Ionization cross section for a strongly coupled partially ionized hydrogen plasma: variable phase approach

2009 J. Phys. A: Math. Theor. 42 214034

(http://iopscience.iop.org/1751-8121/42/21/214034)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **42** (2009) 214034 (6pp) doi:10.1088/1751-8113/42/21/214034

Ionization cross section for a strongly coupled partially ionized hydrogen plasma: variable phase approach

F B Baimbetov and Z A Kudyshev

Department of Physics, Al-Farabi Kazakh National University, 050012 Almaty, Kazakhstan

E-mail: Fazylhan.Baimbetov@kaznu.kz and Z.Kudyshev@mail.ru

Received 24 September 2008, in final form 28 December 2008
Published 8 May 2009
Online at stacks.iop.org/JPhysA/42/214034

Abstract
In the present work an electron impact ionization cross section is considered. The electron impact ionization cross section is calculated with the help of a variable phase approach to potential scattering. The Calogero equation is numerically solved, based on a pseudopotential model of interaction between partially ionized plasma particles, which accounts for correlation effects. As a result, scattering phase shifts are obtained. On the basis of the scattering phase shifts, the ionization cross section is calculated.

PACS numbers: 34.80.Dp, 52.25.Jm, 52.20.j

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

1. Introduction

Plasma is widely used in different technical applications, such as MHD generators, gas-phase nuclear reactors and gas discharges. There are some natural objects where nuclear fusion reactions take place, namely, stars. In such strongly coupled systems, the collective and quantum-mechanical effects play an important role.

In the present work the electron impact ionization cross section is considered. There are various approaches to the consideration of the ionization process. One of these is the classical method, introduced by Thompson [1]. According to the Thompson model, the ionization process is considered as a collision of two electrons, interacting through the Coulomb potential, one of them collides with the atom's stationary electron. The ionization process in this model is considered with the help of classical motion equations under the assumption that the minimal imparted energy must be equal to the ionization energy of the atom. In contrast to the Thomson model, the Gryzinski model [2] takes into account the velocity dependence of a bound electron with the help of a semi-empirical distribution function. The results of the Gryzinski model give a good qualitative representation of the ionization process.

In most cases, the ionization of an atom is treated as an isolated event. In reality, the presence of other particles (surrounding) should be taken into account.

The scientific goal of the paper is to account for the surrounding and phase shifts during our consideration of the ionization process.

It is very important to select a correct, sufficient model of interaction between plasma particles involved in the process, during the consideration of elementary processes. In most cases, the Coulomb potential is taken to describe the interaction between the impact particle (electron) and the atom. In the present work the influence of the surrounding on the process of ionization is taken into account through the pseudopotential of interaction between plasma particles.

Taking into account correlation effects and quantum mechanical properties of interacting particles leads to modification of potentials of interparticle interactions [3, 4]. In the work [5] the pseudopotentials are evaluated based on a BBGKY (Bogolyubov–Born–Green–Kirkwood–Yvon) hierarchy in the pair correlation approximation.

In [6], we have obtained the ionization cross section with the help of classical and quantum mechanical methods in the Born approximation. It has been shown that in the case of correlation effects being accounted for with the help of interparticle interaction potential, the obtained ionization cross section has its maximum at $E \approx 3E_i$ (E_i is the ionization energy). The results of calculations are in satisfactory agreement with experimental data and the results of authors who used different models of interaction.

2. System parameters

In the framework of this paper the partially ionized hydrogen plasma, which consists of free electrons (with mass m_e, charge $-e$, concentration n_e), free protons (with mass m_p, charge e, concentration n_p) and atoms (with mass m_n, concentration n_n), is considered. A typical partially ionized plasma also contains hydrogen molecules but we neglect their presence.

Number density is considered in the range of $n = n_e + n_p = 10^{20}–10^{24}$ cm^{-3}, and the temperature domain is $10^3–10^7$ K. The average distance between particles is

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

where $n = n_e + n_p$. The density parameter is $r_s = a/a_B$ ($a_B = \hbar^2/m_e e^2$ is the Bohr radius), $\hbar$ is Planck's constant. The intensity of interaction between plasma particles is defined by the coupling parameter $\Gamma = e^2/ak_B T$, where k_B is the Boltzmann constant, and T is the plasma temperature.

