Distribution function of the ion microscopic field in strongly coupled ultracold plasma: Molecular dynamics simulations

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Abstract. The results of calculating the distribution function of the ion-microscopic field at the neutral point of ultracold plasma by the method of molecular dynamics are presented. The calculations are carried out for the model of two-component fully ionized ultracold plasma in a wide range of the Coulomb coupling parameter values. To evaluate the accuracy of the calculations, the distribution function of the ion microscopic field of randomly distributed charged particles was calculated and compared with the exact Holtsmark function. Results obtained for our model can be used for any equilibrium or non-equilibrium strongly coupled plasmas, in which quantum effects are negligible. Comparison with results of other authors is made.

1. Introduction

In low-temperature plasma (LTP), diagnostic methods based on measurements of frequency shift and broadening of the spectral lines of atoms due to electric fields created by plasma electrons and ions are widely used [1,2]. It seems natural to use this approach for diagnostics of ultracold plasma (UCP). However, it is necessary to take into account that the UCP has a number of features that can be important in the quantitative description of the processes in the plasma. Firstly, the concentration of particles in the UCP $n \lesssim 10^{10}$ cm$^{-3}$ is significantly lower than in the LTP. At such concentrations, the quasistatic ion microfield in the UCP is several orders of magnitude smaller than in the LTP. As result, its influence on the spectral line of an atom can be reliably determined only in the case of a highly excited Rydberg state. Secondly, the UCP is a two-temperature non-equilibrium thermodynamic system, where the temperature of electrons can be many times higher than the temperature of ions. It is necessary to know how the temperature difference affects the correlation of charged particles. Finally, it is important to take into account the fact, that the experimental study of the UCP is carried out in a magneto-optical trap, in which the number of trapped particles can vary from $10^3$ to $10^6$. Therefore,
when analyzing the results, it is necessary to take into account the effects of boundary influence on the microfield distribution function.

This paper presents the results of calculations of the distribution function of a quasistatic ion field at a neutral point depending on the strongly coupled parameter using the method of molecular dynamics (MMD). Calculations were performed for a model of a two-component fully ionized ultracold plasma [3, 4]. To assess the accuracy of the obtained results, calculations of the distribution function of the ion microfield of randomly distributed charged particles were performed in order to compare the obtained distribution function with the known Holtsmark function [1, 2, 5].

2. The construction of the distribution function of ion microfield in plasma

Like any quantity that characterizes a physical system consisting of a large number of particles, the ion microfield in plasma is of statistical nature. A method based on the construction of a probability distribution function is traditionally used to describe it, which in general is determined by the relation [6]

\[ P(\beta) = \frac{2\beta}{\pi} \int_{0}^{\infty} x \sin(\beta x) T(x) dx, \]  

(1)

where \( \beta \) is the normalized value of the ion microfield (\( \beta = E/E_H \)), \( E_H \) is the Holtsmark field (\( E_H = 2.603e/h_2^{2/3} \)), where \( e \) is the electron charge, \( n \) is the concentration of ions), and \( T(x) \) is the characteristic distribution function defined in the probability theory. Analytical computation of the function \( T(x) \) is possible only in certain limit cases, one of which is the system of non-interacting charges characterized by the Holtsmark distribution, for which

\[ P(\beta) = \frac{2\beta}{\pi} \int_{0}^{\infty} x \sin(\beta x) \exp(-x^{3/2}) dx. \]  

(2)

In the framework of numerical model, the probability distribution function can be obtained as a normalized histogram of random values corresponding to various possible configurations of the physical system. This raises two main questions: the first is the choice of an effective way to move to the next configuration of the system, and the second is the statistical conditionality and error of the results obtained.

In the present paper, we consider a system of charged particles consisting of electrons and ions, with \( n_e = Z n_i \), where \( n_e \) and \( n_i \) are the concentrations of electrons and ions, and \( Z \) is the charge number of the ion. An algorithm for molecular dynamics of a microcanonical ensemble is used to model the behavior of a system in phase space [7]. The interaction is described by the Coulomb potential without any restrictions on the distance between the particles. The motion equations are integrated in a cubic cell with periodic boundary conditions with numerical method using a variable time step that does not exceed the base step [8]. To preserve the specified particle concentrations, the cell size is defined as \( L_{x,y,z} = (N_e/n_e)^{1/3} \), where \( N_e \) is the number of electrons chosen in the calculation. The initial coordinates of electrons and ions are chosen randomly, and the velocities are determined based on the Maxwell distribution corresponding to the initial temperature of each of the subsystems. In order to eliminate the influence of the initial distribution of particles inside the cell, the phase trajectory is calculated several times with different initial conditions and then averaged. Specific parameter values common to all calculations are shown in table 1.

