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Non-exponential dynamic relaxation in strongly nonequilibrium nonideal plasmas

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Abstract
Relaxation of kinetic energy to the equilibrium state is simulated by the molecular dynamics method for nonideal two-component non-degenerate plasmas. Three limiting examples of initial states of strongly nonequilibrium plasma are considered: zero electron velocities, zero ion velocities and zero velocities of both electrons and ions. The initial non-exponential stage, its duration τ_{nB} and subsequent exponential stages of the relaxation process are studied for a wide range of the nonideality parameter and the ion mass.

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1. Introduction

The Boltzmann equation is a fundamental equation of kinetic theory of gases; there were numerous attempts to modify this equation and extend it to dense systems [1–5]. One could also mention a quite general theory [6], the generalized Langevin theory [7], and renormalized kinetic theories [8]. In fact all these approaches are rather formal and explicit results can be obtained only for weakly nonideal systems or close to equilibrium [7]. For that reason some authors [9–11] tried to compare their experimental results for strongly nonequilibrium nonideal plasmas only with simple modifications of the Landau theory [12], the binary collision approximation extended to strong scattering [13] and the density functional approach [14, 15]. A generalization of the Landau–Spitzer approach to the case of strong binary collisions was recently suggested in [16].

The kinetic theory of gases deals only with probabilities of collisions. Another fundamental assumption is the molecular chaos hypothesis (Stosszahlansatz) which means that molecules are statistically independent between collisions. This leads, for example, to the exponential relaxation to equilibrium for a two-temperature system. It is evident, however, that the stochastic motion is preceded by the dynamical stage [1, 4, 5, 17]. The problem of stochastic properties of dynamical systems has been argued since Boltzmann's time [1, 17, 18]. The

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predictability time or the dynamical memory time t_m was introduced in [19, 20]. It determines the maximum time interval during which the evolution of a dynamical system can be predicted from initial conditions and deterministic equations of motion. The value of t_m was calculated numerically for equilibrium two-component nonideal plasmas [21]. It is closely related to the Lyapunov divergence of particle trajectories. The latter was studied for OCP in [22]. One may expect the Boltzmann-like exponential relaxation in kinetic processes to be valid only for times greater than t_m.

The method of molecular dynamics (MD) can be a powerful tool for studying relaxation phenomena in dense many-particle systems on arbitrary time scales. In the case of nonideal plasmas the method of molecular dynamics is more efficient than a numerical solution of kinetic equations. Some nonequilibrium processes in systems of neutral particles were studied by MD [23–25]. Exponential relaxation to equilibrium in two-component nonideal plasmas was simulated by MD in [26, 27]. The damping oscillation regime was observed in one-component nonideal plasmas [28]. Note, however, that neither oscillations nor their transition to exponential decay were studied in the framework of MD.

In the present work MD is used to study the relaxation of the electron and ion kinetic energies in strongly nonequilibrium nonideal plasmas. Non-exponential relaxation is observed for different initial conditions and its transition to the exponential regime is confirmed.

2. Simulation technique

We consider a fully ionized system of $2N$ single-charged particles: electrons and ions with masses m and M, respectively. The nonideality is characterized by the parameter $\gamma = e^2 n^{1/3}/kT$, where $n = n_e + n_i = 2n_e$ is the total density of charged particles, and T is the temperature. The values of γ range from 0.3 to 6. The relaxation in the system of free charges is studied. For that reason we choose an effective pair electron–ion potential which excludes the possibility of the formation of low energy bound states in the Coulomb well. Another potential with a very deep (with respect to temperature) cut-off of the Coulomb potential was used in the study of the recombination relaxation in ultracold plasmas [29, 30]. It was shown in [31, 32] that such a model overestimated the absolute values of three-, four- and many-particle cluster energies remarkably because this pair potential did not account for quantum effects in such clusters. So the model [29, 30] was able to reproduce only the initial stage of the recombination relaxation when only pair bound states were formed. The details of the plasma models were described in [21, 32–34].

