq k}^{(z+1)n} f_{kl}(r_k^0 - r_l^0).$$

In order to reduce the computation size, one should take into account Newton's third law: $f_{kl} = -f_{lk}$. After that, one finds for each particle the two others: the first is the nearest positively charged particle neighbour, and the second is the nearest negatively charged particle neighbour. The force acting on each particle is calculated in the form of a sum of two terms $F_k = F_k^{(F)} + F_k^{(N)}$. The $F_k^{(N)}$ is due to the given particle interaction with its nearest neighbours and with the particles for which the given particle is the nearest neighbour. $F_k^{(F)}$ is a result of the interaction with all the other particles. Then, the Newton equations are integrated over the time interval Δt using a Runge–Kutta fourth order of accuracy procedure with an internal (small) time step $\tau = \Delta t/N_\tau$, where N_τ represents the number of internal steps. Only the forces $F_k^{(N)}$ are variable in the course of the integration:

$$F_k(t) = F_k^{(F)}(t_0 + \Delta t/2) + F_k^{(N)}(t), \quad t_0 < t < t_0 + \Delta t.$$

Having calculated $r_k(t_0+\Delta t)$ and $v_k(t_0+\Delta t)$, one should verify whether there are particles outside the cube volume. With particles having penetrated through the cube wall, one should proceed according to the above formulated boundary conditions.

Time steps in the range of $0.005 < \Delta t/\tau_{ep} < 0.1$ and $N_\tau \sim 30$were usually used in the calculations. Time evolution of the up to 8,000 particle systems were traced over the time interval $t \sim (200-1,000)\cdot\tau_{ep}$. The total energy conservation law was fulfilled in these conditions, with an accuracy better than 0.5% (usually 0.1%). The proposed algorithm provided the reversibility of the system motion at time intervals of the order τ_{ep}. The time of the system evolution tracing is usually far greater than τ_{ep}, so the system motion is irreversible. However, the energy conservation in the reversibility tests was very fine—better than 0.1% for a time interval of the order e-p collision time τ_e.

The non-ideality index of the classical Coulomb system is defined as follows:

$$\Gamma = \frac{Z^2 e^2}{a\,T} \sim \frac{Z^2 n^{1/3}}{T}, \tag{1}$$

where $a = (3/4\pi n)^{1/3}$ is the Wigner–Seitz radius. Large values of the non-ideality index can be obtained in various ways: due to the large charge Z (the charge of dust particles in the plasma),[26] high ion density n (inertial thermonuclear fusion),[27] and low temperature T (ultracold plasma).[28,29]. For simplicity, we consider the case of singly charged ions $Z = 1$.

If we assume that, at the initial moment of time, the two plasma components have a Maxwell distribution of velocities with different temperatures, then the process of equalization of temperatures due to Coulomb collisions is described by the following equation[30]:

$$\frac{dT_e}{dt} = \frac{T_p - T_e}{\tau_{ep}}, \frac{dT_p}{dt} = \frac{T_e - T_p}{\tau_{pe}}, \tag{2}$$

in which the rate of relaxation of the electron temperature is determined by the temperature difference and the characteristic relaxation time:

$$\tau_{ep} = \frac{1}{\nu_{ep}} = \frac{3 m_e m_p}{8\sqrt{2\pi} n_p e^4 \Lambda}\left(\frac{k_B\,\varepsilon_e}{m_e} + \frac{k_B\,\varepsilon_p}{m_p}\right)^{3/2}. \tag{3}$$

To determine the relaxation time of the temperatures of electrons and ions, it is necessary to know the value of the Coulomb logarithm Λ, which is known to reflect the long-range nature of the Coulomb interaction. For convergence of theoretical results, the so-called cut-off radius was introduced. The Coulomb logarithm expressed in terms of cut-off radius has the form[30]:

$$\Lambda = \ln \frac{b_{max}}{b_{min}}, \tag{4}$$

where b_{max}, b_{min} are maximal and minimal impact parameters, respectively. As the minimal impact parameter, the closest approach distance $b_c = Ze^2/k_B T$ or the de Broglie thermal wave length $L_B = \sqrt{2\pi\hbar^2/m_e k_B T_e}$ is measured. The thermal wave length is measured when it is necessary to take into account the quantum effects. Based on the numerical calculations in the work of Gericke, Murillo, and Schlanges (GMS),[31] the following formula for the Coulomb logarithm was suggested:

