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Interparticle interaction potential in two-component plasmas

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The purpose of this work is to find a pseudopotential of interparticle interaction of charged particles which takes into account quantum and collective effects for an ideal and weakly non-ideal plasma in the framework of linear dielectric response formalism. In the quantum contribution to the potential the symmetry effects are neglected. Fourier transformations are employed in our studies of the potential. The results demonstrate that th e constructed potential is finite at the origin and tends to the Coulomb one when the interparticle distance tends to infinity. In other words, it satisfies established theoretical requirements. The potential we obtain is also compared to the well-known Debye-Hückel and Deutsch potentials. The potential we obtain is also compared to the well-known Debye-Hückel and Deutsch potentials.

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1 Introduction

Non-ideal plasmas are systems of charged particles where the interparticle interactions play a main role. It is known, that the interaction of charged particles in plasmas is different from the Coulomb interaction. If we use the Coulomb potential, problems related to the divergence of collision integrals at scattering angles will appear, since this potential does not take into account the collective effects, screening and quantum effects. To avoid these problems, some effective potentials were introduced in plasma physics. Let us discuss some of them.

The potential energy of the Coulomb interaction between two charged particles is given by [1]:

$$\varphi_{ab} = \frac{e_a e_b}{r}, \tag{1}$$

where e_a and $e_b$are electric charges of the particles involved in the interaction, $r$is the distance between them. Further, as it is usually done in plasma physics, we will call the potential energy of interaction potential.

Interaction force that is due to the Coulomb potential (1) has a long-range nature. However, long-range interactionsare substantially changed by collective effects or shielding effects, due to the influence of surrounding particles. At short distances quantum-mechanical effects of diffraction and exchange are also important. Thus, the so-called effective potentials that take into account these effects are introduced in plasma physics. Let us consider the most common effective potentials:

a) The self-consistent field potential (the Debye - Hückel potential). This potential corresponds to the approximation of pair correlations and it is applicable at small plasma densities:

$$\varphi_{ab} = \frac{e_a e_b}{r} exp\left(-\frac{r}{r_D}\right). \tag{2}$$

b) The Deutsch potential. It takes into account quantum-mechanical effects of diffraction and exchange:

$$\varphi_{ab} = \frac{e_a e_b}{r}\left(1 - e^{-\frac{r}{\lambda_{ab}}}e\right) + \delta_{ae}\delta_{be}k_B T \ln 2\, e^{-\frac{r^2}{\lambda_{ee}{}^2 \pi \ln 2}}, \tag{3}$$

where $\lambda_{ab} = \hbar/(2\pi\mu_{ab}k_b T)^{1/2}$is de Broglie thermal wavelength, $\mu_{ab} = m_a m_b/(m_a + m_b)$is the reduced mass of interacting particles.

c) The authors of [1] proposed a potential which takes into account both screening and quantum-mechanical effects:

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$$\varphi_{ab} = \frac{e_a e_b}{r}\left(exp\left(-\frac{r}{r_D}\right) - exp\left(-\frac{r}{\lambda_{ab}}\right)\right). \quad (4)$$

2 The pseudopotential

The purpose of this paper is to obtain an effective potential, which will analytically take into account not only the screening effects, but also two types of quantum effects: local and statistical.

This effective potential can be obtained in the framework of the linear dielectric response theory. The main idea is as follows. We choose some microscopic potential, to which we want to add a new property and determine its Fourier transform. Next, the Fourier-image of new potential is determined via the ratio of Fourier-images of the microscopic potential and the model dielectric function. Finally, a new effective potential with necessary properties is obtained by the reverse Fourier transformation. Let uscarry out these calculations in practice:

The equation of theeffective or pseudopotential in the Fourier space is then the following:

$$\varphi_{ab}(q) = \phi_{ac}(q)\varepsilon_{cb}^{-1}(q,0), \quad (5)$$

where $\varepsilon_{cb}^{-1}(q,0)$ is the static dielectric function (SDF) of the plasma, $\phi_{ac}(q)$ is the Fourier transform of a micropotential and $\varphi_{ab}(q)$ isthe Fourier transform of the potential we are looking for.

Further, it is necessary to select a micropotential which possesses a part of the required properties, as well as a model for SDF, which complements the above properties.