The number of particles is $N = 100$–200 in our simulations. It is usually taken less than 10^3–10^4 for simulations of weakly nonideal plasmas or plasmas with long-range order, e.g., OCP with $\gamma \sim 100$. Nevertheless, it was already shown in seventies [35–37] that due to the screening effects in two-component plasmas with $\gamma \sim 1$, each particle interacts only with its nearest neighbours, and the exponential Debye law for the effective interparticle interaction remains valid for distances larger than the average interparticle distance even for $\gamma > 1$. For that reason, starting from $\gamma = 0.2$, more than 90% of the interaction energy is contributed from the particles nearer to each other than those with the average interparticle distance. It was found that $N = 50$ was sufficient for such plasmas when calculating thermodynamic properties and correlation functions [35–37]. In the present paper we performed test simulations of the relaxation in strongly nonequilibrium plasmas for N varying from 25 to 800 and found that starting from $N = 50$, the scatter of the relaxation curves for different N is within the simulation error. So $N = 100$ still holds under strongly nonequilibrium circumstances. This model would not hold for long wavelength oscillations but they are not expected for the investigated case.

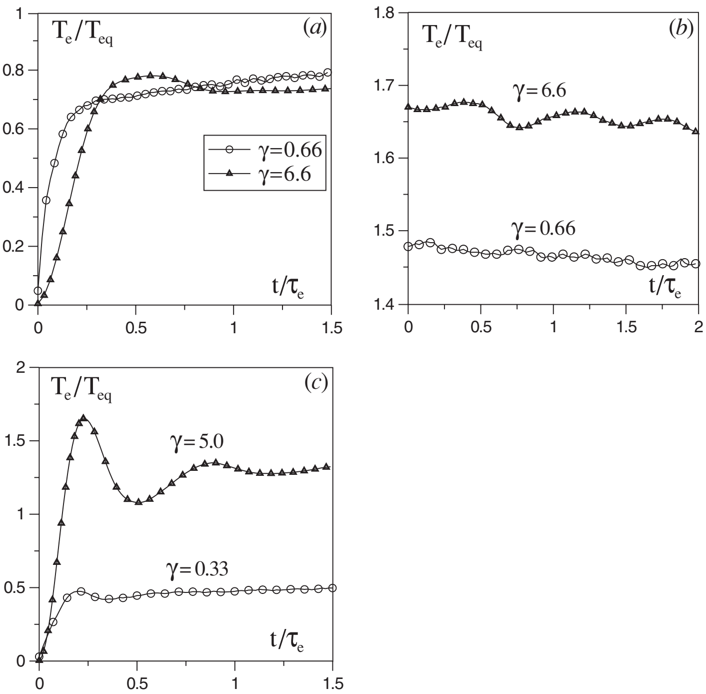

Figure 1. The dependence of the average kinetic energy of electrons T_e on the time for different initial conditions: (*a*) $T_e(0) = 0$; (*b*) $T_i(0) = 0$; (*c*) $T_e(0) = T_i(0) = 0$. $M/m = 100$.

The number of particles chosen is sufficient to study oscillations at plasma frequency and high-order oscillations [21].

The following procedure is used to prepare the ensemble of initial nonequilibrium plasma states. First, an equilibrium trajectory is generated by MD for a given initial value of γ. A set of $I = 50$–200 statistically independent points is obtained from this trajectory. Statistical independence is ensured by the time interval between outputs greater than t_m. Then three sets of the following nonequilibrium configurations are prepared:

- the velocities of electrons are dropped to zero;
- the velocities of ions are dropped to zero;
- the velocities of both electrons and ions are dropped to zero.

These three sets are the limiting cases of strongly nonequilibrium plasmas. The first example corresponds to the primitive model of a strong shock wavefront ($T_e \ll T_i$), the second one to the fast laser heating or electron explosion of wires ($T_e \gg T_i$).

No matter what case of the initial state ensemble is chosen, after the relaxation is simulated, averaging over the initial configurations is performed. Provided the result is N-independent, the relative error is given by $\sqrt{NI}$. The error bars in the figures shown in section 3 correspond to a confidence coefficient equal to 0.95. They are not indicted if they are smaller than the size of the points.

3. Simulation results

Examples of relaxation of the average kinetic energy $T_e(t) = \frac{1}{2NI}\sum_{j,k}^{N,I} m\, v_{jk}^2(t)$ in the initial stage are presented in figure 1. The nonideality parameter in this and other figures

