Effective polarization interaction potentials of the partially ionized dense plasma

2006 J. Phys. A: Math. Gen. 39 4369

(http://iopscience.iop.org/0305-4470/39/17/S10)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 4369–4373 doi:10.1088/0305-4470/39/17/S10

Effective polarization interaction potentials of the partially ionized dense plasma

T S Ramazanov[1], **K N Dzhumagulova**[1], **Yu A Omarbakiyeva**[1] **and G Röpke**[2]

[1] IETP, Al Farabi Kazakh National University, Tole Bi 96a, 050012 Almaty, Kazakhstan
[2] Institute of Physics, University of Rostock, D-18051 Rostock, Germany

E-mail: ramazan@physics.kz

Received 18 September 2005
Published 7 April 2006
Online at stacks.iop.org/JPhysA/39/4369

Abstract
The effective polarization interaction potential between charged and neutral particles is considered for a partially ionized plasma. This pseudopotential is deduced taking into account quantum-mechanical effects at short distances as well as screening effects at large distances. Furthermore, a cutoff radius is obtained using a modified effective-range theory. Explicit results for parameters describing the interaction of the atom with charged particles are given.

PACS numbers: 52.20.Hv, 52.27.Gr

1. Introduction

A partially ionized hydrogen plasma (number density of electrons and ions $n_e = n_i = 10^{21}$–10^{24} cm^{-3}, temperature $T = 10^3$–10^6 K) is considered, with $a = (3/4\pi n)^{1/3}$ denoting the average distance between particles, where $n = n_e + n_i$. The state of the system depends greatly on the coupling parameter $\Gamma = e^2/ak_BT$, which describes the ratio of the potential energy of charged particles' interaction at an average distance to their thermal energy. The plasma becomes non-ideal at $\Gamma > 1$. Furthermore, we introduce the density parameter $r_S = a/a_B$ (a_B is the Bohr radius), which decreases with increasing densities.

To calculate the thermodynamic and transport properties of partially ionized plasmas, we can use the chemical picture where atoms are considered as new constituents in addition to free electrons and ions. Therefore, effective potentials have to be introduced for the different interactions between neutral atoms and charged particles. We will focus on the polarization potential describing the interaction between charged particles (electrons) and neutrals. In particular, we consider the inclusion of screening and quantum-mechanical effects into the polarization potential.

2. Polarization potential

As well known, at large distances the interaction between an isolated atom and a charged particle is given by

$$\Psi_0(r) = -\frac{e^2\alpha}{2r^4}, \tag{1}$$

where α is the polarizability of the atom.

However, this potential is not appropriate for dense plasmas. At short distances, it becomes singular. It has to be modified if r is of the order of the extension of the atom as given by the Bohr radius a_B. According to Buckingham, a cutoff radius $r_{1,B}$ can be introduced leading to the potential

$$\Psi_B(r) = -\frac{e^2\alpha}{2\left(r^2 + r_{1,B}^2\right)^2}, \tag{2}$$

with

$$r_{1,B}^4 = \frac{\alpha a_B}{2}. \tag{3}$$

We obtain a finite value $\Psi_B(0) = -e^2/a_B$.

At large distances, also a modification is necessary. In dense plasmas, the Coulomb interaction between charged particles is screened. The well-known Debye formula $(e^2/r)\exp(-r/r_D)$, with $r_D = \sqrt{k_BT/(4\pi ne^2)}$ being the Debye radius, gives an exponential decrease of the interaction. This leads to the contradiction that the interaction between charged particles becomes smaller than the polarization potential at large distances. Therefore, we have to screen also the polarization potential. Redmer *et al* [1] found the expression

$$\Psi_{B,S}(r) = -\frac{e^2\alpha}{2\left(r^2 + r_{1,B}^2\right)^2}\exp\left(-\frac{2r}{r_D}\right)\left(1 + \frac{r}{r_D}\right)^2. \tag{4}$$

In our previous paper [2], we proposed a pseudopotential for the interaction between charged particles and atoms, which also considers the polarization of atom in an external field:

$$\Psi(r) = -\frac{e^2\alpha}{2r^4\left(1 - 4\lambda^2/r_D^2\right)}\left(\mathrm{e}^{-\mathrm{Br}}(1 + \mathrm{Br}) - \mathrm{e}^{-\mathrm{Ar}}(1 + \mathrm{Ar})\right)^2, \tag{5}$$

where $A^2 = \left(1 + \sqrt{1 - 4\lambda^2/r_D^2}\right)/(2\lambda^2)$, $B^2 = \left(1 - \sqrt{1 - 4\lambda^2/r_D^2}\right)/(2\lambda^2)$ are coefficients, $\lambda_{ab} = \hbar/(2\pi\mu_{ab}k_BT)^{1/2}$ is the thermal de Broglie wavelength of electrons.

This effective polarization potential takes into account quantum effects by averaging over the thermal wavelength. Similar to the Kelbg or Deutsch potential for the interaction between charged particles, it can be used to perform classical molecular dynamics calculations.