It is worth noting that the plasma state can be fully described by these two dimensionless plasma parameters: coupling parameter and density parameter.

3. Numerical solution of the Calogero equation for phase shifts

In a common case, the scattered wave is not a plane wave. It is necessary to take into account phase shifts. One has to solve the Calogero equation to evaluate the phase shift [7]:

$$\frac{\mathrm{d}}{\mathrm{d}r}\delta_l^{ab}(r) = -\frac{2\mu_{ab}}{\hbar^2 k}\Phi_{ab}(r)\big[\cos\delta_l^{ab}(r)j_l(kr) - \sin\delta_l^{ab}(r)n_l(kr)\big]^2 \tag{1}$$

with initial condition $\delta_l^{ab}(0) = 0$. Here $\delta_l^{ab}(r)$ is the phase shift of the scattering process (a and b are the particle sort indices); $J_l(kr)$ and $n_l(kr)$ are the Bessel functions of the first and

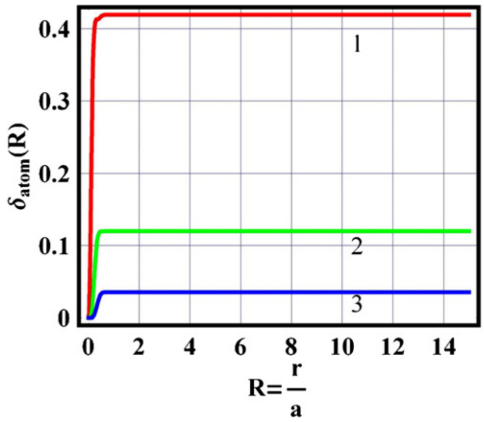

Figure 1. Dependence of the electron–atomic phase shift on the dimensionless interparticle distance ($r_s = 5$, $\Gamma = 1$ and $K = ka = 8$). Red curve (1), $l = 0$; green curve (2), $l = 1$; blue curve (3), $l = 2$.

second kinds correspondingly; $E = \hbar^2 k^2/2\mu_{ab}$ is the relative kinetic energy of the interacting particles with reduced mass $\mu_{ab} = m_a m_b/(m_a + m_b)$; Φ_{ab} is the potential of interaction.

The Calogero equation (1) is numerically solved, based on the pseudopotential model of interaction between the partially ionized hydrogen plasma particles, which accounts for correlation effects. The results of calculations are represented in figure 1.

Phase shifts are weakly dependent on the coupling parameter. At the same time, in the case of a fixed coupling parameter and the reduction of the density parameter, the phase shifts slightly increase. This fact indicates the decay of the correlation effects' influence on the scattering process. In all cases, phase shifts decrease with increase of quantum number l, because increase of quantum number l, by fixed energy of impact electron, signifies the increase of the impact parameter.

4. Ionization cross-section calculation: variable phase approach

The differential cross section is determined as follows:

$$d\sigma = |f(\theta)|^2 \, d\Omega. \tag{2}$$

In expression (2), the scattering amplitude $f(\theta)$ can be calculated through phase shifts with the help of the following formula:

$$f(\theta) = \frac{1}{2iK} \sum_{l=0}^{\infty} (2l+1)[e^{2i\delta_l(\infty)} - 1] P_l(\cos[\theta]), \tag{3}$$

where $P_l(\cos[\theta])$ is the Legendre polynomial of the l order; $\delta_l(\infty)$ is the phase shift in the infinite distance [8, 9]. It is worth noting that summation over l in the expression (3) is done until $l = 20$ and the phase shift in the infinite distance $\delta_l(\infty)$ is determined at $R = 14$, where the phase shifts have a constant value (figure 1). The result of numerical calculations of the differential cross section is represented in figure 2.