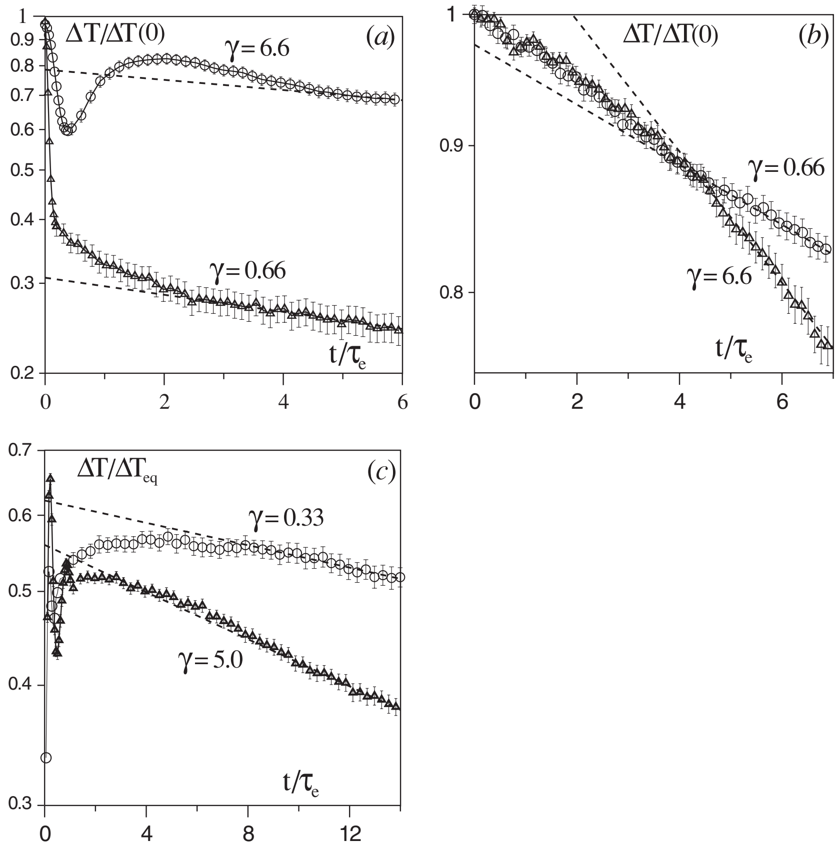

Figure 2. The difference between kinetic energies of electrons and ions $\Delta T = |T_e - T_i|$ depending on the time for different initial conditions: (*a*) $T_e(0) = 0$; (*b*) $T_i(0) = 0$; (*c*) $T_e(0) = T_i(0) = 0$. The value of ΔT is normalized either by its initial value $\Delta T(0)$ or by the equilibrium temperature T_{eq}. In order to define τ_{nB} and the beginning of exponential decay the long time scale relaxation is fitted by the dashed straight line. $M/m = 100$.

is defined as $\gamma = e^2 n^{1/3}/kT_{eq}$, where T_{eq} is the kinetic energy of electrons and ions in the final equilibrium state. The time here and below is measured in periods of electron plasma oscillations $\tau_e = 2\pi/\Omega_e$. Figure 2 shows the transition to the exponential relaxation. The possibility of two stages of relaxation was noted in [27].

Though the relaxation character in the beginning stage depends on the initial conditions, there are common features also. The electron kinetic energy passes through the maximum and undergoes several damping oscillations which are more pronounced for greater γ (figure 1). The initial increase of kinetic energy of ions presented in figure 3(*b*) shows that the ion subsystem are no longer in the nonequilibrium state after the electrons are stopped. The amplitude and the frequency of this 'oscillation' of ions depend on the mass ratio. The comparison of the curves in figures 1(*a*), 2(*a*), 3(*a*) and 3(*b*) gives the following picture of initial relaxation for $\gamma = 6.6$ and $T_e(0) = 0$. Electrons are heated for $0.2\tau_e$, and the ion temperature does not change remarkably during this period of time. So electrons take energy from the initial excess of the potential energy and the value of ΔT decreases. The rapid increase of electron kinetic energy excites damping oscillations. Since both electron and ion energies do not change monotonically, it means that nonideal plasma is a system with

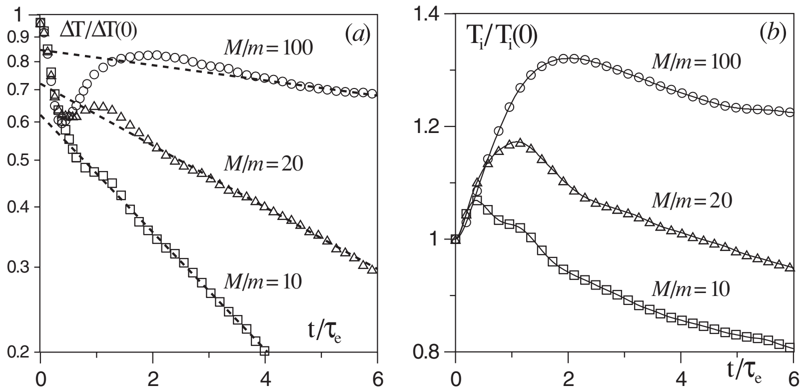

Figure 3. The oscillations of the energy difference (*a*) and kinetic energy of ions (*b*) for different mass ratios. $T_e(0) = 0$, $\gamma = 6.6$.

