Evolution of Temperature in the Ultracold Strongly-Correlated Plasmas

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Abstract

We present a theoretical interpretation of the recently revealed features of temperature evolution in the ultracold plasma clouds released from a magneto-optical trap, namely: (a) its independence at the sufficiently large times on the initial plasma parameters and (b) the asymptotics close to $t^{-1}$ instead of $t^{-2}$, expected for a rarefied ideal gas. It is shown that both these properties can be well explained by the model of virialization of the charged particle velocities in the regime of strong electron–ion correlations, while heating due to inelastic processes (e.g. three-body recombination) should be of secondary importance. These conclusions are confirmed also by the results of ab initio computer simulations.

Key words: Ultracold plasma, Temperature evolution, Virialization

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1 Introduction

A new interesting branch of plasma physics, emerged in the last decade, is studying the clouds of rarefied ultracold plasmas produced by the laser capture and cooling of gases in the magneto–optical traps (MOT) and their subsequent ionization (for general review see, for example, [1,2,3] and references therein). These are the classical (non-quantum) gaseous systems with characteristic temperatures from a fraction to a few Kelvin, in which the Coulomb’s coupling parameter $\Gamma = e^2 n^{1/3}/k_B T$ can reach considerable values. For example, the measured values of this parameter for the ions $\Gamma_i$ are about 2÷3 [4]; the

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estimates of $\Gamma_e$ for the electrons are less accurate and model dependent, but they also result in the values comparable to unity.

The possibility of existence of such metastable plasmas was theoretically predicted a quite long time ago (e.g. article [5] and references therein), but they were created experimentally only after sufficient development of the technology for laser cooling of atoms. Besides, it was proposed to produce similar plasma states by the artificial release of the ionized gas clouds from spacecraft [6,7], but the possibility of diagnostics in cosmic space remains too limited by now.

One of the most interesting recent results in the experimental study of ultracold plasmas is the behavior of temperature in the clouds released from a trap and expanding freely in space. It was unexpectedly found that, firstly, the law of decrease of the electron temperature became universal at large times, i.e. did not depend on the initial conditions. (For example, when the initial temperatures $T_e$ varied by 30 times, their difference after a few microseconds was only 2 ÷ 3 times and decreased further in the course of the subsequent evolution [8].) Secondly, which is even more interesting, the asymptotics was measured to be $T_e \propto t^{-(1.2 \pm 0.1)} \approx t^{-1}$ instead of $t^{-2}$, which would be expected for an ideal rarefied gas without internal degrees of freedom ($\gamma = 5/3$) at the inertial stage of its expansion (i.e. when the plasma cloud expands with a constant velocity, so that its characteristic size increases linearly with time, $R \propto t$).

The most straightforward way to interpret the substantially slower decrease in the electron temperature is to take into account a heat release by the recombination of charged particles. In the particular case of atomic ions, the most efficient channel should be three-body recombination $A^+ + e + e \rightarrow A + e$, when one electron is captured by the ion, while the second electron carries away the excessive energy. Unfortunately, the recent attempts of numerical simulation of the observed law of temperature evolution with the three-body recombination did not lead to the satisfactory results; see, for example, Fig. 3a [9].

The aim of our paper is to show that all the experimentally observed features of temperature evolution (namely, both the establishment of the universal asymptotics, independent of the initial conditions, and its particular form, close to $t^{-1}$) can be naturally explained by the model of virialization of the charged particle velocities, i.e. actually due to changing the equation of state of the ultracold plasma under the presence of strong electron–ion correlations.

\footnote{Let us mention that the method of plotting the temperature curves in Fig. 3a [9] is slightly confusing. According to the physical sense of the problem, the various laws of evolution should be compared at the same initial temperature; while in the above-mentioned figure they were presented at various initial temperatures. As a result, at first sight, the disagreement between the curves appears at small rather than at large times.}
Thereby, in the first approximation, it is not necessary to take into account any inelastic processes, such as heat release by the three-body recombination.

