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The electron–atom interaction in partially ionized dense plasmas

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Abstract

The electron–atom interaction is considered in dense partially ionized plasmas. The separable potential is constructed from scattering data using effective radius theory. Parameters of the interaction potential were obtained from phase shifts, scattering length and effective radius. The binding energy of the electron in the H^- ion is determined for the singlet channel on the basis of the reconstructed separable potential. In dense plasmas, the influence of the Pauli exclusion principle on the phase shifts and the binding energy is considered. Due to the Pauli blocking, the binding energy vanishes at the Mott density. At that density the behavior of the phase shifts is drastically changed. This leads to modifications of macroscopic properties such as composition and transport coefficients.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The electron–atom interaction is one of the main problems in calculating the physical properties of a partially ionized dense plasma, such as thermodynamical, transport and optical properties. It is known that the form of the interaction potential plays an important role to obtain accurate data calculating such properties. In particular, many-particle effects have to be considered in dense plasmas such as collective modes, strong collisions and quantum effects. The main modifications in the electron–atom interaction are due to polarization and exchange processes. Several polarization models of the interaction potential between electron and atom were introduced in the past. The screened Buckingham potential model is very often used in theoretical works [1–4]. In the case of semi-classical plasmas the polarization pseudopotential

$$V_{ea}(r) = -\frac{e^2\alpha}{2r^4\left(1-4\lambda^2/r_D^2\right)}\left(e^{-Br}(1+Br) - e^{-Ar}(1+Ar)\right)^2 \qquad (1)$$

was suggested [5], where α is the polarizability of atoms, $A^2 = \left(1 + \sqrt{1 - 4\bar{\lambda}^2/r_D^2}\right)/(2\bar{\lambda}^2)$, $B^2 = \left(1 - \sqrt{1 - 4\bar{\lambda}^2/r_D^2}\right)/(2\,\bar{\lambda}^2)$ and $\bar{\lambda}_{ab} = \hbar/\sqrt{2\pi\mu_{ab}k_BT}$ is the thermal de Broglie wavelength of electrons. This pseudopotential considers screening and quantum-mechanical effects, which take place in a dense semi-classical plasma. On the basis of the pseudopotential (1) the elastic scattering of electrons on hydrogen atoms was considered in [6, 7].

Treating the interaction of an electron with an atom, one has also to consider exchange effects. In principle, there are two possibilities for the spin orientation 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. Of special interest are non-local interactions which are necessary to describe exchange interaction. It is possible to solve the inverse scattering problem, since the phase shifts as a function of incident electron energy describe the interaction between particles at different distances. Such an inverse scattering problem is solved in nuclear physics to describe the nucleon–nucleon short-range interaction [8, 9]. We will give the results for Coulomb systems below.

Essential features of dense plasmas are many-particle effects, such as Pauli blocking, screening, correlations and bound state formation. The influence of these effects is fundamental in deriving thermodynamic and transport properties. The electron–ion interaction was reconstructed and the influence of Pauli blocking on transport properties of a dense plasma was considered in [10]. Here we will consider the electron–atom interaction.

We will focus on the reconstruction of the e–a interaction on the basis of scattering data using the Ernst–Shakin–Thaler (EST) separable approximation method [11]. A partially ionized hydrogen plasma in the parameter-range region $T = 10^3$–10^6 K, $n_e = 10^{18}$–10^{22} cm^{-3} will be considered.

2. Reconstruction of e–a interaction

We introduce the interaction potential of an electron with a hydrogen atom on the basis of scattering data taking into account spin orientation of incident and bound electrons. At first the low-density limit is considered. It is possibly to solve the inverse scattering problem using the effective radius theory (ERT). Within ERT, the following expansion

$$k \cot \delta(k) = -\frac{1}{a} + \frac{k^2 r_0}{2} \tag{2}$$

of the scattering phase shift $\delta(k)$ can be used, where $k = \sqrt{2m_r E/\hbar^2}$, a is the scattering length and r_0 is the effective radius. This expansion is applicable for low-energy scattering (small k) and for the S wave. One of the difficulties in solving of this problem is the absence of exact experimental data for a and r_0. Therefore we consider theoretical works on calculations of these data. Among the great number of theoretical works on the investigation of electron–atom scattering at low energies [12–16] the work of Schwartz [12] is notable. The Kohn's variational principle was used to calculate S-wave elastic scattering of electrons from atomic hydrogen. Phase shifts and scattering lengths for triplet and singlet scattering states were obtained. Results for the phase shifts, obtained in this work, is the most accurate at low energies of the incident electron. There are also data obtained on the basis of different theoretical methods [13–15] as R-matrix, density functional theory (DFT), adiabatic local density approximation (ALDA), etc.