collective degrees of freedom which cannot be separated into electron and ion degrees of freedom. Oscillations damp more slowly and their amplitudes increase with increasing γ. It correlates with the decrease in the damping decrement of plasma waves with increasing γ for $\gamma \gtrsim 1$ which was found both analytically [16] and in simulation [38] for the equilibrium plasmas. A collective description of nonideal plasmas was drafted in [16].

The description of the relaxation process in the case when the electrons and ions are initially stopped ($T_e(0) = T_i(0) = 0$) is supplemented by the kinetic energy distributions for electrons and ions, figure 4. The Maxwellian energy distribution for electrons builds up very fast after $t = 0.03\tau_e$. During the non-exponential stage of relaxation only the distribution for electrons is Maxwellian as shown in figure 4(*b*). Figure 4(*c*) corresponds to the subsequent exponential stage where both distributions are Maxwellian except the ion tail but the temperatures are still different.

The exponential character of the long time scale relaxation agrees with the earlier results [26, 27]. The exponential decay of the difference between the electron and ion temperatures does not depend on the initial state and is given by $\Delta T = |T_e - T_i| \sim \exp\{-t/\tau_B\}$. The dependences of both relaxation times τ_B and τ_{nB} on the mass ratio and γ are presented in figure 5.

The scatter of τ_{nB} values in figures 5(*b*) reveals the apparent dependence of the non-exponential relaxation on the initial conditions. The values of τ_{nB} increase with γ in a similar way as the dynamic memory time t_m. Note that t_m was calculated in [21] for electrons in an equilibrium plasma and therefore does not deal with a relaxation process. Nevertheless, the close correspondence of t_m and τ_{nB} in figure 5(*b*) points to a deep relation between stochastization of electron trajectories and the transition to exponential relaxation. The increase of t_m with increasing γ correlates with the decrease of the damping decrement mentioned above. Remember that the divergencies of both the electron and ion trajectories are defined by the same Lyapunov exponent for $t < t_m$ [21]. It gives an additional argument for the collective nature of nonideal plasmas.

The value of τ_B is fitted in figure 5(*a*) by $\tau_B/\tau_e \sim (M/m)^{0.86}$ which is slightly different from the Landay–Spitzer formula $\tau_B/\tau_e \sim \gamma^{-3/2}(M/m)$. The dependence of τ_B on γ (figure 5(*b*)) is rather weak. The dependences of τ_B/τ_e on both mass ratio and γ are close to each other for different initial states. Independence of the relaxation process from the initial states supports the idea that the electron trajectories forget the initial conditions for $t > \tau_{nB} > t_m$.