In particular, as for the Buckingham potential (2), the singularity of the simple potential (1) at $r = 0$ is removed. A finite value $\Psi(0) = -e^2\alpha/(8\lambda^4)$ is obtained, which differs from $\Psi_B(0)$ for the Buckingham potential. At large distances, for $\lambda^2/r_D^2 \ll 1$ the screening behaviour is reproduced.

The short-range behaviour of the effective interaction between the atom and an electron needs more detailed consideration. In principle, we have to consider two possibilities for the spin orientations of the electrons. If the spins of the free as well as the bound electrons are parallel, due to the Pauli exclusion principle we have a strong repulsion at short distances. Therefore, we introduce an effective polarization potential which has a finite cutoff (hard core) radius. Conventionally, this radius is obtained using a modified effective-range theory. The detailed description of this theory is beyond the scope of the present work and we just refer to original works [3, 4], see also [5]. In the following we will not consider the electron spin explicitly, which can be understood as performing an averaging over the spin orientations. The interaction between charges and neutrals has also been considered recently [6]. The concept of the excluded volume was used to take into account that because of the Pauli blocking a part of the total volume, which is already occupied by atoms, is not accessible for free electrons. The smallest distance to which free electrons can approach atoms was estimated within 1 a_B and 2 a_B.

3. Cutoff radius

As already noted above, to obtain the effective radius we use the so-called modified effective-range theory. The interaction potential

$$V(r) = V_1(r) + V_2(r) \tag{6}$$

is represented as a sum of a short-range hard sphere potential $V_1(r) = \infty$ for $r < r_1$, $V_1(r) = 0$ for $r > r_1$, and a polarization potential $V_2(r) = 0$ for $r < r_1$, $V_2(r) = \Psi(r)$ for $r > r_1$, where r_1 is the cutoff radius.

As the short-range part of the potential we considered hard spheres [7]. The potential that describes the impervious sphere of radius r_1 is equal to $+\infty$ at $r < r_1$. The condition of the sphere impermeability into the sphere $r < r_1$ may be expressed as a boundary condition imposed on the wavefunction, $\psi(k, r) = 0$ at $|\vec{r}| = r_1$. Considering the potential $\Psi(r)$ as small, in first approximation we have for $l = 0$ the phase shift

$$\delta_{01} = -kr_1, \tag{7}$$

where k is the wave number.

The modified effective-range theory provides the following scattering length for the potential $V(r)$ [5]:

$$L = L_1 + \frac{m}{2\pi\hbar^2}\int V_2(r)\,\mathrm{d}\vec{r}, \tag{8}$$

where m is the mass of electron and L_1 is the scattering length for the short-range potential $V_1(r)$.

For arbitrary short-range potentials, the s-wave phase shift behaves for small k like $\delta_0 = -Lk$. Using (7) we find that $L_1 = r_1$, and substituting it into (8) we get

$$L = r_1 + \frac{m}{2\pi\hbar^2}\int V_2(r)\,\mathrm{d}\vec{r}. \tag{9}$$

Taking the pseudopotential (5) for the potential $V_2(r)$ we obtain

$$L = r_1 - \frac{m}{4\pi\hbar^2}\int_{r_1}^{\infty}\frac{\mathrm{e}^2\alpha}{r^4\left(1-4\lambda\!\!\!^{-2}/r_D^2\right)}(\mathrm{e}^{-\mathrm{Br}}(1+\mathrm{Br}) - \mathrm{e}^{-\mathrm{Ar}}(1+\mathrm{Ar}))^2\,\mathrm{d}\vec{r}. \tag{10}$$

On the other hand the scattering length is equal to

$$L = \sqrt{\alpha/a_B}\cot[\sqrt{\alpha/a_B}I/e^2], \tag{11}$$

where I is the ionization potential of the atom [8].

Inserting this relation, the final equation we need to solve to get the cutoff radius takes the form

$$r_1 - \frac{m}{4\pi\hbar^2}\int_{r_1}^{\infty}\frac{e^2\alpha}{r^4\left(1-4\lambda\!\!\!^{-2}/r_D^2\right)}(\mathrm{e}^{-\mathrm{Br}}(1+\mathrm{Br}) - \mathrm{e}^{-\mathrm{Ar}}(1+\mathrm{Ar}))^2\,\mathrm{d}\vec{r} \\ - \sqrt{\alpha/a_B}\cot[\sqrt{\alpha/a_B}I/e^2] = 0. \tag{12}$$

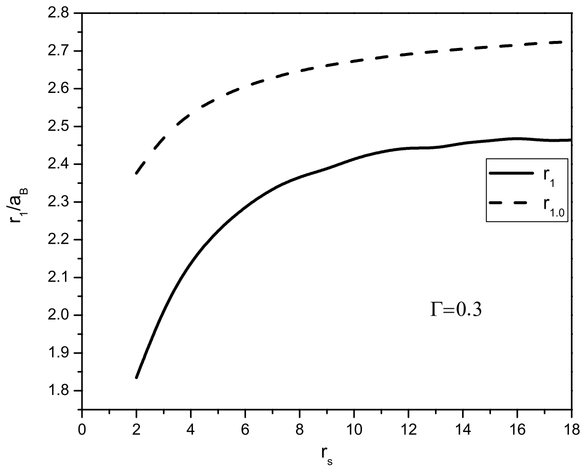

Figure 1. Cutoff radius for the polarization interaction potential between charged particles and hydrogen atom, $\Gamma = 0.3$.