$$\Lambda_{GMS} = \frac{1}{2}\ln(1 + [\lambda_D^2 + R_{ion}^2]/[\Lambda^2/8\pi + b_C^2]), \tag{5}$$

where $R_{ion} = (3/4\pi n_p)^{1/3}$ is the distance of closest approach. This formula has a good agreement with the results obtained in the framework of the T matrix theory. Based on dimensional continuation, Brown, Preston and Singleton (BPS)[32] derived a Coulomb logarithm:

$$\Lambda_{BPS} = \log\left(\frac{\lambda_D}{L_B}\right) + \frac{1}{2}[\log(16\pi) - \gamma - 1], \tag{6}$$

where γ is the Euler constant.

3 | CALCULATION OF TEMPERATURE EQUALIZATION

Let us first consider the influence of the following factors on the process of temperature equalization in the Coulomb system: the type of boundary conditions and the number of particles in the system. Figure 1 shows the graphs of electron and ion

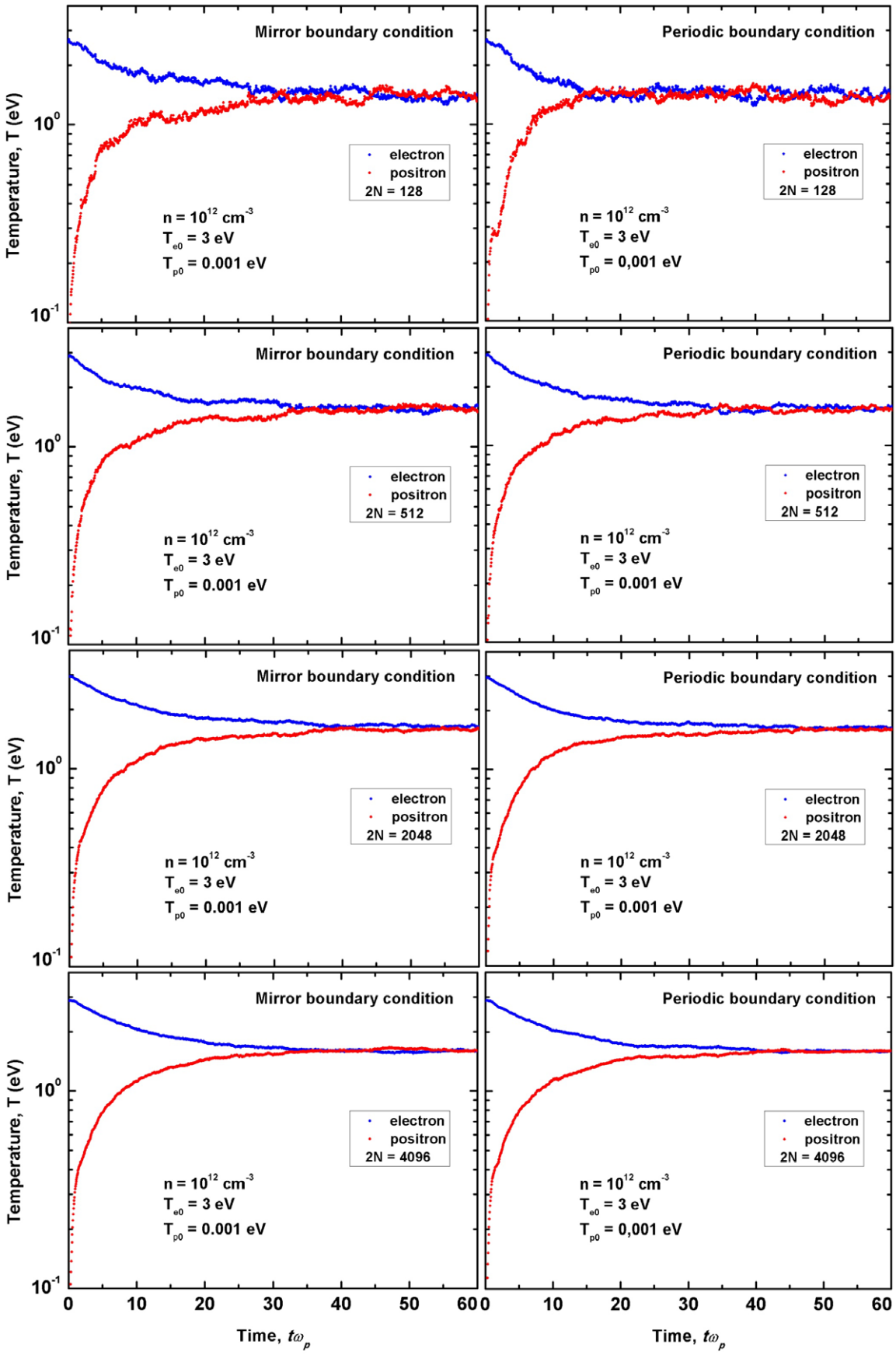

FIGURE 1 Time dependence of electron and ion temperatures for two types of boundary conditions and for a different number of particles in the system: the left panel—mirror; the right panel—periodic

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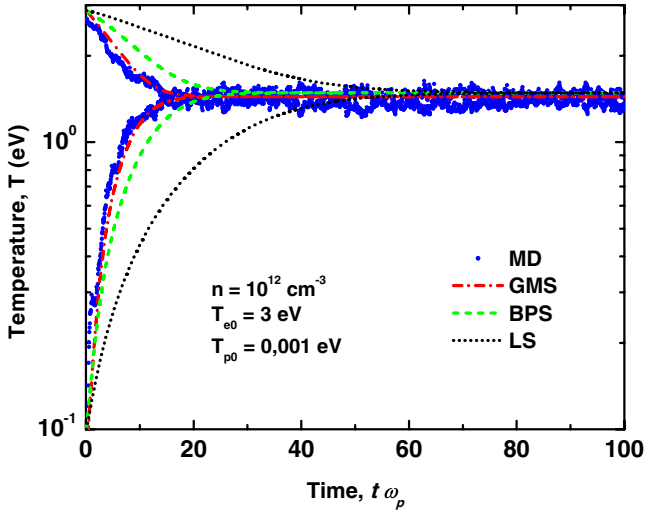

FIGURE 2 A comparison of the values of temperature relaxation calculated on the basis of MD simulations with theoretical approaches of LS[30], GMS[31], and BPS[32]

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temperatures for two types of boundary conditions: the left panel—mirror; the right panel—periodic. Different vertical graphs correspond to different numbers of particles in the system $2N = 128,\ 512,\ 2048,\ 4096$.

