Self-diffusion and conductivity in an ultracold strongly coupled plasma: Calculation by the method of molecular dynamics

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Abstract. We present results of calculations by the method of molecular dynamics of self-diffusion and conductivity of electron and ion components of ultracold plasma in a comparison with available theoretical and experimental data. For the ion self-diffusion coefficient, good agreement was obtained with experiments on ultracold plasma. The results of the calculation of self-diffusion also agree well with other calculations performed for the same values of the coupling parameter, but at high temperatures. The difference in the results of the conductivity calculations on the basis of the current autocorrelation function and on the basis of the diffusion coefficient is discussed.

1. Introduction
Self-diffusion and conductivity of the charged particles in the low-temperature plasmas are being intensively investigated by experimental, analytical and numerical methods [1–10]. In experiments on low-temperature plasmas [1] (at a temperature of more than 1000 K), the conductivity of the charged particles depends on the collisions between them and collisions with neutral particles. It is usually quite difficult to determine the contribution of the Coulomb conductivity (i.e. conductivity that is determined by charged particles collisions only) in the conductivity of the plasma, as there is no accurate enough data on cross sections for interactions of electrons and ions with neutrals. In addition, it is extremely difficult to obtain a fully ionized low-temperature dense plasma in experiments [1].

Theoretical approaches to calculate the Coulomb conductivity also have difficulties under strong coupling conditions [2–5], i.e. when the Coulomb coupling parameter $\Gamma_k = e^2/(T_k a)$ (where $a = (4\pi n_k/3)^{-1/3}$, $e$ is the electron charge, $n_k$ and $T_k$ are the density and temperature of particle species $k$ respectively) of the order or greater than unity. The analytical expressions obtained for small coupling parameters include the Coulomb logarithm which becomes negative already at $\Gamma \geq 0.45$.

As for the numerical calculations of models of Coulomb systems, the results depend on the choice of the model. The papers [6, 7] published in recent years are among the papers in which the diffusion coefficients and the conductivity of strongly coupled plasma were calculated.

In [6] for the calculation of transport coefficients, a hypernetted chain effective potential and a modified-Enskog correction were used.
In paper [7], an equilibrium two-component system of electrons and ions was considered at high temperatures and densities. The potential of the interaction of unlike charged particles was the Kelbg pseudopotential, which depends on temperature and at small distances is finite because paired quantum effects were taken into account. For particles of the same charge, Coulomb’s law was used. Below we discuss the results of these studies.

In order to determine the most satisfactory model of a Coulomb plasma, reliable experimental data is needed. As was said above in experiments on a low-temperature plasma, it is very difficult to single out the non-Coulomb part of diffusion and conductivity because of the unsatisfactorily determined contribution of the charge-neutral interaction.

The pure Coulomb self-diffusion was obtained in the study of ultracold plasma [8–10]. Ultracold plasma is created by ionization of the narrow-band laser of an ultracold gas of atoms in a magnetic optical trap. Ultracold plasma is non-equilibrium, since the equilibrium plasma does not exist at temperatures of 1 K and less. However, the experimental equipment allowed the study of ultra-cold plasma processes at a very small time scale of about 0.1–1 \( \mu s \). During these short periods of time the temperatures of electrons and ions are established and changed only slightly. It is important to note that the temperatures of electrons and ions are substantially different, since at the initial moment of ionization the ions have the kinetic energy of atoms, the temperature of which is \( \sim 10^{-3} \) K, and the kinetic energy of the electrons is determined by the excess of photon energy above the ionization threshold, which can be tuned in the range 1–1000 K.

It is possible to achieve large coupling in the ultracold plasma during short period of its existence, despite a low density of charged particles \((10^8–10^{10} \text{ cm}^{-3})\), and due to the very low temperatures. Moreover, the coupling parameter for ions is significantly higher than for electrons. Also it is important to note that at this time scale electron-ion recombination is negligible.

In the work [10] an ultracold plasma of alkaline earth element \(^{88}\text{Sr}\) was studied. The choice of this element is due to the fact that the ion transition from the ground state to the first excited state is in the optical part of the spectrum. This allowed to conduct a laser visual monitoring of the particle movement and therefore to obtain the velocity of the ions. In the experiments [10] the self-diffusion coefficient values of ions were obtained in a wide region of conditions of strong coupled plasma.

2. Physical model and molecular dynamics simulation

In the present work we used the physical model of ultracold plasma in which the charged particles interact according to Coulomb’s law without any restrictions at large or small distances. There are also no additional parameters in this model. The calculations were carried out by molecular dynamics method with a variable time step.

In this paper we give some results of calculations of self-diffusion and conductivity of electrons and ions in a region of parameters, which is wider than the region of the experiment. A good agreement with experimental data was obtained. It was compared with some analytical theories and numerical calculations.

We considered the model of a system of charged particles consisting of protons and electrons with concentration \( n_e = n_i \), interacting according to the Coulomb law. We considered electron-proton system as neutral two-temperature plasma. A similar model, but for one-temperature plasma, was considered in [11–13]. In our simulations classical equations of motion were solved for 200–500 electrons and 200–500 ions in the simulation cell using \( NV E \) ensemble. The number of particles in the cell was chosen so that the screening length was less than the cell size. To simulate continuous plasma we applied periodic boundary conditions to the cell. The particle density in the calculations was equal to \( 10^{10} \text{ cm}^{-3} \). The electron temperature was varied between 10 and 50 K, and the temperature of protons between 1 and 10 K. We calculated the velocity
autocorrelation functions (VAF) of the electron and the proton depending on time.