In addition to set the parameters described above, one must determine the error of the resulting distribution function values. In the most general case, the accuracy of the results depends on the relation between the number of particles, the number of configurations of the
Table 1. Parameters of the molecular dynamics calculations.

| Parameter                       | Value         |
|---------------------------------|---------------|
| Number of electrons, $N_e$      | 500           |
| Number of ions, $N_i$           | 500           |
| Electron concentration, $n_e$   | $10^{10}$ cm$^{-3}$ |
| Charge number of an ion, $Z$    | 1             |
| Basic time step, $\tau$        | $10^{-14}$ s   |

Figure 1. Distribution function of the ion microfield in a system of non-interacting charged particles: red curve—random points; black curve—Holtsmark distribution.

...physical system, the number of initial conditions, the number of probe points, the histogram step, and the largest fixed microfield. However, it should be clarified that the set of values for all parameters has the determining role: specifying the parameters for constructing the distribution function (the histogram step and the largest fixed microfield) without increasing the statistics of molecular dynamic calculation (the number of particles, the number of configurations, and the number of initial conditions) will only lead to the accumulation of errors in the final result. To determine the error value corresponding to the selected combination of these parameters, an approach based on relation (2) is used. Although the behavior of a system in which there is no interaction between particles cannot be modeled using the MMD, it is well known that the Holtsmark distribution corresponds to an equally probable location of charged particles in the studied volume. Thus, various configurations of such a system can be obtained using a random number generator. Comparing the distribution function obtained from them with the values calculated using relation (2) allows us to determine the error introduced by the limitations of the accumulated statistics. Figure 1 shows the result of the described procedure for parameters...
Table 2. Parameters of the ion microfield distribution function.

| Parameter                    | Value |
|------------------------------|-------|
| Number of configurations, \(N_c\) | 150   |
| Number of probe points, \(N_p\)     | 79,507|
| Maximum field, \(\beta_{\text{max}}\) | 30    |
| Histogram step, \(S_h\)            | 0.05  |

Figure 2. Dependence of the ion microfield distribution function upon the electron temperature: red curve—\(T_e = 52.0\) K, \(T_i = 6.8\) K; green curve—\(T_e = 33.1\) K, \(T_i = 6.8\) K; blue curve—\(T_e = 14.9\) K, \(T_i = 6.1\) K; purple curve—\(T_e = 10.7\) K, \(T_i = 6.2\) K.

from table 2. It can be seen that the largest discrepancy with the exact values is located in the maximum distribution region and equals 4% and 5% for \(P\) and \(\beta\), correspondingly.

3. The results of calculations

The main goal of this work is to perform a primary search for patterns in the behavior of ion microfield distribution functions in the UCP and compare them with the results obtained for the LTP. All calculations were performed using the parameters shown in tables 1 and 2.

As we have already noted, a significant difference in the temperatures of the electron and ion subsystems is possible in the case of UCP. Accordingly, first of all, it is necessary to evaluate the influence of various electronic temperatures on the correlation of ions. Figure 2 shows the distribution functions of the ion microfield at a neutral point at various electronic temperatures. It can be seen that despite of significantly difference in electronic temperatures, the difference in the obtained results does not exceed the calculation error. The main numerical characteristics corresponding to figure 2 are shown in table 3.
Table 3. Distribution function of the ion microfield with a change in the electron temperature.

| Curve  | $T_e$, K | $T_i$, K | $\beta_0$               | $P(\beta_0)$               |
|--------|---------|---------|-------------------------|---------------------------|
| Red    | 52.0    | 6.8     | $1.375 \pm 0.069$       | $0.410 \pm 0.016$         |
| Green  | 33.1    | 6.8     | $1.375 \pm 0.069$       | $0.409 \pm 0.016$         |
| Blue   | 14.9    | 6.1     | $1.425 \pm 0.071$       | $0.398 \pm 0.016$         |
| Purple | 10.7    | 6.2     | $1.525 \pm 0.076$       | $0.399 \pm 0.016$         |

Figure 3. Dependence of the ion microfield distribution function upon the strongly coupled parameter: black curve—$\Gamma_i = 0$; red curve—$\Gamma_i = 0.11$; blue curve—$\Gamma_i = 0.85$; purple curve—$\Gamma_i = 2.19$.