The above figures show that, for a small number of particles in the system, the temperature relaxation time strongly depends on the type of boundary conditions. As expected, when the number of particles in the system increases, the dependence decreases. It is interesting to note that, with a small number of particles in the system with periodic boundary conditions, the temperature is equalized faster. This result can be explained by the fact that, under mirror boundary conditions, the particle distance to the wall is significantly shorter than the average inter-particle distance $n^{-1/3}$, and the average value of the micro-field acting on the particle is $2^{2/3}$ times smaller than the average micro-field. With a large number of particles at the initial time, the temperature relaxation curves for periodic and mirror boundary conditions are the same, with great accuracy, but at large times, differences arise due to the fact that the periodic system has better conditions for the appearance of large-scale fluctuations.

Figure 2 shows the values of the temperature of positrons and electrons using MD methods at $n = 10^{12}$ cm^{-3} in comparison with the theoretical results of other authors such as GMS,[31] BPS,[32] and Landau-Spitzer (LS).[30] GMS investigated various approximations in the evaluation of Λ, including issues with trajectories and cut-offs, and provided different evaluations of the relaxation rate based on quantum kinetic theory. BPS used dimensional continuation to obtain expressions for the electron–ion coupling rate accurate to the second order in the plasma coupling parameter. The MD data in Figure 2 are most closely matched by GMS followed by BPS. The LS[30] model predicts the slow relaxation. For the positronium plasmas, the simulations are consistent with both GMS and BPS.

