Diffusion coefficient for electrons in magnetized ultracold plasmas

B B Zelener, B V Zelener, D R Khikhluhka, S Ya Bronin and A A Bobrov

Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
E-mail: abobrov@inbox.ru

Abstract. The diffusion coefficients for electrons in an ultracold plasma in strong magnetic field were calculated for the first time by the molecular dynamics method. Earlier, we reported our results on the diffusion coefficients without magnetic field and obtained good agreement with experiment. In contrast to a convenient low-temperature plasma, strong magnetic field affects transport coefficients in an ultracold plasma event for field magnitudes $10^3 - 10^4$ G. In the present paper a model of a system of charged particles consisting of electrons and protons interacting according to the Coulomb law without any correction of the potential at large or small distances was considered. Density of particles was varied from $10^{10} \text{cm}^{-3}$; the initial temperature of the electrons was from 5 to 100 K, the temperature of the ions was from $10^{-3}$ to 2 K; induction of the magnetic field was from 0 to $5 \times 10^4$ G.

1. Introduction

In weak magnetic fields $B$, when the impact parameter for charged particles collisions is smaller than the Larmor radius $r_B = V/\omega_B$, where $\omega_B = eB/(mc)$ is the Larmor frequency ($m$ and $e$ are respectively the mass and charge of the electron, $c$ is the speed of light) and $V$ is the velocity of the charged particle, one can use the approximation in which the action of the Coulomb center is considered as a weak perturbation to the initial cyclotron rotation of the particle [1–4]. In this case, the Larmor radius is taken as the maximum impact parameter in the Coulomb logarithm instead of the Debye radius.

The condition for strong magnetic fields in the classical description of collisions between electron with a certain velocity and ion (see, for example, [5]) can be written in the following form:

$$\frac{B}{B_0} \left( \frac{V}{c} \right)^{-3} \gg 1, \quad (1)$$

where $B_0 = m^2 c^4/e^3 = 6.05 \times 10^{15}$ G. This condition corresponds to the value of $B$ and the electron velocity $V$, at which the Larmor frequency is greater than the frequency of near collisions $V/(e^2/T_e)$, where $r_L = e^2/T_e$ is the Landau length. For electrons in the low-temperature plasma with a temperature of $\sim 10^4$ K, the value of $B$ satisfying inequality (1) is $10^8$ G, since the characteristic electron velocity $\sim 10^8$ cm/s. At present, the induction of homogeneous magnetic fields experimentally obtained in laboratory conditions reaches $5 \times 10^5$ G. At the same time, for electrons in Rydberg atoms, excitons in semiconductors, and also for free electrons in ultracold
plasma, with velocities of about $10^6$ cm/s, the value of $B$ satisfying inequality (1) is $10^4$ G. In strong magnetic fields, the nature of collisions varies for all impact distances in comparison with a weak magnetic field. This does not allow the use of perturbation theory methods. In this case, it is of interest to carry out molecular dynamics calculations of the coefficients of diffusion and conductivity of an ultracold plasma in a magnetic field, taking into account the possibility of carrying out experimental studies. The results of calculations by the molecular dynamics method of the electron diffusion coefficient of ultracold plasma in the electron temperature range 1–60 K and the magnetic field induction range from 0 to $5 \times 10^4$ G are presented.

2. Physical model and molecular dynamics simulation

We considered the model of a system of charged particles consisting of protons and electrons as neutral two-temperature plasma with concentration $n_e = n_i$. In the present work as well as in previous works [6–8] 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 contrast to [6], instead of the Verlet algorithm, a leapfrog algorithm with a variable time step was used, and the Lorentz magnetic force was taken into account using the Boris algorithm [9], specially developed for solving the equations of motion in the electric and magnetic fields. As mentioned above, we used the variable step $\delta t$, which depended on the interaction force between the two particles. If the particles were close to each other, the step was chosen so that the total energy of the particle system was maintained with the required accuracy, and in the case of an increase in the distance, it increased to $\sim 10^{-13}$ s (the choice of the maximum time step is determined by the Larmor period for electrons, which for the field $B = 5 \times 10^4$ G is $\sim 10^{-12}$ s).

We used a calculation method that preserves the total energy of the system. Therefore, the criterion for estimating the error of the method can be regarded as the deviation of the total energy of the system from the initial value. For the results of the calculations presented in this paper, the deviation of the total energy of the system was in the range 0.1–1%.