Here we choose as the micropotential the Deutsch potential, which takes into account local quantum-mechanical effects (without the exchange contribution). ItsFouriertransformis simple:

$$\phi(q) = \left(\frac{4\pi\alpha}{q^2} - \frac{4\pi\alpha}{k_{ab}^2 + q^2}\right). \quad (6)$$

We acquire the SDF model including quantum-statistical effects from [2]:

$$\varepsilon(q,0) = 1 + \frac{1}{(q/k_D)^2 + (q/k_q)^4}. \quad (7)$$

Here
$k_D^2 = 4e^2\beta n_{tot,} n_{tot} = n_e + \sum_i n_i Z_i^2\, , k_q^4 = 16\,\pi e^2/h^2(n_e m_e + \sum_i n_i m_i Z_i^2)$.

Now, on the basis of these formulas, we carry out the inverse transform:

$$\varphi_{ab}(r) = \frac{1}{(2\pi)^3}\int \boldsymbol{dk}\varphi_{ab}(q)\, exp(i\,\boldsymbol{qr}). \quad (8)$$

Thus weobtain the following expression for the potential:

$$\varphi_{ab}(r) = \frac{e_a e_b}{r}\big(A\, exp(-r\, k_{ab}) + B_1\, exp(-r\, K_1) - B_2\, exp(-r\, K_2)\big), \quad (9)$$

where

$$A = \frac{1-\beta}{\Delta}\ ;\ B_{1,2} = \frac{C_{1,2}(C_{1,2}-\beta)}{(2C_2-1)\Delta}\ ;\ K_{1,2} = k_{ab}\sqrt{\frac{C_{2,1}}{\beta}};$$

$$\Delta = \gamma + \beta - 1;\, C_{1,2} = \frac{1\mp R}{2}\,; R = \sqrt{1-4\,\alpha}\,;$$

$$\alpha = \frac{k_D^4}{k_q^4}\ ;\ \beta = \frac{k_{ab}^2 k_D^2}{k_q^4};\ \gamma = \frac{k_D^2}{k_{ab}^2}\,.$$

This potential is presented in figures 1-2 for various dimensionless coupling, Γ and density, r_s parameters,

$$\Gamma = \frac{e^2}{ak_B T},$$

where $a = \left(\frac{3}{4\pi n}\right)^{1/3}$,

$$r_s = \frac{ame^2}{\hbar}.$$

Comparison between potentials is displayed in figures 3-5 for various Γ, r_s and degeneracy parameter,θ,

$$\theta = \frac{k_B T}{E_F} = 2\left(\frac{4}{9\pi}\right)^{2/3}\frac{r_s}{\Gamma}.$$

3 The plasma thermodynamic properties

A system in a thermodynamic equilibrium can be described by using the measured macroscopic parameters, such as pressure and internal energy.

From energy we can derive other thermodynamic values, such as heat capacity, free energy, etc.

It is well known, that the internal energy can be calculated as

$$E = \frac{3}{2}Nk_BT + U_N,$$

where N is the total number of particles in the system and the correlation energy U_N is determined via the radial function distribution$g_{ab}(r)$ (RDF). In turn, the plasma pressure is also determined through the RDF. Let us write these two equations down; they link the effective potential and the macro parameters:

a) The correlation energy of the plasma:

$$U_N = 2\pi V\int_0^\infty \sum_{a,b} n_a\, n_b \varphi_{ab}(r) g_{ab}(r) r^2 dr \qquad (10)$$

where V is the volume of the system, $\varphi_{ab}(r)$ is the effective potential, $g_{ab}(r)$ is the radial distribution function of the system.

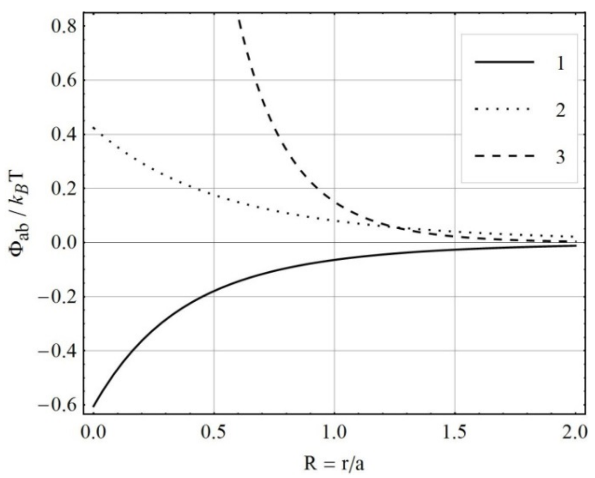

Figure 1 – The hydrogen plasma potential plots (9). 1 stands for the electron-electron interaction; 2 for the electron-protoninteraction, 3 for the proton-proton interaction at the parameters: Γ = 3, rs =0.5.

