Diffusion in ultracold strongly coupled multiply charged plasma: Calculation by molecular dynamics method

A A Bobrov, A M Bunkov, S Ya Bronin, A B Klyarfeld, B B Zelener and B V Zelener
Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
E-mail: abobrov@inbox.ru

Abstract. We present the results of calculations of electron and ion diffusion by the method of molecular dynamics in an ultracold multiply charged plasma. The calculations were carried out in a wide range of Coulomb coupling parameter. The problems of similarity for a Coulomb multiply charged plasma are discussed. It is shown that in a multiply charged classical plasma for the diffusion coefficients in a wide range of coupling parameter, the similarity assumption is valid.

1. Introduction

Diffusion and conductivity of charged particles in low-temperature plasmas are being intensively investigated by experimental, analytical and numerical methods [1]. 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 [1], 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) is of order or greater than unity. The analytical expressions [2,3] obtained for small coupling parameters include the Coulomb logarithm which becomes negative already at $\Gamma \gtrsim 0.45$. As for the numerical calculations of models of Coulomb systems, the results depend on the choice of the model. The papers [4,5] published in recent years are among the papers in which the diffusion coefficients and the conductivity of strongly coupled plasma were calculated. In [4] for the calculation of transport coefficients a hypernetted chain effective potential and a modified Enskog correction were used. In [5] 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, the Coulomb law was used. In order to
determine the most satisfactory model of the Coulomb plasma, reliable experimental data is
needed. As was said above in the 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 non-Coulomb contribution.

Pure Coulomb diffusion was obtained by studying ultracold plasma [6]. Ultracold plasma is
created by ionization of an ultracold gas of atoms in a magnetic optical trap with a narrow-
bond laser. 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 µs. 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 from 1 to 1000 K.

It is possible to achieve strong coupling in ultracold plasma in a short period of its existence,
despite of the low density of charged particles (\( 10^8 - 10^{10} \) cm\(^{-3} \)), and because of 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 [6], ultracold plasma of alkaline earth element \(^{88}\)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 conducting a laser visual monitoring of the particle
movement and therefore to obtain the velocity of the ions. In the experiments [4,6] the diffusion
coefficient values of ions were obtained in a wide range of the plasma coupling.

In our previous work [7], the experimental data for the ion diffusion coefficient of ultracold
plasma [6] gave us the opportunity to verify our calculations by the molecular dynamics of
transfer coefficients for our model of a nonequilibrium ultracold plasma. This plasma model
considers a system of electrons and ions interacting via the Coulomb potential without any
restrictions at large and small distances. This physical model can be realized only because very
low density of ultracold plasma is considered. The comparison of the calculation results with
the experiment data showed that our model reliably reflects the physical reality.

The agreement of the experiment and the calculation results allowed us to assume that other
properties of the ultracold plasma, which cannot yet be determined experimentally due to the
absence of diagnostic methods, will also be close to reality. We carried out calculations of the
electron diffusion coefficient and conductivity. This results agree well with calculations [5] by
the molecular dynamics method of an equilibrium low-temperature plasma in the region where
quantum effects can be neglected (ion diffusion coefficients also are similar). Moreover, the
calculations of conductivity [7] are in a quite good agreement with the experiment for strong
coupled low-temperature plasma in the temperature range of several tens of thousands of K and
densities greater than \( 10^{18} \) cm\(^{-3} \).

The reason for the present work was the conclusion in [1, section 7.5] that there is no similarity
for the Coulomb component of electrical conductivity in the case of multiple ionization when
the coupling parameter is of the order or greater than unity.

In the present work, we used the molecular dynamics model of the classical two-component
two-temperature plasma, in which the interaction between charges is Coulomb without any
restrictions at small and long distances and without any additional parameters. We applied
our model to calculate the transport properties of a nonequilibrium ultracold double and triple
charged plasma. The ion charge is \( z = 2 \) or \( 3 \). The diffusion coefficients of electrons and ions
were calculated.
2. Physical model and molecular dynamics simulation

We considered physical model of ultracold plasma in which the charged particles (\(z\)-charged ions and electrons with concentrations \(n_e = zn_i\)) interacting according to the Coulomb law without any restrictions at large or small distances. There are also no additional parameters in this model. The calculations were carried out by the method with a variable time step with the base time step value \(10^{-14}\) s. A similar model and simulation method were considered by us for the ultracold plasma diffusion calculation in [7]. We considered electron-ion system as a neutral two-temperature plasma. In our simulations classical equations of motion were solved for 500–1100 electrons and 250–350 ions in the cubic simulation cell using constant number of particles, constant volume and constant full energy (\(NVE\)) 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 electron density in the calculations was equal to \(10^{10}\) cm\(^{-3}\). The electron temperature was varied in the range from 10 to 250 K, and the temperature of ions from 1 to 250 K. We calculated the time-dependent velocity autocorrelation functions (VAF) for the electrons and the ions.

The electron velocity autocorrelator vanished with an accuracy of \(1/\sqrt{N}\) for ten nanoseconds. For ions, this time was an order of magnitude longer. Length of the calculations (in the base time steps) was varied from \(5 \times 10^5\) for strong coupling to \(5 \times 10^6\) for weak coupling.