The energy exchange between impact and bound electrons is taken into account through the energy conservation law [3, 4]. One can easily obtain the following expression, which

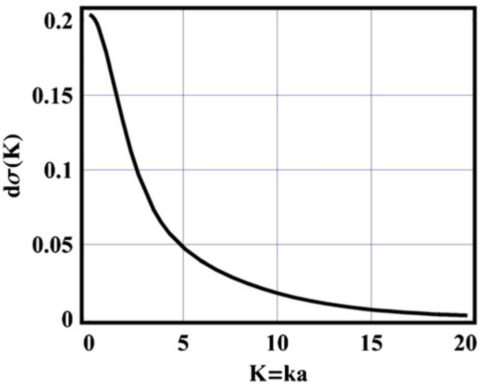

Figure 2. Dependence of the differential cross section on a dimensionless wave vector of the impact electron ($r_s = 5$ and $\Gamma = 1$).

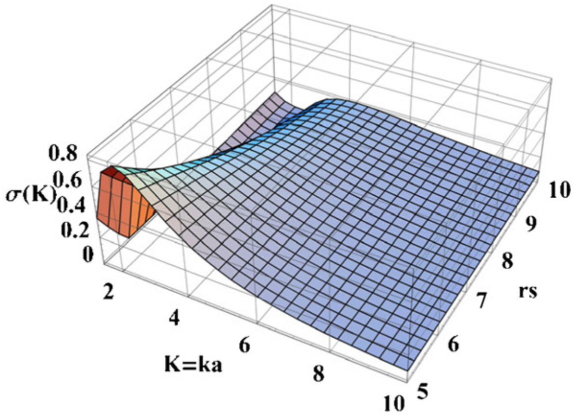

Figure 3. Dependence of the ionization cross section on a dimensionless wave vector of impact electron and on the density parameter ($\Gamma = 1$).

determines the dependence of minimal scattering angle on ionization energy:

$$\begin{aligned} &\Delta E_k = E_i \Rightarrow E_i = E_k \sin^2\left[\frac{\theta_{\min}}{2}\right], \\ &\theta_{\min} = 2\arcsin\left[\sqrt{\frac{E_i}{E_k}}\right]. \end{aligned} \tag{4}$$

Corresponding to the Thompson model, the differential scattering cross section (2) is used for ionization cross-section calculations. During the ionization cross-section calculation the lower limit of solid angle integration has to be replaced by a minimal angle, determined by (4):

$$\sigma_i = 2\pi \int_{\theta_{\min}}^{\pi} \mathrm{d}\sigma \sin[\theta]\,\mathrm{d}\theta. \tag{5}$$

The result of numerical calculations is represented in figure 3.

As is shown in figure 3, decrease of the density parameter r_s leads to increase of the ionization cross section maximum, in the case of the fixed coupling parameter Γ. First,

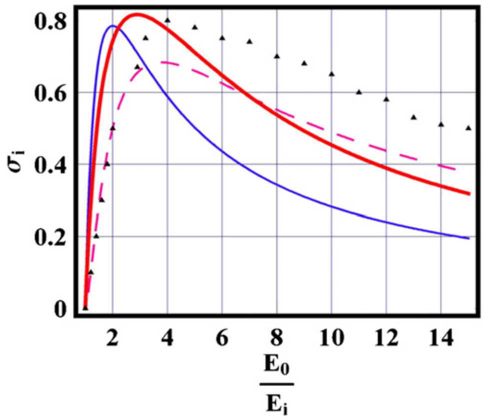

Figure 4. The comparison graph of the obtained ionization cross section (solid red curve; $r_s = 5$ and $\Gamma = 1$) with the corresponding results of Thompson (thin blue curve), Gryzinski (dashed yellow curve), experimental data (point).