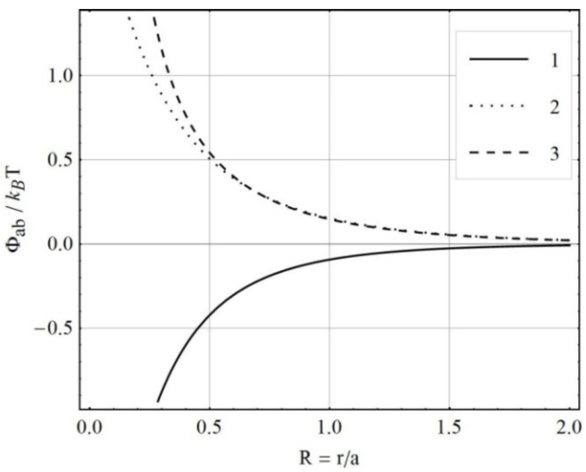

Figure 2 – As in Figure 1 but for Γ = 0.5, r_s =5.

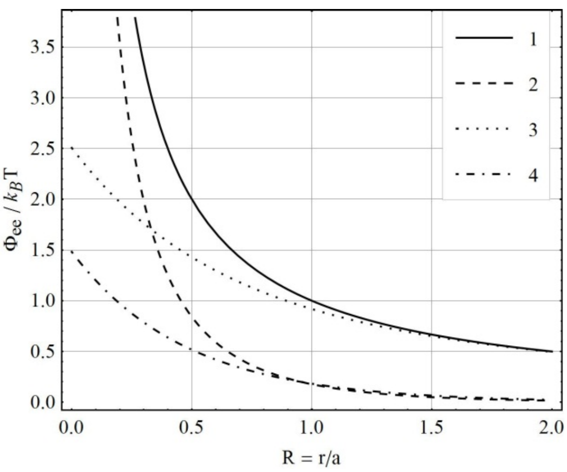

Figure 3 – As in Figure 1 but for Γ =1, r_s = 2.

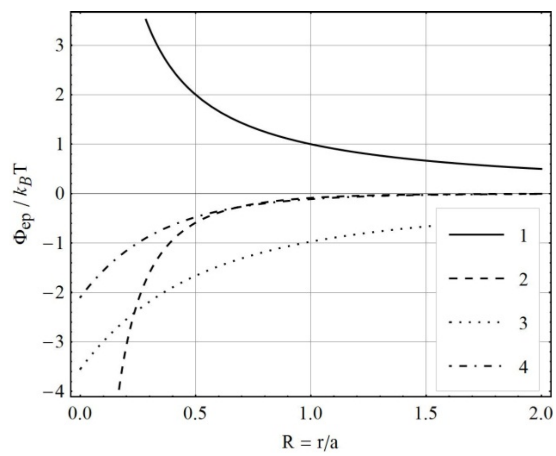

Figure 4 – As in Figure 1 but for Γ=1, r_s = 2.

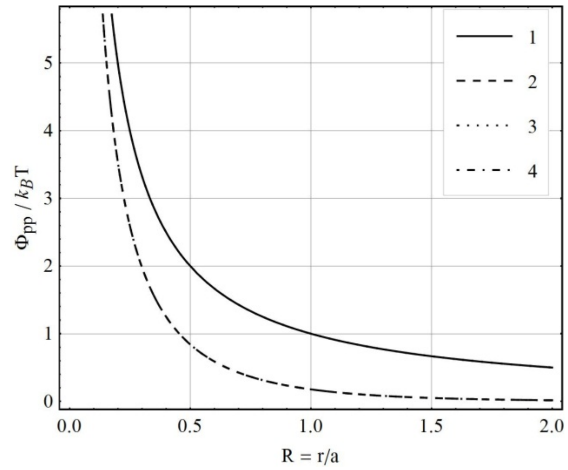

Figure 5 – As in Figure 1 but for Γ=1, r_s = 2.