2 Theoretical Model

Our analysis will consist of the three basic steps. First of all, let us consider a sufficiently small (but macroscopic) element of the expanding plasma where thermodynamic equilibrium is supposed to be established. Then, we can describe it by the multi-particle distribution function of the following general form:

\[
f(r_{e1}, \ldots, r_{eN_e}, v_{e1}, \ldots, v_{eN_e}) = A_f \exp\left\{-\frac{1}{k_B T_e} \left[\sum_{n=1}^{N_e} \frac{m_e v_{en}^2}{2} + U(r_{e1}, \ldots, r_{eN_e}, r_{i1}, \ldots, r_{iN_i})\right]\right\},
\]

where \(r_{en}\) and \(v_{en}\) are the coordinates and velocities of electrons, \(r_{in}\) are the coordinates of ions, and \(A_f\) is the normalization factor. (Kinetic energy of the ions is ignored here, since it is usually much less than the kinetic energy of electrons in the particular experimental setups. In principle, the same consideration can be conducted with the kinetic energy of ions if the thermodynamic equilibrium is established between all kinds of the charged particles.)

Despite a very complex form of the potential energy \(U\) in the regime of strong Coulomb’s interaction, the average value of some quantity \(F\) depending only on the velocities \(v_{en}\) can be calculated quite easily:

\[
\langle F(v_e) \rangle = \frac{\int F(v_e) \exp\left\{-\frac{1}{k_B T_e} \left[\sum_{n=1}^{N_e} \frac{m_e v_{en}^2}{2}\right]\right\} dv_e}{\int \exp\left\{-\frac{1}{k_B T_e} \left[\sum_{n=1}^{N_e} \frac{m_e v_{en}^2}{2}\right]\right\} dv_e},
\]

because the integrals \(\int \exp\{-U(r_e, r_i)/k_B T_e\} dr_e\) in the numerator and denominator exactly cancel each other. (Here, \(v_e, r_e,\) and \(r_i\) designate the entire sets of velocities and coordinates of the electrons and ions, respectively.)

Therefore, the average kinetic energy per one particle will be

\[
\langle k \rangle = (3/2) k_B T_e.
\]

This formula looks exactly as for the ideal gas, but it is actually applicable for a plasma with arbitrary strong Coulomb’s interaction \(U\) between the particles.
Next, at the second step of our consideration, the average kinetic energy \( \langle k \rangle \) can be related to the average potential energy \( \langle u \rangle \) by the virial theorem for the Coulomb’s field [10]:

\[
\langle k \rangle = \frac{1}{2} \left| \langle u \rangle \right| ,
\]

which is also valid at the arbitrary strength of interparticle interaction. Strictly speaking, the virial theorem is applicable only to the system of particles experiencing a finite (i.e. restricted in space) motion. Nevertheless, we can expect that this theorem will be sufficiently accurate also for a freely expanding plasma cloud if the characteristic time of variation in its macroscopic parameters (\( \gtrsim 10^{-5} \) s for the particular experimental setup [9][11]) is considerably greater than the microscopic periods of motion of the electrons (\( 10^{-9} \div 10^{-7} \) s).

Finally, at the last step of our consideration, the average potential energy can be evidently expressed through the characteristic distance between the particles:

\[
\langle u \rangle \sim \frac{e^2}{\langle r \rangle} \sim e^2 n^{1/3} .
\]

Therefore, combining all the above formulas, we get \( T_e \propto n^{1/3} \). In particular, if the cloud expands inertially (i.e. linearly in time) and, consequently, its concentration changes as \( t^{-3} \), we get:

\[
T_e \propto t^{-1} .
\]

In summary, we conclude that the presented model of virialization of the charged particle velocities well explains both experimental features of thermal evolution of the plasma, namely: (a) the system “forget” in the course of time about its initial temperature, i.e. the plasma clouds with various initial temperatures evolve by the same way; and (b) the particular functional dependence is close to \( t^{-1} \) instead of the intuitively expected \( t^{-2} \). The inelastic processes, such as three-body recombination, are not of importance in this model.

3 Numerical Simulations

To verify the above theoretical estimates, we performed \( ab \) initio simulation of the plasma dynamics, based on the numerical solution of the equations of

\[\text{[Note: Since the virial theorem directly relates the energies averaged over time, we need to assume also that the system is ergodic, i.e. the quantities averaged over time are equal to the ones averaged over ensemble.]}\]
classical mechanics for the multi-particle system. Our approach differed from the earlier works in the following aspects.

