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Pair Interaction Potential of Particles for Two-Component Plasma

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In this work the semiclassical potential for plasma particles pair interactions, which takes into account the diffraction effects due to the uncertainty principle in two-component plasma (the region of temperatures $10^4\mathrm{K} < T < 10^8\mathrm{K}$ and densities $10^{21}\mathrm{cm}^{-3} < n \leq 10^{24}\mathrm{cm}^{-3}$), was proposed. The values of this potential were numerically calculated and an interpolation formula was obtained.

1 Introduction

The theoretical study of the quantum effects in a dense high-temperature plasma is important for investigation and explanation of the phenomena in a so-called semiclassical plasma, for example, in space plasmas, in laser shock plasma etc. Properties of the semiclassical plasma can be studied on the basis of the theoretical and computer simulation methods, which use an interaction potential taking into account the quantum effects. For the two-component system in work [1] the pair interaction potential taking into account the quantum effects in a wide region of temperatures was obtained by means of the generalization of the Kelbg potential (see work [2]). Now, the Deutsch potential [3], which takes into account the diffraction effects and has a very simple form, is widely used. The Deutsch potential is valid only for a dense plasma at high temperatures ($T > 10^6\mathrm{K}$). In this paper the semiclassical potential, which takes into account the diffraction effects and is valid for temperatures ($T > 10^4\mathrm{K}$), was obtained. It should be noted, that this potential additionally takes into account the influence of the density effects on the diffraction term. So, this potential depends on temperature and density. It was obtained on the basis of the Slater sum:

$$S(r_1, ..., r_N) = c \sum_n \Psi_n^* e^{-\beta E_n} \Psi_n \,, \tag{1}$$

here:

$$c = \Pi N_\nu ! \lambda_\nu^{3N_\nu}, \lambda_\nu^2 = 4\pi\alpha_\nu\beta, \alpha_\nu = \hbar^2/8\pi^2 m_\nu, \beta = 1/kT \tag{2}$$

In these equations N_ν is the number of particles of the ν-th sort, which have a mass m_ν and thermal wavelength λ_ν. The wave function is a properly symmetrized eigenfunction for the total macroscopic system with eigenvalue E_n, where n represents a complete set of quantum numbers. In order to derive the semiclassical potential the Slater sum eq.(1) is equated to the classical Boltzmann factor (see work [4]).

2 Differential equations for the semiclassical potential

The Thomas Fermi approximation for wave function was used [4]. The Hamiltonian is

$$H = -\sum_j \alpha_j \nabla_j^2 + V, \tag{3}$$

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where $\sum_j \alpha_j \nabla_j$ is $3N$-dimensional vector operator and the interaction potential V is:

$$V = \sum_{i<j} u_{ij} = \sum_{i<j} Z_i Z_j e^2 / r_{ij}. \tag{4}$$

One can write $S = e^{-B}$ and expand B in terms of the two-body functions, the three-body functions, etc. :

$$B = \sum_{i<j} \omega_{ij} + \sum_{i<j<k} \omega_{ijk}^{(3)} ... \tag{5}$$

In the limit of the infinite temperature the Slater sum transforms to the classical Boltzmann factor : $\omega_{ij} \to \beta v_{ij}$, where v_{ij} is the Coulomb potential.

Since the Slater sum is invariant under unitary transformation eq.(1) can be rewritten as :

$$S = c \sum_n (e^{-\beta H/2} \Psi_n)^* (e^{-\beta H/2} \Psi_n) \tag{6}$$

After differentiating (6) by β the following expression can be found:

$$\frac{\partial B}{\partial \beta} = V + 1/2 \sum_j \alpha_j \nabla_j^2 B - 1/4 \sum_j \alpha_j \nabla_j B \nabla_j B + Y, \tag{7}$$

where:

$$X = c \sum_n (\sum_j \alpha_j \nabla_j e^{-\beta H/2} \Psi_n)^* (\sum_j \alpha_j \nabla_j e^{-\beta H/2} \Psi_n), \tag{8}$$

$$Y = X/S - 3N/2\beta - 1/4 \sum_j \alpha_j \nabla_j B \nabla_j B. \tag{9}$$

The same procedure was used to derive the equation like (7) for the mixture of the gases:

$$\frac{\partial B_I}{\partial \beta} = V + 1/2 \sum_j \alpha_j \nabla_j^2 B_I - \sum_j \alpha_j \nabla_j B_I \nabla_j B_I + Y_I, \tag{10}$$

Taking the difference of (7) and (10) one can obtain for $U = B - B_I$:

$$\frac{\partial U}{\partial \beta} = V + 1/2 \sum_j \alpha_j \nabla_j^2 U - 1/4 \sum_j \alpha_j \nabla_j U \nabla_j U - 1/2 \sum_j \alpha_j \nabla_j U \nabla_j B_I + Y - Y_I, \tag{11}$$

B_I is the symmetry effective potential. So, U takes into account only the diffraction effect. Let us substitute the following expressions instead of B_I, U and $Y - Y_I$:

$$B_I \approx \sum_{i<j} s_{ij}, \tag{12}$$

$$U_I \approx \sum_{i<j} u_{ij}, \tag{13}$$

$$Y - Y_I \approx \sum_{i<j} y_{ij}, \tag{14}$$

By the Fourier transforming the following differential equation for Fourier transformations denoted as $\tilde{u}$ was obtained:

$$\frac{\partial \tilde{u}_{ab}}{\partial \beta} = \tilde{u} - 1/2(\epsilon_a + \epsilon_b)\tilde{u}_{ab} - \tilde{Q}_{ab} - 1/2(\alpha_a - \alpha_b)(\nabla \tilde{u}_{ab} \nabla s_{ab} + \tilde{y}_{ab})$$

$$-1/2\frac{1}{\Omega}\sum_k \epsilon_k(\tilde{u}_{ak}\tilde{u}_{bk}+\tilde{u}_{ak}\tilde{s}_{bk}+\tilde{u}_{bk}\tilde{s}_{ak}))\,, \tag{15}$$

where: $\epsilon_a = \alpha_a x^2$, $Q_{ab}(r) = 1/4(\alpha_a - \alpha_b)\nabla u_{ab}(r)\nabla u_{ab}(r)$