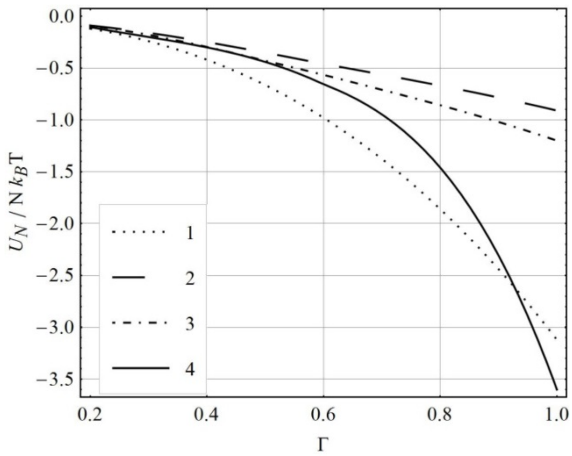

Figure 6 – Correlation energy of plasma. $\theta = 10$. 1 corresponds to the data of [11], 2 –to the Debye-Hückel theory, 3 – to [10], 4-to formula (10) with (9).

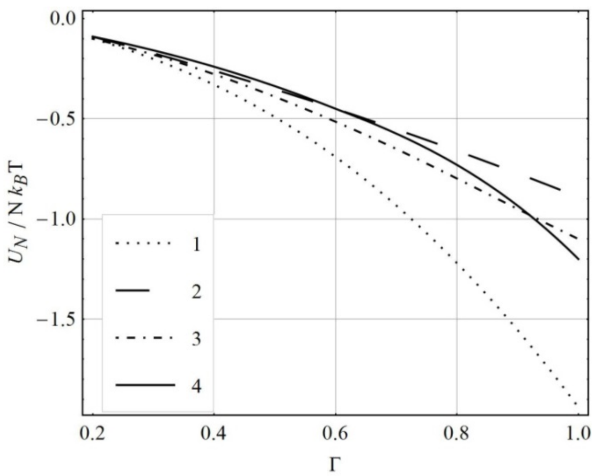

Figure 7 – As in Figure 6 but for $\theta = 5$.

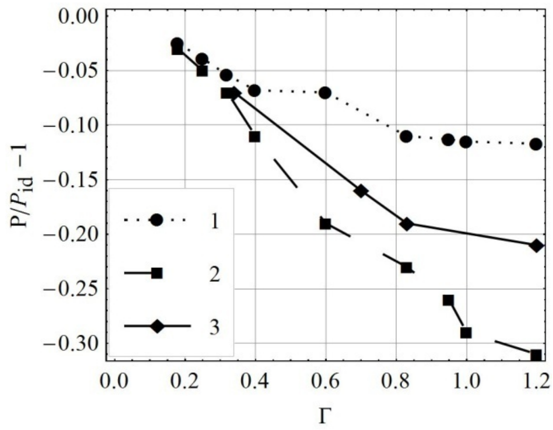

Figure 8 – Pressure isotherms. T=125000K. 1 – formula (11) with (9), 2 – PIMC data [8], 3 – HFMW.

Our results for the correlation energy are presented in Figures6 and 7 for the hydrogen plasma vs. the coupling parameter Γ. Comparison between the data of the [11] and those of other theories is displayed in these figures as well. In the present work, the bound states were considered within the HNC approximation. It can be seen that formula (10) with the potential (9) is in an agreement with the simulation data.

b) The pressure of the plasma or the plasma equation of state (EOS):

$$P = P_{id} - \frac{2\pi}{3}\int_0^\infty \sum_{a,b} n_a n_b \frac{d\varphi_{ab}(r)}{dr} g_{ab}(r) r^3 dr \qquad (11)$$

where $P_{id} = \sum_a n_a k_B T$is the ideal gas pressure.

Figure 5 represents the pressure isotherms for 125kK. These isotherms were derived in the framework of the PIMC simulation [8]. One can observe, hence, that the potential (9) is in a relatively good agreement with the experimental data found in the Hartree-Fock and Montroll-Ward (HFMW) approximations, especially at small values of the coupling parameter.

4 Conclusions

An effective pair interaction potential for ideal and weakly non-ideal plasmasis obtained. It takes into account not only screening and dynamic quantum effects, but also statistical quantum effects. It is in a good agreement with the Deutsch potential at high temperature. Also, we used this potential for the calculation of thermodynamics properties of plasma and for the comparison with some simulation data.

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