In our simulations classical equations of motion were solved for 100–500 electrons and 100–500 ions in the simulation cell using $NVE$ 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 particle density in the calculations was equal to $10^{10}$ cm$^{-3}$. The initial electron temperature was varied between 1 and 15 K, and the temperature of protons between $10^{-3}$ and 2 K. We calculated the velocity autocorrelation functions (VAF) along $\langle V_z(0)V_z(t) \rangle$ and across $\langle V_x(0)\bar{V}_x(t) \rangle$ the direction of the magnetic field.

If the only nonzero component of magnetic field is $B_z$ the diffusion tensor $D_{\alpha\beta}$, is diagonal so that

$$ D_{zz} = \frac{1}{N} \int_0^{\infty} \left\langle \sum_i V_z^i(0)V_z^i(t) \right\rangle dt, \tag{2} $$

and

$$ D_{xx} = D_{yy} = \frac{1}{2N} \int_0^{\infty} \left\langle \sum_i \left( V_x^i(0)V_x^i(t) + V_y^i(0)V_y^i(t) \right) \right\rangle dt, \tag{3} $$

where

$$ \langle V_z^2(0) \rangle = V^2(0)/3 = V_\perp^2, \langle V_x^2(0) \rangle = \langle V_y^2(0) \rangle = V^2(0)/3 = V_\perp^2/2. \tag{4} $$

Until the first collision the velocities $V_\alpha^i(t)$ are

$$ V_x^i(t) = V_\perp \sin(\phi_i + \omega_B t), V_y^i(t) = -V_\perp \cos(\phi_i + \omega_B t). \tag{5} $$
Figure 1. Electron velocity autocorrelators along the magnetic field for different values of the field: $B = 5 \times 10^2$ (a), $5 \times 10^3$ (b) and $10^4$ G (c). Black solid line is the result of molecular-dynamics (MD) calculations, red dashed line is exponential function fit.

Phase $\phi_i$ is the initial angle of $\vec{V}_\perp$ in the $X$–$Y$ plane. It is natural to assume that the velocity autocorrelator in the direction of the magnetic field will not depend explicitly on $\omega_B$, and in the perpendicular direction this dependence will have the form of a damped periodic function.

3. Results
The calculations carried out showed, first of all, that the magnetic field in the range from 0 to $5 \times 10^4$ G only affects the diffusion of electrons in the ultracold plasma. Therefore, we present the calculation results only for electrons. In addition, the calculations showed that the electron temperature at first the same in all three coordinates in the presence of the field is different in the direction of the field and perpendicular to it. And this difference increases with increasing induction. This is related to the fact that the Maxwell distribution in each direction is due to fast electron–electron collisions relaxation, and the energy exchange between the degrees of freedom of the electron along and across is significantly slowed down [5]. For equilibrium plasma, with time, the temperature should become the same and independent of the direction, but in our case of nonequilibrium quasistationary plasma we consider a small time interval in which the temperature is constant in each direction.

Figure 1 presents an example of the results of calculations for velocity autocorrelators along the field at a given temperature $T_e = 15$ K and density $n_e = 10^{10}$ cm$^{-3}$, depending on the value of the magnetic field induction. As seen from the graphs, these results are approximated fairly well by the exponential function.

Figure 2 presents an example of the results of calculations for velocity autocorrelators across the field at a given temperature $T_e = 15$ K and density $n_e = 10^{10}$ cm$^{-3}$, depending on the value of the magnetic field induction. As can be seen from the graphs, these results are approximated fairly well by the product of the damped exponential function by periodic function, depending on $\omega_B$, since the oscillations of the autocorrelator are due to the Larmor frequency, which is established in the process of numerical analysis.

Approximation formulas reliably describe the results of calculating the velocity autocorrelators. This allows us to calculate the diffusion coefficients along and across the magnetic field. For the velocity autocorrelator along the field, the diffusion coefficient has the form:

$$D_{zz} = \frac{V^2(0)}{3} \int_0^\infty \exp(-t/\tau)dt = \frac{V^2(0)}{3} \tau,$$

where $\tau$ is the decay time of the correlator; $\tau$ is inversely proportional to the electron collision frequency in the field direction.
Figure 2. Electron velocity autocorrelators across the magnetic field for different values of the field: $B = 5 \times 10^2$ (a), $5 \times 10^3$ (b) and $10^4$ G (c). Black solid line is the MD calculations result, red dashed line is dumped sine function fit.

