Electrical current and conductivity in ultracold plasma: Study by molecular dynamics method

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Abstract. Calculation of electrical current in ultracold strongly coupled plasma was studied by using molecular dynamics method. The current was induced by electric field applied to the plasma. Simulations were made for different values of coupling parameter. Conductivity was defined as a ratio of current and electric field. Comparison with results of other calculations was made. Our results for conductivity differ from calculations based on a diffusion coefficient and an auto-correlation function for the electric current.

1. Introduction
For the first time, ultracold plasma was created and observed in 1999 [1]. Ultracold plasma has features, which allow studying kinetics of strongly coupled Coulomb systems. It is completely ionized neutral plasma and properties of this plasma are determined by collisions of charged particles only. This is one of important differences between the laser prepared ultracold plasma and the usual low-temperature plasma where charge-neutral collisions are important.

Ultracold plasma can be made strongly coupled since the plasma will be produced from ultracold atomic gas with high number density. Atoms will be ionized by laser emission and electron temperature will be determined by difference between laser photon energy and ionization threshold. This excess energy depends on laser detuning and it can be made quite low, just several kelvins.

Theoretical investigation of strongly coupled plasma is complicated problem due to the lack of small parameters and to solution of this problem various calculation methods should be used. Previously we reported our results of calculation of an ion self diffusion coefficient in strongly coupled plasma [2]. Our theoretical results agree with results of the recent work [3], where for the first time the ion self-diffusion coefficient was measured in coupled ultracold plasma. We also calculated electron diffusion coefficient which is not measured yet.

In the frame of one electron approximation by using electron diffusion coefficient we estimated the electrical conductivity in the wide range of coupling parameter.

We would like to note that our results for diffusion in ultracold plasma agree with results of [4], where the calculations were made by using molecular dynamics method for hot dense strongly coupled plasma with the same values of coupling parameter. In [4] the conductivity was also calculated by using the current autocorrelation function. The results differ from our recent results. It is important to note that in both our previous calculations [2] and calculations of [4] we used indirect methods for the conductivity estimation. In the present paper, we present
our recent results of calculation of the conductivity by using the direct simulation of electrical current in plasma.

2. Theoretical model

Ultracold plasma produced in experiments is essentially a non equilibrium and non stationary system. Equilibrium ionization degree which follows from Boltzman distribution must be zero for such low temperatures. But as was observed in experiments and shown in theoretical works the main recombination process which is three body recombination is strongly suppressed in the ultracold plasma. The reason of the very low recombination rate is strong coupling of the plasma. The ultracold plasma with high ionization degree observed in experiments can exist for long times up to tens of microseconds.

In typical experimental conditions the ultracold plasma is not in thermal equilibrium as well. The electron temperature $T_e$ and ion temperature $T_i$ are established separately but due to high ion to electron mass ratio energy exchange rate is very slow.

In the present paper, we considered kinetics of fully ionized ultracold strongly coupled plasma. We simulated the plasma for times much less than characteristic recombination time and electron–ion energy exchange time. Due to short timescale we considered the plasma as being in quasi stationary and quasi equilibrium state for a simulation duration.

To simulate the ultracold plasma by using the molecular dynamics method we placed charged particles in a cubic cell. Then we solved equations of motion for the charged particles. Neutral plasma of electrons and protons was considered. The Coulomb potentials were used for all charged particles. In order to take into account behavior of particles at the short distance between particles during the collisions we used a leapfrog integration with variable time step.

Classical equations of motion were solved for the particles in the selected cell. In our case the classical approach is correct due to the average distance between particles is much more than de Broglie wavelength. In our case the main recombination process that occurs in such a plasma is three-body recombination in which only highly excited states can be formed. These Rydberg states can be described by classical mechanics with good accuracy.

In the present paper, we considered 1000 particles in the simulation cell ($N_e = 500$ electrons and $N_p = 500$ protons). Cell size was selected to correspond to electrons number and given electron density $n_e$. Initial positions of electrons and protons in the simulation cell where chosen randomly. Initial particles velocities directions were set also randomly, velocities absolute values were selected in such way, that initial total kinetic energies of electrons and protons were equal to the given initial values $E_e(0)$ and $E_p(0)$ respectively. For more simulation details see [2].

To simulate electrical current in the plasma electrical field $E$ was applied at some time after starting point of integration (the delay was to provide electron temperature equilibrium). Electrical field was directed along one of the edges of the simulation cell (parallel to the x-axis).

3. Results and discussion

In the present paper, we report our results of calculations for electron density $n_e = 10^{10}$ cm$^{-3}$ and initial electron energies $E_e(0) = 2–30$ K. These values correspond to strongly coupled plasma. The strong coupling leads to a well known disorder induced heating effect [5]: after start of the simulation kinetic energy of electrons rapidly grows on timescale of inverse plasma frequency

$$\omega_p^{-1} = \sqrt{\frac{m_e}{4\pi n_e e^2}},$$

where $m_e$ is the electron mass, $e$ is the elementary charge. After heating, electrons gain energy of about $e^2/n_e^{-1/3}$, the temperature of electrons establishes, and electrical field is switched on.

Electrical field generate current in the plasma along the x-axis. To avoid possible non-linear effects due to massive run-away electrons formation we applied low values of electrical field $E$. 