According to the EST method each potential can be presented by a sum of separable potentials. We consider a potential, which is separable in momentum representation:

$$V(p, p') = \lambda w(p) w(p'), \tag{3}$$

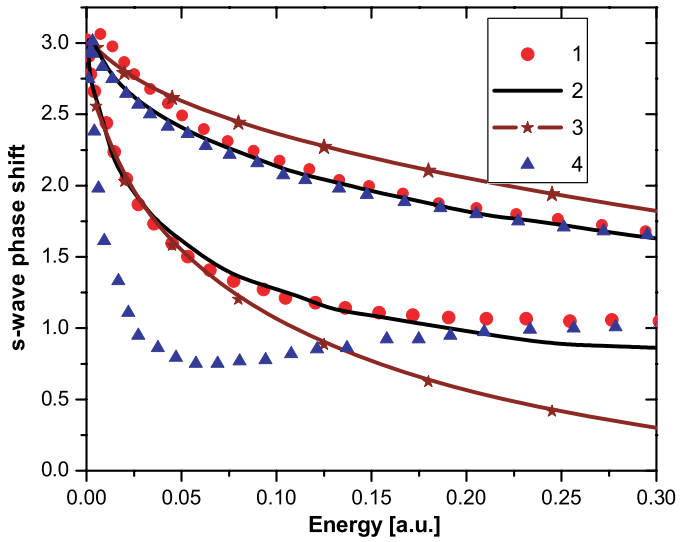

Figure 1. Singlet and triplet scattering phase shifts of electron on the hydrogen atom. 1, ALDA [15]; 2, accurate data [12]; 3, present work and 4, ALDA SPA [15].

where $w(p)$ is the atomic form-factor. In our calculation we use the following Gaussian form:

$$w(p) = \exp(-p^2/b^2). \tag{4}$$

The parameters λ, b can be determined from the e–a scattering data. For the separable interaction the T-matrix has the form [8, 19]

$$t(p, p', E) = \frac{\lambda w(p) w(p')}{1 - \lambda \sum_{p''} \frac{w(p'')^2}{E - p''^2/2m_r}}. \tag{5}$$

The phase shifts in this formalism are defined as ($E = p^2/2m_r$)

$$\tan\delta(p) = \frac{\Im t\left(p, p', \frac{p^2}{2m_r}\right)}{\Re t\left(p, p', \frac{p^2}{2m_r}\right)} = \frac{\Im\left(1 - \lambda \sum_{p''} \frac{w(p'')^2}{E - p''^2/2m_r}\right)}{\Re\left(1 - \lambda \sum_{p''} \frac{w(p'')^2}{E - p''^2/2m_r}\right)}. \tag{6}$$

Using scattering data as scattering length and effective radius from [12], the parameters of the separable potential were obtained. The results are presented in table 1. Figure 1 shows the phase shifts for the singlet and triplet scattering channels obtained by the separable potential. There are also results obtained from TDDFT within ALDA and with the single-pole approximation (SPA) [15] and also data of Schwartz [12]. The behavior at high values of k (respectively E) is improved if more terms in the separable potential are taken into account. Using the properties of the T-matrix (see [8, 19]), the binding energy E_0 of the H^- ion can be obtained solving

$$1 - \lambda b \frac{2}{\pi^2} \int_0^\infty \frac{\mathrm{e}^{-2k^2} k^2 \,\mathrm{d}k}{E_0/b^2 - k^2} = 0. \tag{7}$$

With the parameters fitted to the scattering phase shifts, the binding energy for the singlet state is found as $E_0 = -0.0474$ H ($-1.280\,448$ eV). The experimental value of the binding energy is $E_0 = -0.0277$ H (-0.7542 eV) [17]. The comparison shows that the simple separable potential with Gaussian form-factor gives already reasonable results which may be improved using more terms in the interaction potential and dispersive forces instead of a static potential.

Table 1. Parameters of the separable potential.

	λ	b	a/a_B	r_0/a_B
$S=0$	−45.399	0.4705	5.965	3.32
$S=1$	77.67	0.9	1.77	1.1

3. Pauli blocking

In the previous section we have considered the plasma in the low-density limit. In this section we pass on to investigate a partially ionized dense hydrogen plasma. The Pauli blocking has to be taken into account in a dense system. The Pauli exclusion principle helps to explain a wide variety of physical phenomena. The Mott effect, which is defined as destruction of bound states at high densities, is caused by screening or the Pauli blocking. The Pauli exclusion principle suppresses the probability for the free electrons to penetrate into atoms or molecules. At high densities the atoms become ionized because of the pressure from the free electrons. Recently an article [20] has been published, devoted to the role of the energy shifts on thermodynamics and phase transitions in a dense hydrogen plasma. The binding energy of the hydrogen atom was calculated as well as the ionization equilibria of the system, taking into account the Pauli shifts and Fock shifts of the ground-state energy level due to the interaction with the medium.