4 | RESULTS OF CALCULATIONS OF THE AUTOCORRELATION FLOW FUNCTION

Consider the autocorrelation flow functions of positively and negatively charged particles (positrons and electrons). As in the general case, our system is strictly neutral, and its total momentum is zero in the periodic system and oscillates around zero in the system with mirror boundary conditions; we will consider the autocorrelation functions for a flow of particles with only one sign:

$$J(t) = \sum_i^N q_i v_i(t), \tag{7}$$

where q_i, v_i are the charge and velocity of the i particle, respectively. Then, the autocorrelator of the particle flux is determined by the formula:

$$Z(\tau) = \langle J(0) \cdot J(\tau) \rangle / \langle J^2(0) \rangle. \tag{8}$$

The flow autocorrelator is an important characteristic of the considered Coulomb system. Its dependence on the number of particles and the type of boundary conditions is of great interest. Therefore, calculations were carried out with a different number of particles and two types of boundary conditions: mirror and periodic. Figure 3, the top panel, shows the dependence of the autocorrelation function of the flow in the cube with mirror boundary conditions for the number of particles $2N = 128$,

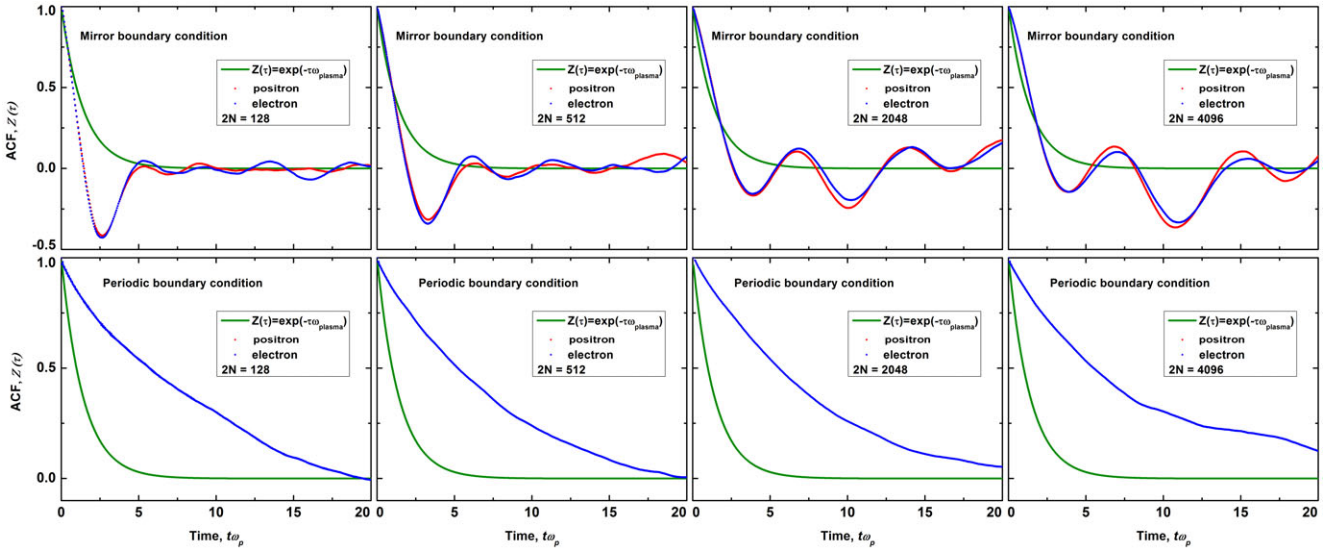

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FIGURE 3 Time dependence of the autocorrelation flow function for two types of boundary conditions and for a different numbers of particles in the system: the top panel—mirror; the bottom panel—periodic; solid curve—(9)