Figure 1. Electrical current (a) and kinetic energy per one electron (b) during one of the simulations for $n_e = 10^{10}$ cm$^{-3}$, $T_e(0) = 10$ K, $E = 3 \times 10^{-4}$ statV/cm (critical field value for $T_e = 16$ K is $E_c \approx 6 \times 10^{-3}$ statV/cm).

We used values of $E$ much less than critical field value $E_c$ at which fraction of run-away electrons become significant [6]:

$$E_c = \frac{4\pi e^3 L n_e}{T_e},$$

where $L$ is the Coulomb logarithm:

$$L = \ln \left( \frac{\sqrt{T_e/4\pi n_e e^2}}{e^2/T_e} \right).$$

Total current was calculated using following formula:

$$\vec{I}(t) = \sum_{j=1}^{N_e} e \vec{v}_j(t),$$

where $\vec{v}_j(t)$ is the $j$-th electron velocity in the moment of time $t$.

In figure 1, typical dependences of current and corresponding electrons total kinetic energy on time during the simulation are shown for one of the runs for $n_e = 10^{10}$ cm$^{-3}$ and $T_e(0) = 10$ K. Electric field $E = 3 \times 10^{-4}$ statV/cm was switched on at $t = 1$ ns. Critical field value can be estimated as $E_c \approx 6 \times 10^{-3}$ statV/cm that is about 20 times higher than $E$ for this calculation. In figure 1(b), fast rise of electron energy is due to disordered induced heating which is clearly seen followed by the process of the Joule heating. Since the low electrical field value was used electron temperature growth due to the Joule heating is very slow.

In figure 2, velocities distributions for electrons along coordinate axes are shown for the same simulation as in figure 1. It is clearly seen from the figure that velocity distribution distortion along the $x$-axis is negligible and run-away electrons are not formed for such a low value of applied field.

To estimate electrical conductivity $\sigma$ the following relation for current density $J_x$ can be used:

$$J_x = \sigma E = \frac{I_x n_e}{N_e}.$$  

It is convenient to plot electrical conductivity in dimensionless form

$$\sigma^* = \frac{\sigma}{\omega_p}.$$
Figure 2. Electrons velocities distributions along the coordinate axes for the same molecular dynamics run as in figure 1 for the moment of time $t = 5$ ns. Points are the result of calculations, dashed line is the Maxwell distribution for $T_e = 16$ K.

Figure 3. Dimensionless conductivity as a function of the parameter $\Gamma$. The Landau–Spitzer conductivity is estimated from the collision frequency from [7].

Figure 3 presents our results of study of dimensionless conductivity as a dependence on the coupling strength $\Gamma = e^2/(T_e a)$, where $a = (4\pi n_e/3)^{-1/3}$. The Landau–Spitzer conductivity is plotted by solid line. To calculate conductivity we averaged molecular dynamics trajectories for relatively short times, so that the growth of the electron temperature due to Joule heating is not exceed 10%. The resulting error in $\Gamma$ is not exceed symbol size in figure 3. But this in turn
lead to rather high uncertainty in electrical current value which is the main source of error for resulting conductivity as shown in figure 3. For all the results electrical field value $E$ was at least an order of magnitude lower than corresponding critical field $E_c$.

Plotting conductivity in dimensionless form in dependence on $\Gamma$ allows us to compare our results for ultracold plasma conductivity to molecular dynamics results for hot dense plasma \cite{4}. In \cite{4} conductivity was calculated using current autocorrelation function. It is seen from the figure that our present results agree well with \cite{4} for moderate coupling but for $\Gamma \sim 0.5$ the results are different. We attribute this difference to the modified potential used in simulations \cite{4}. In \cite{4} the Kelbg potential was applied to describe electron–ion interaction instead of the Coulomb potential and possibly it affects the calculations in the region of high density and strong coupling.

In figure 3, our previous results \cite{2} for conductivity are shown. In paper \cite{2}, we used molecular dynamics method to calculate velocity autocorrelation functions (VAF) for electrons in ultracold plasma. From the VAF we calculated the diffusion coefficient and effective collision frequency. From the collision frequency we estimated electrical conductivity in one electron approximation. It is seen from the figure that results based on collision frequency differ both from our current results and from \cite{4}. The difference can be explained by the fact that conductivity is influenced by electron–ion collisions only. When two electrons collide their total momentum is conserved and the electrical current is unchanged. But the effective collision frequency includes both electron–ion and electron–electron scattering. This leads to underestimation of conductivity in \cite{2} as seen from the figure. The similar influence of electron–electron collisions account on plasma transport properties was also discussed in the recent paper \cite{8} where electrical and thermal conductivities for weakly coupled plasma were studied by density functional theory.

4. Conclusion

The current in ultracold strongly coupled plasma was simulated by using molecular dynamics method. The electrical conductivity was estimated by analyzing a dependence of the current density on the applied electrical field. The dimensionless conductivity is compared with conductivity obtained using two different indirect methods: one electron approximation and current autocorrelation function. It is shown that both approaches give results which are different from the results of direct method described in the present paper.

The calculation error is rather high for our current simulation results. We plan to reduce the error in two ways. The first one is to increase particle number in the simulation cell to reduce fluctuations. The second one is to calculate conductivity independently from the Joule heating kinetics.

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