Table 1. Cutoff radius for the polarization interaction potential between charged particles and hydrogen atoms.

			r_1	
N	r_s	$r_{1,0}$	$\Gamma = 0.5$	$\Gamma = 1$
1	2	2.3760	1.7222	1.5586
2	3	2.4756	1.9029	1.7025
3	4	2.5364	2.0168	1.7920
4	5	2.5775	2.0995	1.8535
5	6	2.6064	2.1552	1.8972
6	7	2.6292	2.1945	1.9180
7	8	2.6472	2.2200	1.9384
8	9	2.6613	2.2446	1.9512
9	10	2.6730	2.2650	1.9660
10	11	2.6829	2.2792	1.9635
11	12	2.6916	2.2752	1.9632
12	13	2.6988	2.2815	1.9630
13	14	2.7048	2.2848	1.9600
14	15	2.7105	2.2905	1.9608

4. Results

We performed calculations for hydrogen where $\alpha = 4.5\ a_B^3$ and $I = 13.6$ eV. We have solved equation (12), considering for $r > r_1$ the simple polarization interaction $\Psi_0(r)$, equation (1), as well as for the new expression $\Psi(r)$, equation (5), which was derived in [2]. The corresponding solutions for the cutoff radius $r_{1,0}$ and r_1, respectively, as a function of r_s are given in table 1 in units of a_B for different values $\Gamma = 0.5$ and $\Gamma = 1$. For two further values of $\Gamma = 0.3$ and $\Gamma = 0.8$ the corresponding solutions are presented in figures 1 and 2.

It is seen that in the low-density limit $r_s \to \infty$, the calculated values for r_1 approach a limiting value which is larger than the Buckingham parameter $r_{1,B} = 1.2246$ and also larger than the value 1.5 used in [6].

The results for r_1 are smaller than $r_{1,0}$ and decrease with increasing Γ.

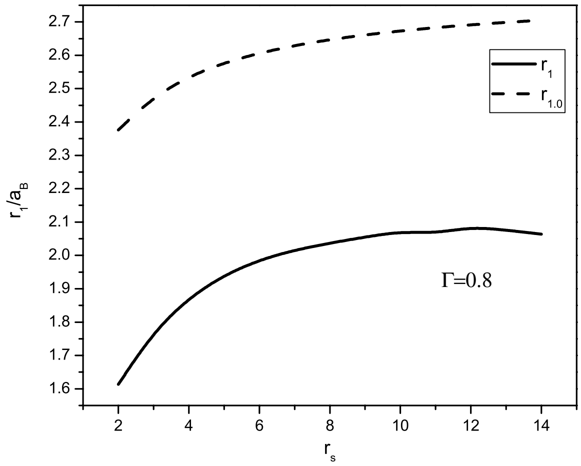

Figure 2. Cutoff radius for the polarization interaction potential between charged particles and hydrogen atom, $\Gamma = 0.8$.

5. Conclusions

The effective polarization interaction potential between charge and neutral particles is considered. The cutoff radius for hydrogen atom has been obtained on the basis of a modified effective-range theory for the pseudopotential model (5). Compared with the concept of the excluded volume, our approach may be considered as a more systematic approach to the interaction between electron and neutrals.

Acknowledgments

The authors would like to thank Professor A G Khrapak and Professor V S Vorobyev for their suggestions, and Professor C Deutsch for a useful discussion.

References

[1] Redmer R 1999 *Phys. Rev.* E **59** 1073
[2] Ramazanov T S, Dzhumagulova K N and Omarbakiyeva Yu A 2005 *Phys. Plasmas* **12** 092702
[3] O' Malley T F, Spruch L and Rosenberg L 1962 *Phys. Rev.* **125** 1300
[4] O' Malley T F 1963 *Phys. Rev.* **130** 1020
[5] Khrapak A G and Iakubov I T 1981 *Electrons in Dense Gases and Plasma* (Moscow: Nauka) (in Russian)
[6] Ebeling W, Hache H, Juranek H, Redmer R and Röpke G 2005 *Contrib. Plasma Phys.* **45** 160
[7] Newton R G 1969 *Scattering Theory of Waves and Particles* (Moscow: Mir) (in Russian)
[8] Iakubov I T and Khrapak A G 1995 *Phys. Rev.* A **51** 5043