The Calculation of the Photo Absorption Processes in Dense Hydrogen Plasma with the Help of Cut-Off Coulomb Potential Model

Nenad M. Sakan
Institute of Physics, Pregrevica 118, Zemun, Belgrade, Serbia
E-mail: nsakan@ipb.ac.rs

Abstract. Extensive work was done in the application of a cut-off Coulomb model on the description of the optical processes of the photo ionization and inverse bremsstrahlung. Present work deals with the usage of a cut-off Coulomb model pseudo potential for the calculation of the optical absorption process in dense hydrogen plasma as a entirely quantum mechanical process. Although the mentioned processes are strongly influenced by the collective process in dense plasma, the used pseudo potential enables to model the described interaction with the plasma system as a binary process. There are several advantages of such approach: the existence of the exact analytical solutions for the wave functions in the described potential enables to eliminate one of the several sources of numerical error. Also, more complex processes of the interaction inside plasma could be considered, and they have been added in presented work. The work on description of such processes has been started. The collective phenomena of the plasma are here described as an additional shifting and broadening of a bond states levels. Furthermore, with the adding of mentioned broadening and additional shifting of the bond states as free external parameters the good agreement between the analyzed experimental data and our model solutions occurs. The method of determination of the cut-off radius was developed and applied in our considerations. The presented model is a good approach for the description of dense hydrogen plasma of moderate and high non-ideality. It presents an easily extendable model, in which is easy to introduce additional processes and effects.

1. Introduction
In this paper is studied a new model method of the describing of the continuous absorption of electromagnetic (EM) radiation in dense strongly ionized hydrogen plasma, caused by the atomic photo-ionization processes

\[ E_{h\nu} + H^*(nl) \rightarrow H^+ + e_{q'}, \]  

(1)

and electron-ion inverse ”bremsstrahlung” processes

\[ E_{h\nu} + e_{\vec{q}} + H^+ \rightarrow e'_{\vec{q'}} + H^+, \]  

(2)

where \( E_{h\nu} \) is the energy of the photon with the wavelength \( \lambda \), \( n \) and \( l \) - principal and orbital quantum numbers of hydrogen excited states, \( \vec{q} \) and \( \vec{q'} \) - the momentum of the free electron before and after scattering on the considered ion \( H^+ \).
While in weakly and moderately non-ideal plasma, this absorption is caused by the neutral atoms and electron-ion collision complex which interaction with the neighborhood can be neglected, as for example in Solar photosphere [5, 6], or described within the framework of a perturbation theory [18, 12, 13, 15, 16] in the dense strongly non-ideal plasma the situation is in principle different.

By now a lot of effort was aimed to the development of the quantum-statistical methods for the description of the thermodynamical and transport properties of dense strongly non-ideal plasma [9, 11, 8, 7, 10, 14] while the absorption processes was treated only for plasma with electron densities \( N_e < 10^{18}\text{cm}^{-3} \), where the approximation of electron-atom and electron-ion binary collisions is still applicable. The area of really dense plasma with \( N_e > 10^{19}\text{cm}^{-3} \) was not systematically studied from the aspect of the bound-bound, bound-free and free-free absorption processes, excluding some efforts of semi-empirical describing of such processes [25, 26]. Because of that the development of a model method which describes the mentioned absorption process in dense strongly non-ideal plasma on a simple and physically acceptable way is the one of the actual tasks. Within this work as a landmark is taken the hydrogen plasma with the electron density \( N_e = 1.5 \cdot 10^{19}\text{cm}^{-3} \) and the temperature \( T = 23000K \), which was experimentally studied in [26]. The direct result of this work is a new model method for the determination of absorption coefficients \( \kappa_{\text{bf}}(\lambda) \) and \( \kappa_{\text{ff}}(\lambda) \), characterizing the bound-free and free-free absorption processes (1) and (2) in the strongly non-ideal hydrogen plasma, which is based on a cut-off Coulomb pseudo-potentials, similar to the one used for the determination of the non-ideal plasma conductivity. The presented method is tested in the optical range of photon wavelengths \( 350\text{nm} \leq \lambda_{\nu} \leq 550\text{nm} \).

2. Theory
2.1. The cut-off Coulomb potentials

The obvious way of simplification of principally many body processes of photo absorption transitions inside plasma was transformation to the corresponding transitions of the electron in an adequately chosen pseudo-potential, which replaces the considered ion and the rest of the system. In [22], in order to obtain the method of the describing of such process which would be practically applicable, generally non-local pseudo-potential in usual way was soughed in the form of the corresponding local one-particle potential. As such potential was chosen one of model screening Coulomb potential, namely cut-off potential (4).