Common to most of the considered works [5, 6, 9–12], the aim of the present research is to find a regularity in the behavior of the calculation results depending on the strongly coupled parameter, which is defined as

$$\Gamma_i = \frac{Z^2 e^2}{k_B T_i} \left( \frac{4\pi}{3} n_i \right)^{1/3}. \quad (3)$$

Despite the difference in the methods and parameters used for performing calculations, we can distinguish a general pattern in the presented results: with the growth of $\Gamma_i$, the maximum position of the distribution shifts towards weaker fields, and the corresponding probability density monotonically increases. As can be seen in figure 3, this pattern persists in the case of the UCP. The corresponding numerical characteristics are shown in table 4.

4. Discussion of results

Figure 4 shows a comparison of the obtained results with the results given in the works [9–12]. In this case, one should note the following. The UCP is classical plasma in which the quantum
Table 4. Distribution function of the ion microfield with a change in the ionic strongly coupled parameter.

| Curve   | $\Gamma_i$ | $T_i$, K | $\beta_0$ | $P(\beta_0)$ |
|---------|------------|----------|----------|--------------|
| Black   | 0          | —        | 1.600    | 0.366        |
| Red     | 0.11       | 55.0     | $1.425 \pm 0.071$ | $0.394 \pm 0.016$ |
| Blue    | 0.85       | 6.8      | $1.375 \pm 0.069$ | $0.409 \pm 0.016$ |
| Purple  | 2.19       | 2.65     | $1.325 \pm 0.067$ | $0.422 \pm 0.017$ |

Figure 4. Comparison of the obtained results with those from [9–12]: black curve—$\Gamma_i = 2.19$ [9]; blue curve—$\Gamma_i = 0.21$ [10, 11]; purple curve—$\Gamma_i = 1$ [12].

effects are insignificant even at large values of strongly coupled parameter. On the other hand, with large strongly coupled parameters, it is necessary to account for the Coulomb interaction between particles as accurately as possible, without any restrictions on the distance between them. This is not possible with the parameters typical for the LTP, since large values of particle concentrations, when numerically solving the motion equations lead to the need to use a very small time step. In the presented model of the UCP, it is possible to perform calculations using Coulomb’s law as the interaction potential for both equally and oppositely charged particles. As it was shown in [4], the calculations of kinetic properties obtained within the framework of this model coincide with the results for the LTP in the area where quantum effects can be ignored. In this regard, the results obtained in this paper can be used as reference in relation to calculations where the Coulomb potential changes due to taking into account the various corrections (including the quantum ones). According to them, one can trace the trend of changing the microfield distribution functions when using these corrections. In addition, these results allow us to judge the applicability of the well-known single-component plasma model.
5. Conclusion
This paper presents the results of calculating the distribution functions of the ion microfield in an ultracold strongly coupled plasma, performed using the method of molecular dynamics. The obtained results can be used to study the influence of microfields on the broadening of spectral lines of highly excited atoms and to refine the spectral properties of transitions between the nearest Rydberg levels. Currently, the majority of studies which considered the effect of a microfield on the shift of transition lines in ultracold alkaline metal plasma uses the Holtsmark distribution as the ion microfield distribution. The temperature of ions in such experiments is approximately 1 K, which in our opinion requires taking into account a contribution of the strongly coupled parameter $\Gamma_i$ to the calculations, which is usually not done in these works.

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References
[1] Griem H R 1999 Spectral Line Broadening by Plasmas (New York: Academic Press)
[2] Lisitsa V S 1977 Sov. Phys. Usp. 122 449–95
[3] Bobrov A A, Vorobei V S and Zelener B V 2018 Phys. Plasmas 25 033513
[4] Bobrov A A, Bunkov A M, Bronin S Ya, Klyarfeld A B, Zelener B B and Zelener B V 2019 Phys. Plasmas 26 082102
[5] Demura A V 2010 Int. J. Spectrosc. 2010 671073
[6] Sadykova S P, Ebeling W, Sokolov I M and Valuev I A 2010 Prikl. Fiz. 1 37–42
[7] Heerman D W 1986 Computer Simulations Methods in Theoretical Physics (New York: Springer-Verlag)
[8] Aarseth S J 2003 Gravitational N-Body Simulations (Cambridge: University Press)
[9] Kurilenkov Yu K and Filinov V S 1980 Teplofiz. Vys. Temp. 18 657–67
[10] Mozer B and Baranger M 1960 Phys. Rev. 118 626
[11] Hooper C F J 1968 Phys. Rev. 165 215–22
[12] Nersisyan H B and Zwicknagel G 2006 J. Phys. A: Math. Gen. 39 4677–81