The equations for the Fourier transforms of the semiclassical interaction potentials of the two component plasma particles can be written as:

$$\frac{\partial \tilde{u}_{ii}}{\partial \beta} = \tilde{u} - \delta\epsilon\tilde{u}_{ii} - \tilde{Q}_{ii} - 1/2\delta\rho\epsilon\tilde{u}_{ii}^2 - 1/2\rho\epsilon\tilde{u}_{ie}^2 + \tilde{y}_{ii}, \tag{16}$$

$$\frac{\partial \tilde{u}_{ie}}{\partial \beta} = -\tilde{u} - 1/2(1+\delta)\epsilon\tilde{u}_{ie} - \tilde{Q}_{ie} - 1/2\delta\rho\epsilon\tilde{u}_{ie}\tilde{u}_{ii} - 1/2\rho\epsilon\tilde{u}_{ie}(\tilde{u}_{ee} + 1/2\tilde{s}) + \tilde{y}_{ie}, \tag{17}$$

$$\frac{\partial \tilde{u}_{ee}}{\partial \beta} = -\tilde{u} - 1/2\epsilon\tilde{u}_{ee} - \tilde{Q}_{ee} - 1/2\delta\rho\epsilon\tilde{u}_{ie}^2 - 1/2\rho\epsilon\tilde{u}_{ee}(\tilde{u}_{ee} + \tilde{s}) + \tilde{y}_{ee}, \tag{18}$$

where: $\delta = m_e/m_i,\ \epsilon = \epsilon_e = \epsilon_i/\delta$.

3 Semiclassical potential

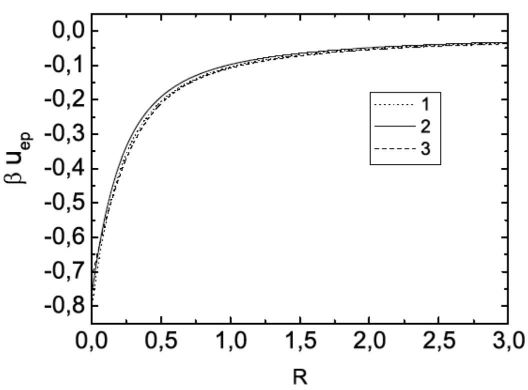

Fig. 1 Proton-electron pair interaction potential. Where: 1 is the potential (21), 2 is the semiclassical potential (20), 3 is the numerical data. $R = r/a_B$,$T = 3.16 \cdot 10^6$K

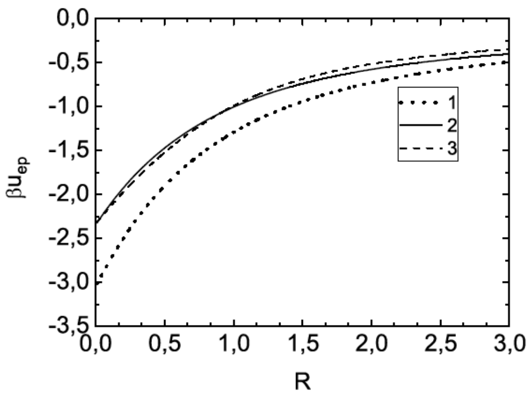

Fig. 2 Proton-electron pair interaction potential. Where: 1 is the potential (21), 2 is the semiclassical potential (20), 3 is the numerical data. $R = r/a_B$,$T = 210000$K

The equations (16)-(18) were solved numerically using the boundary conditions :

$$\tilde{u}_{ab}(x)|_{\beta\to 0} = \frac{4\pi\beta Z_a Z_b e^2}{x^2} \tag{19}$$

For a wide range of temperatures and densities the following interpolation formula was obtained:

$$u_{ab}(r) = \frac{Z_a Z_b e^2}{r}\left(1 - \tanh\left(\sqrt{2}\frac{\lambda_{ab}^2}{a_0^2 + br^2}\right) e^{-\tanh(\sqrt{2}\lambda_{ab}^2/(a_0^2+br^2))}\right)\left(1 - e^{-r/\lambda_{ab}}\right) \tag{20}$$

where $a_0 = (3/4\pi n)^{1/3}$ is an average interparticle distance, $b = 0.033$, $\lambda_{ab} = \hbar/\sqrt{2\pi\mu_{ab}k_B T}$ is the thermal de Broglie wave-length of $a - b$ pair, μ_{ab} is the reduced mass of $a - b$ pair.

In the limit $\beta \to 0$ the potential (20) coincides with the Deutsch potential:

$$u_{ab}(r)|_{\beta\to 0} = \frac{Z_a Z_b e^2}{r}\left(1 - \exp[-r/\lambda_{ab}]\right) \tag{21}$$

Figures 1 and 2 show the curves for semiclassical pair interaction potential (20) and numerical data obtained by solving eqs.(16)-(19) for the different temperatures.

4 Conclusion

Semiclassical interaction potential for particles of the two-component plasma was obtained. It takes into account the diffraction effects in a wide region of temperatures and densities. Semiclassical potential at high densities and temperatures has good agreement with the Deutsch potential.

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