On the occasion of the choosing of the model potential it was taken into account the argumentation from the [22], which shows that often used model Debye-Hückel (DH) potential is not adequate for strongly non-ideal plasma. Let us draw attention that we here do not have in mind some undesirable properties of the DH potential [28, 27], but the way of the obtaining of that potential itself. Namely, in accordance with [19] the DH potential is the average electrostatic potential which is generated by the observed ion and all charged particles from its neighborhood, which are often treated as the screening cloud. Consequently, the electron, that is involved in scattering on the considered ion, also is the part of that cloud. In spite of this fact the DH potential, as it is known, is used often in weakly non-ideal plasma when the number \( n_D \gg 1 \), where \( n_D \) is the number of the electrons inside the sphere with the Debye radius \( r_D \).

However, in the case of strongly non-ideal plasmas, when \( n_D \cong 1 \), as it is in the considered plasma, practically, the complete cloud is consisted of the free electron that is involved in scattering, and the DH potential could not be used any more. Contrary to that, in the case \( n_D \cong 1 \) the application of the cut-off Coulomb potential, as it was noted in [22], is physically completely justified, since it automatically provides: just Coulomb behavior of the potential in the close vicinity of the considered ion; the lowering of the atom ionization potential caused by the influence of the neighborhood, which is equal to the average potential energy of a free electron in plasma; non Coulomb asymptotic of the wave function of a free electron.

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All mentioned have caused that one of the considered here model cut-off Coulomb potentials has the form, which is shown in the Fig. (1a), where $e$ is the absolute value of electron charge, $r$ - the distance from the origin of the chosen reference frame, $r_c$ - corresponding screening radius, and the value $U_p = -e^2/r_c$ has to be interpreted as the above mentioned the average potential energy of a free electron in plasma. Other model cut-off Coulomb potential is considered here because the fact that in the case of the first model the average potential energy of the electron in the region $0 < r < r_c$, for the difference of the region $r_c < r < \infty$, is not equal to the energy $U_p$, which is illustrated by Fig. (1 a). However, in the plasma the moving of the electron from the region occupied by the one ion to the region occupied by the nearest neighbor ion is realized in the potential with the maximal value (between the position of the mentioned ions), which is greater than average values of potential. Because of that the average potential energies of the electron in the region occupied by the one ion and in the rest of the plasma have to be equal to the average energy of the free electron in the whole system denoted here by $U_p$. One can see that this condition can be satisfied in the case of other cut-off Coulomb potential, which is shown in Fig. (1b), when the parameter $k = 1/2$. Namely, it can be shown that
\[
\int_0^{(k+1)r_c} U(r)4\pi r^2 dr = U_p V = -\frac{e^2}{r_c} \cdot \frac{4\pi}{3} [ (k+1)r_c ]^3 ,
\]
is only valid for $k = 1/2$, where $V$ is the volume of sphere with radius $r_c$, which is determined on the basis of the result from [28].

In further consideration we will take the value $-e^2/r_c$ as the zero of the energy. After that, the potentials shown in the Figs. (1a) and (1b) are transformed to the forms $U_0(r; r_c)$ and $U_k(r; r_c)$, respectively, where
\[
U_0(r; r_c) = \begin{cases} 
-\frac{e^2}{r} + \frac{e^2}{r_c} & : 0 < r \leq r_c, \\
0 & : r_c < r ,
\end{cases}
\]
\[
U_k(r; r_c) = \begin{cases} 
-\frac{e^2}{r} + \frac{e^2}{r_c} & : 0 < r \leq (k+1)r_c , \\
0 & : (k+1)r_c < r
\end{cases}
\]
where $U_0(r; r_c)$ is the same potential as in [22]. Because of the above mentioned, in the case of the potential $U_k(r; r_c)$ we will consider that $k = 1/2$.

Let us denote that the form of the potential (5) is not caused by the presence of some new mechanism that increases the barrier in the region $r > r_c$ for the electron in the complex $(H^+ + e)_{nl}$ or $(H^+ + e)_{q\bar{q}}$, but exclusively by the requirement for the satisfying of the condition (3).