First of all, the authors of most of the previous simulations of ultracold plasmas tried to include into consideration as many particles as possible. Unfortunately, to reduce the computational cost, they had to use some simplifications of the equations of motion of the light particles (electrons), such as the particles-in-cell (PIC) method [12] or Vlasov approximation for the electrons [13]. Both these approaches are based on the introduction of average electric fields and, therefore, completely ignore strong individual electron–ion interactions (large-angular scattering), which are just responsible for the virialization of velocities. As distinct from these approximations, we did not intend to simulate as many particles as possible but tried to integrate the equations of motion of the electrons in the real electric microfields as accurately as possible, without using any extra simplifications. (The ions were assumed to be very heavy and moved by a purely inertial law.)

Yet another well-known problem in modeling of the expanding plasmas is a considerable change of the spatial scale of the system (and, therefore, the amplitude of Coulomb’s forces) during its evolution. As a result, it is quite difficult to choose the method of numerical integration ensuring a reasonable accuracy in the entire time interval. We resolved this problem by introducing a “scalable” coordinate frame, expanding in space with the average velocity of plasma outflow. In other words, the initial equations of the electron motion

$$d^2\mathbf{r}_{ek}/dt^2 = \mathbf{F}_{ek}, \quad k = 1, \ldots, N_e$$

(7)

(where $\mathbf{F}_{ek}$ is the total Coulomb’s force acting on $k$’th electron from all other electrons and ions) after the introduction of dimensionless variables $r^* = r/\tilde{l}$, $t^* = t/\tau$ and transformation to the coordinate frame expanding with plasma, $\tilde{l} = \tilde{l}_0(1 + u_0^* t^*)$, can be reduced to

$$\ddot{\mathbf{r}}_{ek} + 2 u_0^* (1 + u_0^* t^*)^{-1} \dot{\mathbf{r}}_{ek} = (1 + u_0^* t^*)^{-3} \mathbf{F}_{ek}^*.$$  

(8)

Here, $\tau = (m/Ze^2)^{1/2} \tilde{l}_0^{3/2}$ is the characteristic plasma time (on the order of the inverse Langmuir frequency), $\tilde{l}$ is the characteristic distance between the particles ($\tilde{l}_0$ is its value at the initial instant of time); $u_0^*$ is the dimensionless velocity of the inertial expansion of the plasma cloud, determined by the relation $u_0^* = u_0 \tau/L_0$, where $L_0$ is the size of the computational cell used in our simulations, and $u_0$ is the velocity of its boundary; $\mathbf{F}_{ek}^*$ are the dimensionless Coulomb’s forces, and the dot denotes derivative with respect to the dimensionless time $t^*$.

Therefore, as follows from equations (8), the effect of inertial plasma outflow in the expanding coordinate system looks like an effective dissipative force, proportional to the electron velocities. Consequently, the temperature of the
Fig. 1. Simulated electron temperature as function of time in the logarithmic scale. The inclined dashed lines show the power-like dependences $T_e \propto t^\alpha$; the values of $\alpha$ being presented near the respective lines.

electron gas is determined by the competition between two effects: (a) acceleration and heating of the electrons due to Coulomb’s interactions with ions and (b) their deceleration and cooling by the above-mentioned dissipative forces.

It is important to emphasize also that transformation from the equations (7) to (8) enabled us to perform a numerical integration in the fixed region of dimensionless coordinates and, therefore, to avoid the problem of quick losing the computational accuracy when the spatial scale of the system changes very much.

The results of our simulations are presented by crosses in Fig. 1. If we do not take into account the earliest time interval, when the relaxation processes occur, the computational points in logarithmic coordinates are located almost along a straight line, corresponding to the power law of evolution of the electron temperature: $T_e \sim t^\alpha$. The corresponding exponent was estimated to be within the limits $\alpha = -(1.08 \div 1.25)$. This is quite close to the value $\alpha = -1$, following from the simple virial estimate, and is in excellent agreement with the experimental values $\alpha = -(1.1 \div 1.3)$ [9].
4 Conclusions

Analysis of the available data on the evolution of the electron temperature in the freely expanding ultracold plasma clouds shows that a heat release due to three-body recombination cannot explain quantitatively the experimental results. On the other hand, taking into account the strong electron–ion correlations and the resulting virialization of the charged particle velocities (i.e. modification of the equation of state of the plasma) leads to the perfect agreement with the experimental data.

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