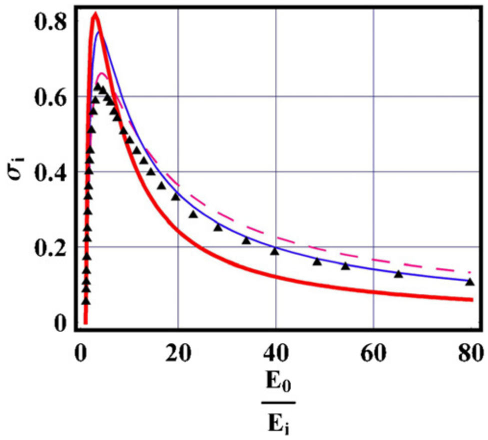

Figure 5. Comparison graph of calculated results (solid red curve: $r_s = 5$ and $\Gamma = 1$) with the corresponding results of Gryzinski (thin blue curve), experimental data [11] (point), results of other authors [10] (dashed pink curve).

decrease of the density parameter r_s signifies increase of the scattering centers (atoms). Second, decrease of r_s leads to increase of the plasma density around interacting particles, i.e. increase of surrounding's influence on the ionization process. Apparently these facts lead to increase of the ionization probability.

5. Comparison with experimental data and results of other authors

The comparison of obtained results of the suggested model of interaction between the electron and the atom with results of other authors and experimental data is represented in figures 4 and 5. A comparison graph of the obtained ionization cross section with the corresponding results of Thompson [4], Gryzinski [5], and experimental data of Fite and Brackmann, represented in work [8], is shown in figure 4. Within this work, the ionization occurs as a result of collision of two crossed beams of electrons and hydrogen atoms in the vacuum chamber.

In figure 5, the obtained results are compared with the results of [10] and [11]. In [10] the suggested model combines the binary-encounter theory with the dipole interaction of the Bethe theory for fast incident electrons. Within this model, the differential cross section for each subshell is calculated using the binding energy, average kinetic energy and the differential dipole oscillator strengths for that subshell. Then the singly differential cross section is integrated over the ejected electron energy to obtain the total ionization cross section. In [11], a pulsed crossed-beam technique incorporating time-of-flight spectroscopy has been applied to measurements of the electron impact ionization cross sections of atomic hydrogen.

From these graphs, one can easily conclude that accounting for the plasma surrounding leads to qualitative changes in the energy dependence of the ionization cross section. First, the curve has a rapid slope at the high energies under all acceptable values of Γ and r_S. If one compares the computed cross section with the corresponding results of our previous work [6], one can conclude that the account of phase shifts leads to a rapid slope at the high energies of the ionization cross section. At the same time, the position of the maximum is in the same area of energies, in agreement with the results of other authors and experimental data.

6. Summary

We have calculated an ionization cross section with the help of a variable phase approach based on the model of interaction between plasma particles, which takes into account the plasma surrounding. It has been shown that accounting for the surroundings leads to some qualitative changes in the energy dependence of the obtained ionization cross section. We believe that one has to take into account the influence of the plasma surroundings during elementary process consideration.

References

[1] Thompson J J 1912 *Phil. Mag.* **6** 23449

[2] Gryzinski M 1965 *Phys. Rev.* A **336** 138

[3] Golant V E, Zhilinskii A N and Sakharov I E. 1977 *Fundamentals of Plasma Physics* (Moscow: Atomizdat) p 62

[4] Smirnov B M 1968 *Atomic Collisions and Elementary Processes in Plasma* (Moscow: Atomizdat) pp 157–78

[5] Baimbetov F B *et al* 2005 Ionization equilibrium and equation of state of partially ionized hydrogen plasmas: Pseudopotential approach in chemical picture *Phys. Plasmas* **12** 082701

[6] Baimbetov F B and Kudyshev Z A 2008 *J. Phys.: Conf. Ser.* **112** 042085

[7] Calogero F 1967 *Variable Phase Approach to Potential Scattering* (New York: Academic) (translated into Russian in 1972)

[8] Mott N and Massey H 1949 *The Theory of Atomic Collisions* (Oxford: Oxford University Press)

[9] Davidov A S 1973 *Quantum Mechanics* (Moscow: Nauka) pp 536–50

[10] Kim Y-K and Rudd M E 1994 *Phys. Rev.* A **50** 3954

[11] Shah M B, Elliott D S and Gilbody H B 1987 *J. Phys. B: At. Mol. Phys.* **20** 3501