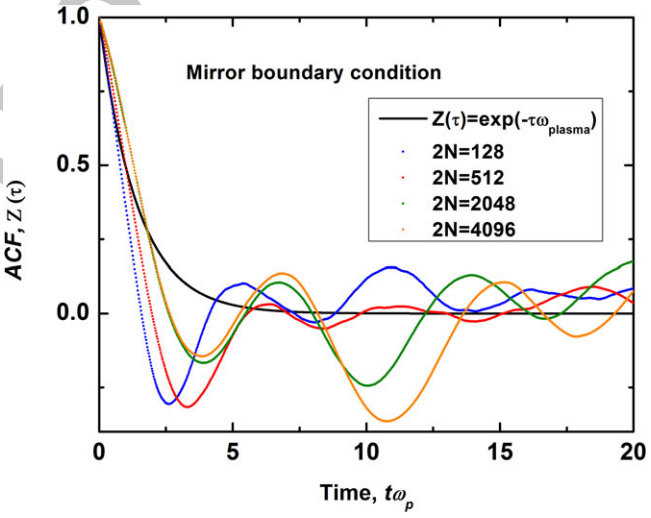

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FIGURE 4 Time dependence of the autocorrelation flow function for a system with mirror boundary conditions in the linear scale

512, 2, 048, 4, 096. In Figure 3, the bottom panel presents similar graphs for the periodic system. In all figures, the solid curves represent the dependence

$$Z(\tau) = \exp(-\tau\,\omega_{\text{plasma}}), \tag{9}$$

where ω_{plasma} is plasma frequency. Comparison of the curves in the lower row shows that they do not differ significantly from each other, that is, the dependence of the ACF flow on the number of particles is rather weak for periodic boundary conditions. However, the graphs in the upper and lower rows differ significantly, that is, the dependence on the type of boundary conditions is very strong.

Another interesting fact, as seen from the figures, is that the correlation decay time in the system with periodic boundary conditions is much longer, and the autocorrelation functions are more monotonic.

For a more explicit demonstration of this effect, Figure 4 shows the dependencies of the autocorrelation flow functions for a system with mirror boundary conditions in a linear scale. Figure 5 shows similar results for a system with periodic boundary conditions in a semi-logarithmic scale. For the system with mirror boundary conditions, a solid curve with dependence (9) demonstrates that the initial period of the ACF is well described by an exponent with a characteristic correlation decay time $1/\omega_{\text{plasma}}$. In the abovementioned graph for a system with periodic boundary conditions, the solid curve with the dependence $Z(\tau) = \exp(-\tau\omega_{\text{plasma}}/2\pi)$ shows that, for such a system, the characteristic time for the correlation decay coincides with good accuracy with the Langmuir period.

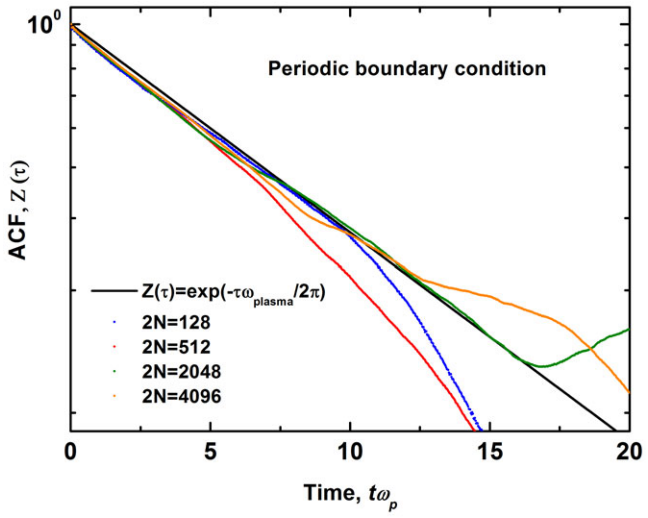

FIGURE 5 Time dependence of the autocorrelation flow function for a system with periodic boundary conditions in the semi-logarithmic scale

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5 | CONCLUSIONS

In this paper, the MD method has been used to study the problem of temperature relaxation in a classical Coulomb system. The dependence of the properties of such a system on the number of particles has been studied, and the cases of mirror and periodical boundary conditions have been considered.

The analysis of the autocorrelation functions of the flux of particles of the same sign in the system showed that the correlation decay time in a system with mirror boundary conditions is reciprocal to the plasma frequency, and in a system with periodic boundary conditions, it has the order of the Langmuir oscillation period. It was also found that, in a system with periodic boundary conditions, the temperature relaxation time is shorter than in a system with mirror boundary conditions. Based on the analysis of the results, the influence of the number of particles on the autocorrelation flux functions is insignificant.

ACKNOWLEDGMENTS

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