2.2. The photo-ionization and inverse "bremsstrahlung" cross-sections
Since under the condition from [26] the considered wavelength $\lambda \gg r_s$, where $r_s = (3/4\pi N_e)^{1/3}$ is the corresponding Wigner-Seitz radius, the dipole approximation in the case of considered processes is valid. According to that, the cross section for these bound-free and free-free absorption processes are given by the expressions from [24], namely
\[
\sigma(nl; E') = \frac{4\pi^2 e^2 k}{3(2l+1)} \sum_{l'=l\pm1} l_{\text{max}} \left( \int P_{nl} r P_{E'l'} dr \right)^2 ,
\]
\[
\sigma(E; E') = \frac{8\pi^4 \hbar e^2 k}{3} \sum_{l'=l\pm1} l_{\text{max}} \left( \int P_{El} r P_{E'l'} dr \right)^2 ,
\]
where $k = \epsilon_{\lambda}/\hbar c$ is the momentum of the absorbed photon with the given $\lambda$, $E = \hbar^2 q^2/2m$ and $E' = \hbar^2 q^2/2m$ - the energies of the free electron, $l_{\text{max}}$ - maximal value of $l$ and $l'$, $m$ - the electron mass, and $c$ - the light velocity. Here the radial wave function of the electron in the model potentials (4) and (5) with $k = 0.5$ is denoted with $P_{nl}/r$, for the bound states with given $n$ and $l$, and with $P_{El}/r$ and $P_{E'l'}/r$ for the free states with the given $E$ and $l$ or $E'$ and $l'$. The functions $P_{nl}$ and $P_{El}$ are obtained in strict analytical form by the means of the expressions for the Whittaker, Coulomb, spherical Bessel, and modified Bessel functions.

In further calculations for the determination of the photo-ionization cross section $\sigma(nl; E')$ is used Eq. 6, while in the case of inverse "bremsstrahlung" cross section $\sigma(E; E')$ is used the expression which is obtained by means of the known relations [24], which connect the matrix elements of the $j$-th components ($j = 1, 2, 3$) of the radius-vector $\vec{r}$, electron momentum $\vec{p}$, and gradient of the potential $\nabla U(\vec{r})$, namely

$$< \langle in | \hat{\nabla} \cdot \hat{U}(\vec{r}) | fin \rangle > = \frac{i}{\hbar} (E_{in} - E_{fin}) < \langle in | \vec{p}_j | fin \rangle >,$$

(8)

$$< \langle in | \vec{p}_j | fin \rangle > = \frac{i m}{\hbar} (E_{in} - E_{fin}) < \langle in | r_j | fin \rangle >,$$

(9)

where $U(\vec{r})$ in the considered case is equal to $U_0(r)$ or $U(r; k)$. Namely, from Eqs. (7), (8) and (9) it follows the expression

$$\sigma(E; E') = \frac{4\pi^4 \hbar^6 e^2}{3 m^3 c E_E E'_{\lambda \nu} \nu_{l \pm 1}} \sum_{l_{\text{max}}} \left( \int_0^{(k+1)r_E} P_{El} \nabla U(r) P_{E'l'} dr \right)^2,$$

(10)

where $E_{E\nu} = E' - E$, and with $U(r) = U(r; k = 0) \equiv U_0(r)$ or $U(r; k = 1/2)$, which enables to use the shape of the potentials (4) and (5) and to avoid all difficulties connected with the calculation of the dipole matrix element in Eq. (7) in the whole region of space $0 < r \leq \infty$. Just Eq. (10) is used here for the calculation of the inverse "bremsstrahlung" cross-section $\sigma(E; E')$.

2.3. The partial and total absorption coefficients

The expressions (6) and (10) for the photo-ionization and inverse "bremsstrahlung" cross-sections enable the direct determination of the partial absorption coefficients, characterizing the bound-free and free-free absorption processes (1) and (2), given by the relations
\[ \kappa_{bf}^{(0)}(\lambda; N_e, T) = \sum_{n=1}^{n_{max}} \sum_{l=0}^{n-1} N_{nl} \cdot \sigma(nl; E'), \]  
\[ \kappa_{ff}^{(0)}(\lambda; N_e, T) = N_l N_e \cdot \int_{0}^{\infty} \sigma(E; E')vf(v)dv, \]

where \( N_{nl} \) is the density of the atoms \( H^* \), e.g. electron-ion pairs in the bound states with the given quantum numbers \( n \) and \( l \), \( T \) - the plasma temperature, and \( n_{max} \) - the principal quantum number of the last realizing bond state for the given \( N_e \) and \( T \). However, while the expression (12) for the free-free absorption coefficient \( \kappa_{ff}^{(0)}(\lambda; N_e, T) \) should generate the purely acceptable results, the situation in connection with Eq. (11) is different. Namely, the results obtained by means of Eq. (11) should be similar to the ones for the diluted plasma (see for example [5]), since, contrary to the existing experimental results [26], the unique serious difference would ensue from the lowering of the photo-ionization limits for the realizing bound states for the value close to \( e^2/r_c \).