The VAF time integral yields the self-diffusion coefficient through the Green–Cubo relation:

$$D = \frac{1}{3} \int_{0}^{\infty} \langle V_j(t) V_j(0) \rangle \, dt,$$

(1)

here, $V_j$ is the velocity of particle $j$, and brackets indicate an equilibrium, canonical-ensemble average. The self-diffusion coefficient in the simplest binary collisions approach is inversely proportional to the collision frequency $\nu$:

$$D = \frac{T_k}{m_k \nu^2}.$$

(2)

In a very short time temperatures of the ions and electrons are increased to a few degrees of K. This is due to the restructuring of the chaotic distribution of particles to a relatively orderly due to the Coulomb interaction. In the literature this process is called “disorder induced heating”. After that for some time the temperatures of ions and electrons remain practically unchanged, and then begin to slowly grow due to the process of recombination. Moreover, the process of recombination within small times is determined by the formation of highly excited states (this allows us to describe the system using classical mechanics approach in the above model of the ultracold plasma). As a result we see in our calculations a relatively weak increase in the temperature of charged particles over time intervals up to about $t \sim 10^{-6}$ s. Considering the time intervals in which the temperature remains relatively constant and calculating VAF in these intervals we obtained the self-diffusion coefficients of charged particles under various values of Coulomb coupling parameter.

The determination of temperature and its stability was carried out using calculation of the velocity distribution function of particles and by comparing it to the Maxwell distribution for a certain temperature.

Previous works [7] on molecular dynamics study of strongly coupled plasma kinetics showed that number of particles $N \approx 150–200$ is sufficient and leads to small simulations errors. In the present work we used overall number of particles not less than 400 and estimated errors of our results is less than symbols size in presented figures.

3. Results

Figure 1 presents an example of our calculations of the velocity distribution function of electrons and ions. It is seen that it is well described by a Maxwell function at $T_e = 10$ K for electrons and
Figure 2. Velocity autocorrelation function for electrons (a) and ions (b).

Figure 3. Dimensionless self-diffusion coefficient.

for ions at $T_i = 11$ K. It should be noted that the Maxwell distribution function for electrons, as expected, established much faster than for protons. Therefore, for protons it is necessary to carry out longer calculations.

Figure 2 presents an example of the calculation of the electrons VAF for $T_e = 10$ K and the ions VAF for $T_i = 11$ K. From the VAF we calculated self-diffusion coefficient $D$ using relation (1). It is convenient to plot self-diffusion coefficient in dimensionless form using following relation:

$$D^* = D/a^2 \omega_p,$$

here $\omega_p$ is the plasma frequency,

$$\omega_p = \left( \frac{4\pi n_k e^2}{m_k} \right)^{1/2}.$$
Figure 3 presents our calculations of self-diffusion coefficient in dimensionless form and data taken from the experimental work [10]. This figure shows the dependence of the dimensionless self-diffusion coefficients for electrons and ions on the coupling parameter $\Gamma$. Theoretical curve plotted by solid line is obtained using classical Landau–Spitzer collision frequency $\nu_0$ divided by a constant factor $C$:

$$\nu = \frac{1}{C} \nu_0 = \frac{1}{C} \frac{4\sqrt{\pi} n_e e^4}{3 \sqrt{m_e T_e^3} \Lambda}, \quad (5)$$

where $\Lambda$ is the Coulomb logarithm,

$$\Lambda = \ln \frac{\sqrt{4\pi e^2 n_e / T_e}}{e^2 / T_e}. \quad (6)$$

Correction factor value $C = 0.582$ similar to correction to electrical resistivity in [2] was used to plot the Landau–Spitzer curve in figure 3. It is interesting to note that as can be seen this correction is in good agreement with molecular dynamics data for electrons.

There is a good agreement between our calculation results for ion self-diffusion coefficient and the experimental data. It should be noted that the results of the works [6, 7] are also consistent with the experimental data, although the calculation models do not describe the ultracold plasma (we used VAF presented in [7] to calculate corresponding values of $D^*$). The fact that our results for self-diffusion of ions agree with the experiment allows us to consider that our calculations of self-diffusion of electrons are also physically correct. This is also indicated by our results agreement with results of [7] for both electrons and ions. This enables us to determine the conductivity of ultracold plasma in the one-electron approximation using the self-diffusion coefficient for electrons. In this case, the dimensionless conductivity is

$$\sigma^* = \frac{\sigma}{\omega_p} = \frac{3}{4\pi} \Gamma D^*. \quad (7)$$

Figure 4 presents our calculations and data [7] of the Coulomb conductivity in dimensionless form. Despite the fact that the physical model of a plasma [7] describes a hot and dense
plasma, there is a reasonable agreement up to parameters at which the difference in the Kelbg pseudopotential from the Coulomb potential begins to affect the calculations.

4. Conclusion
We performed the calculations of self-diffusion and conductivity in a model of ultra-cold plasma of electrons and ions in a region of conditions, which is wider than the region of the recent experiment. Good agreement with experiment was obtained.

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