Figure 3. Dimensionless diffusion coefficient along the field as a function of the parameter $\Gamma$. Landau–Spitzer points are calculated from the collision frequency of [1].

For the velocity autocorrelator across the field, the diffusion coefficient has the form:

$$D_{xx} = D_{yy} = \frac{V^2(0)}{3} \int_0^\infty \exp(-t/\tau) \cos \omega_B t \, dt = \frac{V^2(0) \tau}{3(1 + \omega_B^2 \tau^2)}.$$  

When $\omega_B \tau \gg 1$

$$D_{xx} = D_{yy} = \frac{V^2(0)}{3\omega_B^2 \tau}$$  

and the collision frequency across the field is $\omega_B^2 \tau$.

Figure 3 presents the results of calculating the dimensionless diffusion coefficient of electrons along the direction of the magnetic field $D_z^* = V^2(0) \tau / (a^2 \omega_p)$ depending on the parameter $\Gamma = e^2 / (a T_z)$ for $B = 5 \times 10^4$ G. Here $a = (4\pi n_e / 3)^{-1/3}$ is the size of the Wigner–Seitz cell,
Figure 4. Dimensionless diffusion coefficient across the field for $n_e = 10^{10}$ cm$^{-3}$, $T_e = 14.5$ K, $\Gamma \approx 0.4$.

$\omega_p = (4\pi n_e e^2/m)^{1/2}$ is the plasma frequency. We estimate that calculation error for diffusion coefficient is not more than 10% which is less than symbol size in the scale of figure 3. These results within the limits of accuracy coincide with the diffusion coefficient without a field [10]. This indicates that in the investigated range from 0 to $5 \times 10^4$ G the electron diffusion coefficient along the direction of the magnetic field does not depend on the field.

Figure 4 presents the results of calculating the dimensionless diffusion coefficient of electrons across the direction of the magnetic field $D_{xx} = (V^2(0)/3\omega_B^2 \tau)/(a^2 \omega_p)$ from $\omega_B/\omega_p$ for $\Gamma = 0.4$. It turned out that in the whole range of parameters that we have investigated where $\omega_B \tau \gg 1$, the diffusion coefficient across magnetic field $D_{xx}$ decreases sharply with increasing $B$ and tends to zero in the limit of high values of $B$.

4. Conclusion

The diffusion coefficients for electrons in ultracold plasma in strong magnetic field were calculated for the first time by the molecular dynamics method. It is shown that in the case $\omega_B \tau \gg 1$ the dimensionless diffusion coefficient of electrons along the magnetic field direction is independent of the field, and the dimensionless electron diffusion coefficient across the direction of the magnetic field decreases sharply with increasing $B$ and in the limit of high values of $B$ tends to zero.

Acknowledgments

The work is supported by the Russian Science Foundation (grant No. 14-50-00124).

References

[1] Spitzer L 1967 Physics of Fully Ionized Gases (New York: Interscience)
[2] Lifshitz E M 1937 Zh. Eksp. Teor. Fiz. 7 390
[3] Belyaev S T 1959 Plasma Physics and the Problem of Controlled Thermonuclear Reactions vol 3 ed Leontovich M A (New York: Pergamon)
[4] Silin V P 1960 Sov. Phys. JETP 11 1277
[5] Koryagin S A 2000 J. Exp. Theor. Phys. 90 853
[6] Bobrov A A, Bronin S Y, Zelener B B, Zelener B V, Manykin E A and Khikhlukha D R 2011 J. Exp. Theor. Phys. 112 527
[7] Bobrov A A, Bronin S Y, Zelener B B, Zelener B V, Manykin E A and Khikhlukha D R 2016 Dokl. Phys. 61 440
[8] Bronin S Y, Bobrov A A, Manykin E A, Zelener B B and Zelener B V 2016 J. Phys.: Conf. Ser. 774 012161
[9] Bobrov A A, Bronin S Y, Zelener B B, Zelener B V, Manykin E A and Khikhlukha D R 2017 Plasma Phys. Rep. 43 547
[10] Zelener B B, Zelener B V, Manykin E A, Bronin S Y, Bobrov A A and Khikhlukha D R 2018 J. Phys.: Conf. Ser. 946 012126