In this paper we study the shift of the binding energy of H^- due to Pauli blocking. A Schrödinger equation for the e–a problem is obtained, where medium effects enter by the Pauli blocking

$$\frac{p^2}{2m}\psi(p) + (1 - f(p)) \sum_{p'} V(p, p')\psi(p') = E_0\psi(p), \tag{8}$$

$f(p) = 1\Big/\left(\exp\left[\beta\left(\frac{p^2}{2m} - \mu\right)\right] + 1\right)$ is the Fermi distribution. Quasiparticle self-energy shifts are not of importance here and are neglected. The chemical potential μ is given by the density according to

$$\int_0^\infty \frac{\mathrm{d}^3 p}{(2\pi\hbar)^3} \frac{1}{\exp\left[\beta\left(\frac{p^2}{2m} - \mu\right)\right] + 1} = \frac{n_e}{2}. \tag{9}$$

Using the obtained parameters of the separable potential, the binding energy of the electron in the negative hydrogen ion has been calculated in dependence of the free electron density and the temperature. The numerical results for the energy spectrum are given in figure 2. We find a dependence of the bound-state energy on the density of electrons. We can also see from figure 2 that the binding energy is decreased with increasing electron density. Approximately at the density $n_e = 9.8 \times 10^{21}$ cm^{-3} and temperature $T = 10\,000$ K bound states could not be formed. The influence of the Pauli blocking on the phase shifts is presented in figure 3. It is shown that at $n_e = 9.8 \times 10^{21}$ cm^{-3} for $T = 10\,000$ K the behavior of phase shift is changed. According to the Levinson theorem, the jump of the phase shift $\delta(0)$ at $k = 0$ by π occurs at the same density when the bound state H^- disappears. The formation or disappearance of bound states has an influence on the chemical picture of the system and therefore on the thermodynamical properties. Similar problems, in particular the formation of hydrogen as a bound state in nonideal dense plasmas, were considered in [18].

Let us consider the main results obtained in this paper. (i) We have reconstructed a separable interaction potential between the electron and the atom by using scattering data.

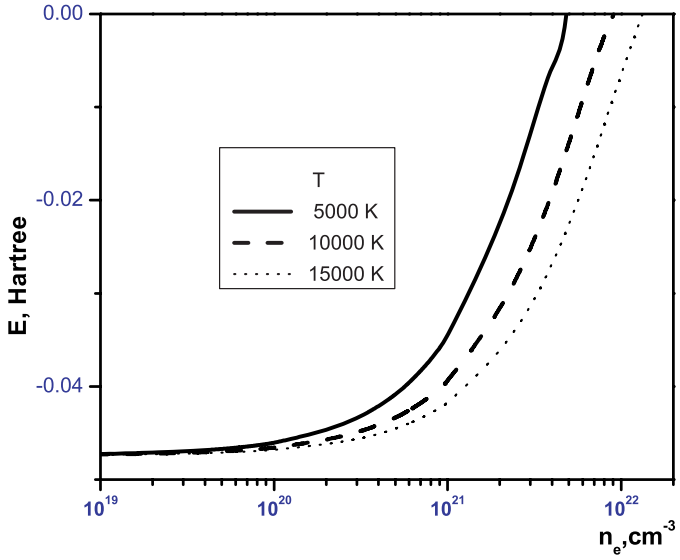

Figure 2. Binding energy in dependence of density number.

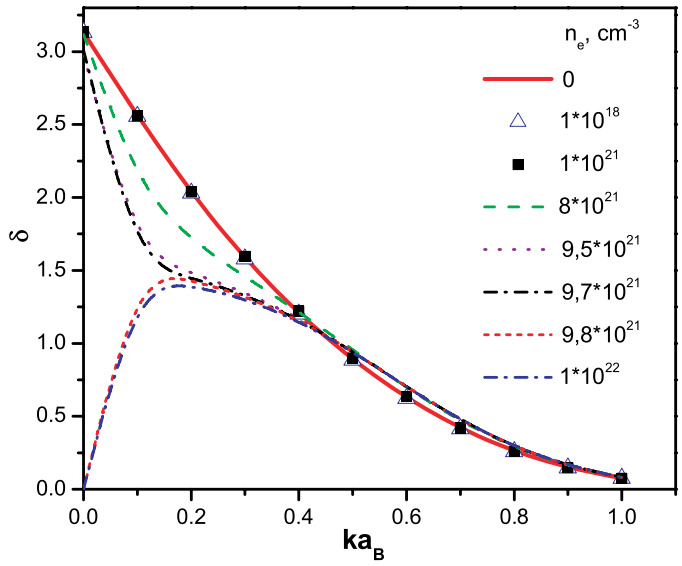

Figure 3. Phase shifts for different electron densities in dependence of k at $T = 10\,000$ K. For comparison, the low-density limit (0) is also shown.

(ii) The binding energy for the singlet state and its shift due to the Pauli blocking effect have been obtained. (iii) The appearance or disappearance of the bound state H^- is also seen in the density-dependent electron–atom phase shifts. (iv) The Pauli blocking effect is essential when investigating dense plasmas. In particular, it can lead to a modification of the recent results for the thermodynamic and transport properties of the dense partially ionized plasma.

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