The criterion for the correctness of the calculations was the conservation of the energy value of the system in the range of 0.1–1%. The possibility of very close collision of electrons with ions is extremely unlikely due to the extreme rarefaction of the plasma, which is taken into account in the initial conditions:

- the coordinates of electrons and ions were set randomly;
- the velocity for each particle was chosen randomly within the framework of the Maxwell distribution at a given initial temperature which was different for electrons and ions;
- the averaging over initial conditions (up to 100 variants) was carried out.

A feature of the calculation of the velocity autocorrelator in ultracold plasma is that this plasma is two-temperature. Considering the time intervals at which the temperature of particles of each type remains almost constant, and calculating the velocity autocorrelators at these intervals, one can obtain the diffusion coefficients of charged particles for various values of the coupling parameter. In our case, the coupling parameter for ions will be significantly higher than for electrons.

Determination of temperature and its stability in the calculation by the method of molecular dynamics was carried out using the formation of the velocity distribution function of particles and its correspondence to the Maxwell function at a certain temperature.

To determine the diffusion coefficient of charged particles in ultracold plasma, autocorrelators of the velocity of ions and electrons were calculated. Based on the well-known Kubo formula [7], the diffusion coefficient is determined by the following expression:

\[
D = \frac{1}{3} \int_0^{\infty} \langle V_i(0) V_i(t) \rangle dt, \tag{1}
\]

where \(V_i(0)\) and \(V_i(t)\) are the \(i\)th particle velocities at the initial moment of time and at the moment of time \(t\). Averaging is carried out over all particles of this class that are considered in a periodic cell. When calculating the diffusion coefficients in a plasma with different ion charges, it was also necessary to find out whether the similarity law is observed for systems of particles with Coulomb interaction in a wide coupling region.

In this regard, we used the following parameters, which allowed us to display the results of calculations for each coefficient regardless of the ion charge in one plot:

- for the ion diffusion coefficient,
– the plasma frequency
\[ \omega_p^i = \sqrt{\frac{4\pi e^2 z^2 n_i}{m_i}}, \quad (2) \]
– the Wigner–Seitz radius
\[ a_i = (4\pi n_i/3)^{-1/3}, \quad (3) \]
– dimensionless ion diffusion coefficient
\[ D_i^* = \frac{D_i}{a_i^2 \omega_p^i}, \quad (4) \]
– the coupling parameter
\[ \Gamma_i = z^2 e^2 (4\pi n_i/3)^{1/3}/T_i; \quad (5) \]

• for the electron diffusion coefficient,
– the plasma frequency
\[ \omega_p^e = \sqrt{\frac{4\pi e^2 n_e}{m_e}}, \quad (6) \]
– the Wigner–Seitz radius
\[ a_e = (4\pi n_e/3)^{-1/3}, \quad (7) \]
– dimensionless electron diffusion coefficient
\[ D_e^* = \frac{D_e}{a_e^2 \omega_p^e}, \quad (8) \]
– coupling parameter
\[ \Gamma_{ei} = ze^2 (4\pi n_i/3)^{1/3}/T_e. \quad (9) \]

It should be noted that the size of the Wigner–Seitz cell is determined by the ion concentration for the diffusion of ions and electrons. This follows from the formulas for weakly coupled plasma.

2.1. Ion diffusion coefficient
Figure 1 shows the results of our calculations of ion diffusion coefficients for \( z = 1, 2 \) and 3 using parameters (2)–(5).

As can be seen in figure 1, such a choice of dimensionless parameters leads to the coincidence of the dimensionless ion diffusion coefficient for various \( z \), values of the coupling parameter and masses. In our calculations the ion mass was equal to the proton mass, in the experiment to the strontium mass, in the calculations \([5]\) to the one hundred electron masses. The good agreement of the results for different masses is consistent with the results of \([5]\). In \([5]\), it was shown that ionic and electronic velocity autocorrelation functions are independent of ion to electron mass ratio for \( m_i/m_e > 100 \).

2.2. Electron diffusion coefficient
Figure 2 shows the results of our calculations of electron diffusion coefficients for \( z = 1, 2 \) and 3 using parameters (6)–(9). The difference between the calculations \([5]\) and our calculations is due to the difference in the electron-ion potential in \([5]\) from the Coulomb potential. Based on the obtained results, it can be assumed that the conductivity in Coulomb plasma, where quantum effects are insignificant, in dimensionless variables will also have the similarity property.
3. Conclusion
We performed the calculations of charged particles diffusion in a model of ultracold multiply charged plasma in a wide region of conditions. It is shown that for Coulomb systems with
different ion charges the law of similarity is valid: for the ion diffusion for $\Gamma_1$ in the range from 0.03 to 10 and for the electron diffusion for $\Gamma_{ei}$ from 0.03 to 0.7.

Acknowledgments
The work is supported by the Presidium of the Russian Academy of Sciences in the framework of the fundamental research program “New approaches to the creation and study of extreme states of matter”.

References
[1] Fortov V E and Iakubov I T 1989 Physics of Nonideal Plasmas (New York: Hemisphere Publishing)
[2] Landau L D 1936 Phys. Z. Sowjet 10 154
[3] Spitzer L 1967 Physics of Fully Ionized Gases (New York: Interscience)
[4] Baalrud S D and Daligault J 2015 Phys. Rev. E 91 062107
[5] Morozov I V and Norman G E 2005 J. Exp. Theor. Phys. 100 370–84
[6] Strickler T S, Langin T K, McQuillen P, Daligault J and Killian T C 2016 Phys. Rev. X 6 021021
[7] Bobrov A A, Vorob’ev V S and Zelener B V 2018 Phys. Plasmas 25 033513