Ionization cross section of partially ionized hydrogen plasma.

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Abstract.

In present work the electron impact ionization cross section is considered. The electron impact ionization cross section is calculated, based on pseudopotential model of interaction between plasma particles which accounts correlation effects. It is calculated with help of two methods: classical and quantum – mechanical (Born approximation). The ionization cross section is compared with corresponding results of other authors and experimental data. It has been shown that it is very important to take into account an influence of the surrounding during consideration of ionization processes.

1. Introduction.

There are various approaches of ionization process consideration. One of them is classical method, introduced by Thomson [1]. According to Thomson model, the ionization process is considered as a collision of two electrons, interacting thought Coulomb potential, one of them collide with atom’s stationary electron. The ionization process, in this model, is considered with help of classical motion equations. Cross section, obtained based on this model, gives a good representation of its dependence from collision energy. In contrast to Thomson model, Gryzinski model [2] takes into account velocity dependence of bound electron with help of semi - empirical distribution function. The results of Gryzinski model also give a good qualitative representation of ionization process. The accounting of bound electron’s motion leads to the shift of the maximum to the area with higher energies and reduce to the slower decrease of cross section with growth of collision energy. The second approach is quantum – mechanical method of ionization process consideration, based on Schrödinger equation. In this case, it is often used Born approximation. The results of this approach are in a good argument with experimental data.

It is well known that charge’s field is screened in plasma. This effect leads to the Debye potential in fully ionized plasma. In partially ionized plasma, the ionization process occurs in neutral particles’ presents, so it is very important to take into account of correlation effects’ influence to the interaction between particles. In work [3], potentials of interaction between particles, which account correlation effects, are obtained. In this work, ionization process and its characteristics, in partially ionized plasma with low degree of ionization, are considered. In this case, the potential of interaction between electron and atom, which accounts correlation effects, takes form as follows:

\[ V_{en}(r) = -\frac{e^2}{\beta_n} \left( \frac{1}{a_B} + \frac{1}{r} \right) \exp\left[ -\frac{2r}{a_B} \right] + \frac{2(1-\beta_n)e^2}{\beta_n^2r} \exp\left[ -\sqrt{2(2-\beta_n)r/a_B} \right] \]  

(1.1)
2. Classical calculation of electron impact cross section.

The classical method of ionization cross section calculation consists of two parts. The first part is differential cross section obtaining. In given work the differential cross section is calculated in the Born approximation. In this method, the electron scattering can be considered as a quantum transition from initial free motion state to another one with different impulse. So, the impact electron’s wave functions for initial and final states are taken as

\[ \varphi_i = \exp(\mathbf{i} \mathbf{k}_i \cdot \mathbf{r}) \]
\[ \varphi_f = \exp(\mathbf{i} \mathbf{k}_f \cdot \mathbf{r}) \]

And the differential cross section can be evaluated using this formula:

\[ d\sigma = \left( \frac{\mu}{2\pi\hbar^2} \right)^2 \left| \langle \varphi_f | V(\mathbf{r}) | \varphi_i \rangle \right|^2 d\Omega \]

(2.2)

where

\[ \left| \langle \varphi_f | V(\mathbf{r}) | \varphi_i \rangle \right|^2 = \int V(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} d^3\mathbf{r} \equiv V(q) \]

(2.3)

\( d\Omega \) - element of the solid angle;

\( V(\mathbf{r}) \) - potential of interaction between electron and atom; \( \mathbf{q} = \mathbf{k}_f - \mathbf{k}_i \)

The second part contains classical ionization cross section calculation. The main idea of this part is to account energy conservation law, i.e. ionization energy. It can be achieved by putting minimal scattering angle, which corresponds to ionization energy, into the lower limit of the solid angle integration:

\[ \sigma_i = 2\pi \int_{\theta_{min}}^{\pi} d\sigma \sin[\theta] d\theta \]

(2.4)

Minimal angle can be obtained from equation that determines the dependence of imparted energy from scattering angle:

\[ \Delta E_k = \frac{1}{2} (1 - \cos[\theta]) E_k = E_k \sin^2[\frac{\theta}{2}] \]

(2.5)

Taking into account that minimal imparted energy is equal to ionization energy, the simple mathematics gives

\[ \Delta E_k = E_i \Rightarrow E_i = E_k \sin^2[\frac{\theta_{min}}{2}] \]

(2.6)

\[ \theta_{min} = 2\arcsin[\sqrt{\frac{E_i}{E_k}}] \]

Actually, this method is based on classical Thomson calculation of corresponding cross section but in represented work it was used mentioned above potential of electron - atom interaction instead of Coulomb’s. In addition, it can be said that the classical ionization cross section is calculated numerically as a function of the impact electron energy.

The dependence of obtained cross section from collision energy is shown in Figure 1.

Generally, the results of classical method are useful only for qualitative analysis, because the maximum and the position of the maximum are not in a good agreement with experimental data. Nevertheless, the account of correlation effects leads to the better description of ionization cross section’s dependence from collision energy, than other similar results (Figure 2.). The comparison of calculated cross section with corresponding results of Thomson and Gryzinski models is represented in Figure 2.
3. Quantum – mechanical method of electron impact ionization cross section calculation.