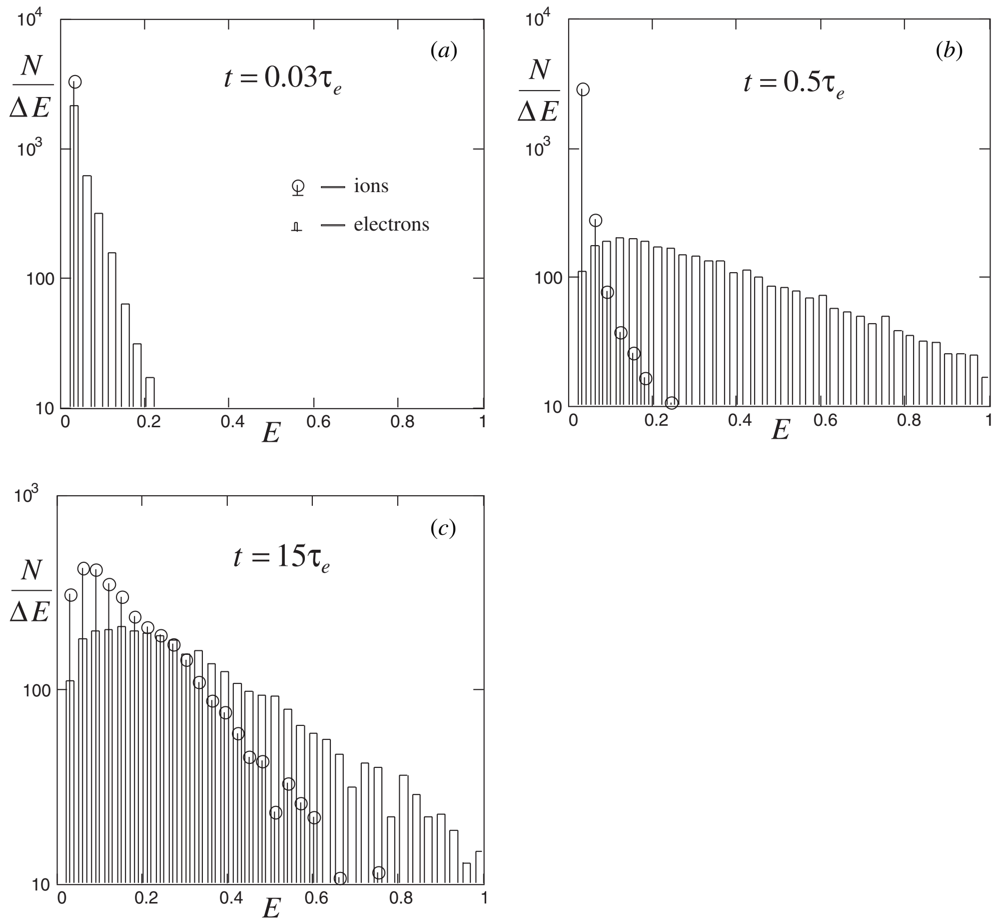

Figure 4. The energy spectrum for electrons and ions at three moments of time corresponding to different stages of relaxation. $T_e(0) = T_i(0) = 0$, $\gamma = 3.3$, $M/m = 100$.

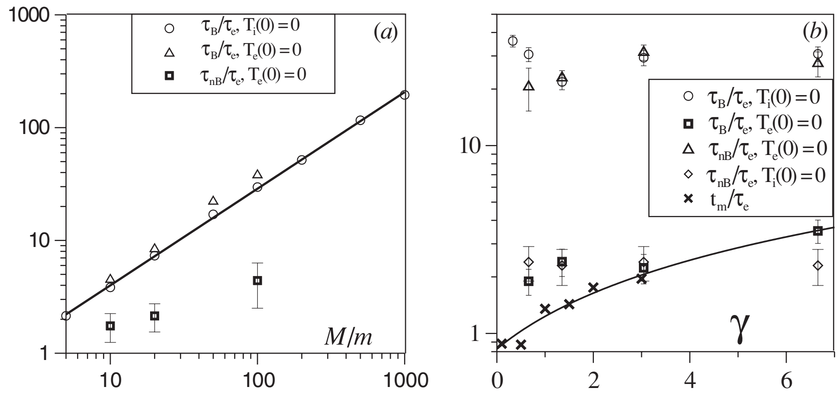

Figure 5. The values of the relaxation time in the exponential stage τ_B and the duration of the non-exponential stage τ_{nB}. (*a*) Mass dependence with power fit: solid line $\tau_B/\tau_e \sim (M/m)^{0.86}$; $\gamma = 0.74$. (*b*) γ-dependence compared with the dependence of dynamical memory time t_m extrapolated by the linear function $t_m \sim \gamma$. $M/m = 100$.

Having the mass dependence and γ-independence of τ_B, we extrapolate the values of the relaxation time to real experimental conditions. Although the degeneracy effects and a possible Z-dependence are not taken into account, the estimated values of the equilibration time 0.1–1 ns agree with experimental data [9, 10].

4. Conclusion

Our results for three types of initial conditions, different γ and the mass ratio can be formulated as follows.

The nonideal plasma is a system with collective degrees of freedom: the initial non-exponential stage of relaxation is related to the relaxation of both electrons and ions; the time behaviour of the kinetic energy depends on the mass ratio and initial conditions used.

The nonideal plasma demonstrates the behaviour of the excitable dynamic system in the initial stage of the relaxation: the greater γ is the more pronounced are the oscillations of the average kinetic energy of electrons and ions, since the damping decrement decreases; the duration of the non-exponential relaxation is closely related to the dynamic memory time; being measured in units of the period of plasma oscillations, the duration grows with γ.

The characteristic time of the exponential relaxation does not show a detectable dependence on the initial conditions used. The mass dependence of the relaxation exponent differs from the linear one; it might point to the collective nature of nonideal plasma as well. The γ dependence is rather a small one in the γ range studied.

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