The plasma-ion interaction at the considered densities is mainly of Stark type, and also it was made a transition from many particle model towards the two particle model. Because of that there should be included and additionally considered a shift and the broadening of a bond state levels, as a result of a many particle interactions. The mentioned shifts and broadenings are treated as the semi-empirical quantities, which appear as the external parameter of the theory. Here, the shift of \((nl)-\)level is denoted by \( \Delta^{sh}_{nl} \), and broadening by \( \Delta^{br}_{nl} \). As it is usual we assume that the electron in atom \( H^*_{nl} \) in the plasma could be in the state with the energies which are dominantly grouped around the energy \( \varepsilon^{max}_{nl} = \varepsilon(nl) + \Delta^{sh}_{nl} \), inside the interval \( (\varepsilon^{max}_{nl} - \Delta^{br}_{nl}/2, \varepsilon^{max}_{nl} + \Delta^{br}_{nl}/2) \). Let \( P_{nl}(\varepsilon) \) is the probability density which characterizes the distribution of the energies of the mentioned state within the interval \( (\varepsilon^{max}_{nl} - \Delta^{br}_{nl}/2, \varepsilon^{max}_{nl} + \Delta^{br}_{nl}/2) \), which satisfies the conditions

\[ \max\{P_{nl}(\varepsilon)\} = P(\varepsilon = \varepsilon^{max}_{nl}) = \int_{\varepsilon^{max}_{nl} - \Delta^{br}_{nl}/2}^{\varepsilon^{max}_{nl} + \Delta^{br}_{nl}/2} P_{nl}(\varepsilon)d\varepsilon = 1. \]

In accordance with above consideration, here we will characterize the bound-free and free-free processes by the photo-ionization and inverse "bremsstrahlung" partial absorption coefficients

\[ \kappa_{bf}(\lambda; N_e, T) = \int_{\varepsilon^{max}_{nl} - \Delta^{br}_{nl}/2}^{\varepsilon^{max}_{nl} + \Delta^{br}_{nl}/2} P_{nl}(\varepsilon) \cdot \tilde{\kappa}_{bf}^{(0)}(\lambda; N_e, T; \varepsilon)d\varepsilon, \]

where \( \tilde{\kappa}_{bf}^{(0)}(\lambda; N_e, T; \varepsilon) \) is obtained from (6) and (11) by replacing free electron energy \( E' \) with \( \tilde{E}' = E' + (\varepsilon - \varepsilon_{nl}) \),

\[ \kappa_{ff}(\lambda; N_e, T) = \kappa_{ff}^{(0)}(\lambda; N_e, T), \]

where \( \kappa_{ff}^{(0)}(\lambda; N_e, T) \) is given by Eq. (12), as well as the corresponding total absorption coefficient

\[ \kappa_{tot}(\lambda; N_e, T) = (\kappa_{ff}(\lambda; N_e, T) + \kappa_{bf}(\lambda; N_e, T)) \cdot \left[ 1 - \exp\left( -\frac{\varepsilon_{kT}}{kT} \right) \right], \]

where it is taken into account the influence of the stimulated emission.
3. Results and discussion

In this paper the calculations of the total absorption coefficient \( \kappa_{tot}(\lambda; N_e, T) \) with the cut-off Coulomb potential (4) were made for the strongly non-ideal hydrogen plasma \( N_e = 1.5 \cdot 10^{19} \text{ cm}^{-3} \) and \( T = 23000 \text{ K} \), as well as \( N_e = 6.5 \cdot 10^{18} \text{ cm}^{-3} \) and \( T = 18000 \text{ K} \) taken from [26].

After process of selection of adequate shift and broadening parameters and comparison with the experimental data, good agreement was found. The good agreement with the experimental data in area where only continuous absorption is present, e.g. at the energies \( E_{h\nu} \geq 2.8 \text{ eV} \), and the form of the total continuous absorption coefficient gives a space for bond-bond transition absorption.

Without further research on bond-bond transition within the frame of this model, there is not much to be said and analyzed for the model of broadening and shifting of bond state levels. Allthow, at this moment, it is just a parameter without further involvement into the processes behind it, it should be emphasized again that good agreement with experimental data exists.

4. Conclusion

Besides the fact that the presented model is still in process of development, a good agreement with the experimental data was shown.

There is a need to develop a model of bond-bond absorptions, which would enable the investigation of form of broadening and shifting of bond state levels. It would enable the studies of the broadening and shifting effects more in detail and develop a more concise model.

Also there is still a need for developing of both faster numerical procedures and code parallelism to improve speed and accuracy.

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