In the Born approximation, the scattering amplitude for an incident electron and an atom is given by

$$ f = -\frac{1}{2\pi} \langle \psi_n | V(r_1, r_2) | \psi_0 \rangle $$

(3.1)

The matrix element is that of the energy of interaction between the incident electron and the atom (1.1).

The wave functions of the initial and final states are given by

$$ \psi_0 = \varphi_0(r_1) \exp(i k r_1) $$

(3.3a)

$$ \psi_n = \varphi_n(r_2) \exp(i k r_2) $$

(3.3b)

where $$ r_1 $$ is the radius vector of the incident electron, $$ r_2 $$ is of the atomic electron, the origin of the coordinate system is at the nucleus of the atom.

It worth to note, that the hydrogen atom’s ground level ($$ \varphi_0(r_2) = (\pi a_0^3)^{-1/2} \exp(-r_2 / a_0) $$) and spherical ($$ \varphi_n(r_2) = (V)^{-1/2} \exp(i k r_2) $$) wave functions are taken to describe bond electron before and after collision correspondingly.

The calculations can be simplified by using the multipole expansion of the expressions $$ e^{-ikr} $$ and $$ \frac{1}{|r_1 - r_2|} $$:

$$ e^{-ikr} = 4\pi \sum_{l,m} (-i)^l j_l(kr) Y^*_{lm}(\theta, \varphi_1) Y_{lm}(\theta, \varphi_2) $$

(3.4)

$$ \frac{1}{|r_1 - r_2|} = 4\pi \sum_{l,m} \frac{1}{r_1} \left( \frac{r_2}{r_1} \right)^l Y^*_{lm}(\theta, \varphi_1) Y_{lm}(\theta, \varphi_2) $$

(3.5)

where $$ j_l(kr) $$ is the spherical Bessel function and $$ Y_{lm}(\theta, \varphi) $$ is a spherical harmonic.

Finally, the electron impact ionization cross section of partially ionized hydrogen plasma can be evaluated using calculated scattering amplitude (3.1):

$$ \sigma_{\alpha \beta} = \frac{k_m}{k_0} \int |f(\theta, \varphi)|^2 d\Omega $$

(3.6)

The analytical formula of quantum - mechanical cross section is obtained and takes form as follows:
Ink aCos

\[ \sigma_{n=0} = \frac{1}{k_0^2} \frac{3072}{\beta_n^2 \pi} \left( 1-2\cos[\theta_p] \right)^2 \left( \frac{a_b^2}{(1-2\cos[\theta_i])^2 + a_b^2 k_n^2} \right)^4 In \] (3.7)

where

\( k_0, k_n \) - wave vectors of impact electron before and after collision correspondingly;

\( k_f \) - wave vector of ionized electron;

\( q_i = k_0 + k_n \); \( q_2 = k_0 - k_n \);

\( \theta_r \) - recession angle of electrons.

\[ In = \frac{1}{6(4+q_1^2 a_b^2)^2} \times ((q_1^2 - q_2^2)^2 \pi q_1^4 q_2^4 a_b^2 (2 - 3 \beta_n) + 48(12 \pi \beta_n + \beta_n - 8 \pi)^2 + + 3 \pi q_1^2 q_2^2 a_b^2 (2 - 3 \beta_n)^2 q_1^2 (q_1^2 - q_2^2)(3 \beta_n - 2)/(24 \pi \beta_n + \beta_n - 16 \pi)) + 12(q_1^2 + q_2^2) a_b^2 (128 \pi^2 - 24 \pi(1 + 16 \pi) \beta_n + + (288 \pi^2 + 36 \pi + 1) \beta_n^2) + + a_b^2 (192 \pi^2 (q_1^2 + 3q_1^2 q_2^2 + q_2^2) - 24 \pi(1 + 35 \pi)(q_1^2 + 3q_1^2 q_2^2 + q_2^2) \beta_n) + + ((1 + 36 \pi + 432 \pi^2) q_1^2 + (1 + 144 \pi + 1728 \pi^2) q_2^2 + (1 + 36 \pi + 432 \pi^2) q_1^2 \beta_n^2)) \]

Figure 3. Dependence of quantum - mechanical ionization cross sections, with given collision parameters (\( \theta_r \) - recession angle of electrons and \( \theta_p \) - output angle of ionized electron), from collision energy

It can be seen from figure 3, that obtained cross section have its maximum at \( E_0 = 3E_i \). The results of calculations are in a good argument with experimental data, represented in figure 4. In addition, it can be said, that taking into account of correlation effect reduces to more rapid slope of the curve at high energies.

References

[1] V. E. Golant, S. A. Sahorov, Plasma Physics,1977, p. 62.
[2] B. M. Smirnov, Atom collisions and elementar processes in plasma,1968, p. 168-171.
[3] Baimbetov F.B., Arkhipov Yu.V., Davletov A.E. Thermodynamics of partially ionized hydrogen plasmas: Pseudopotential approach in chemical models. Phys. Plasma 2005, v.5, p. 315-321
[4] A. S. Davidov, Quantum mechanics // «Nauka». – 1973. p. 536 – 550.
[5] N. Mott and H Massey, The Theory of Atomic Collisions
[6] M. Gryzinski, Classical Theory of Atomic Collisions. I. Theory of Inelastic Collisions, Phys. Rev. 138, A336, 1965

Figure 4. Comparison of the quantum - mechanical cross section with corresponding result of Chandrasekhar, Breen work and experimental data.