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The application of the cut-off Coulomb potential for the calculation of a continuous spectra of dense hydrogen plasma

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Abstract. The continuous optical spectrum of dense hydrogen plasma is modeled with the complete quantum mechanical model based on the cut-off Coulomb potential. Here are presented the results of calculation of a continuous optical spectra of dense hydrogen plasma and compared with the experimental results obtained in "Laboratory for dense plasma" at the Pierre et Marie Curie University in Paris. The cut-off Coulomb potential gives the opportunity to model the most significant effects in dense plasma. The additional effects, including some of time dependent, which influences the spectral characteristics, could be easily added. This work is a continuation of previous works on conductivity of dense plasma based on cut-off Coulomb potential.

1. Theory

In this work the results of calculations of continuous spectra photo absorption coefficients are presented. They are given by

$$k^{tot}(\omega; N_e, T) = \Big(k_{bf}(\omega; N_e, T) + k_{ff}(\omega; N_e, T)\Big) \cdot \left[1 - \exp\left(-\frac{\hbar\omega}{kT}\right)\right]. \quad (1)$$

Here N_e is the electron concentration, while T is electron temperature of investigated plasma. The above coefficient is easily experimentally measured, and it is known as a reduced absorption coefficient. In the equation (1) the $k_{bf}(\omega; N_e, T)$ and $k_{ff}(\omega; N_e, T)$ are the partial bond-free and free-free absorption coefficients, given by following equations

$$k_{bf}(\omega; N_e, T) = \sum_{n,l} N_{nl}\sigma(nl; E), \quad (2)$$

$$k_{ff}(\omega; N_e, T) = N_i N_e \int_0^\infty \sigma(E; E')v f(v) dv. \quad (3)$$

In those equations N_{nl} is the population of the appropriate bound level state, N_i is the positive ion concentration, and in the presented case $N_i = N_e$, and $f(v, T)$ is the Maxwell distribution function.

For the calculation of the absorption coefficient it was necessary to calculate the appropriate cross sections. The formulas for their calculation are adopted from Игорь Ильич

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Собельман (1963), and they are given by the terms

$$\sigma(nl;E) = \frac{4\pi^2 e^2 k}{3(2l+1)} \sum_{l'=l\pm1} l_{max} \left(\int P_{nl} r P_{El'} dr \right)^2 . \quad (4)$$

$$\sigma(E;E') = \frac{8\pi^4}{3} \frac{\hbar e^2 k}{q^2} \cdot \sum_{l'=l\pm1} l_{max} \left(\int P_{E'l'} r P_{El} dr \right)^2 . \quad (5)$$

Here $P_{nl} = rR_{nl}$ is a solution for the bond states of the radial part of Schrödinger equation with the Coulomb cut-off potential given by Eq. (8), P_{El} and $P_{E'l'}$ are the solutions for the free states. The frequency for the bond-free and free-free transitions are given by $\hbar\omega = E' - E(n,l)$ and $\hbar\omega = E' - E$ respectively, and $k = \omega/c$, and also the momentum of the free electron is given by $q^2 = 2mE$.

The cross sections for the inverse processes could be calculated by

$$q^2\sigma(E;nl) = 2(2l+1)k^2\sigma(nl;E)$$
$$q^2 = \frac{2mE}{\hbar^2} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad (6)$$

and

$$q'^2 \frac{d\sigma(E';E)}{d\omega} = q^2 \frac{k^2}{\pi^2} \sigma(E;E'). \quad (7)$$

Here $q^2 = 2mE/\hbar^2$, $q'^2 = 2mE'/\hbar^2$ and $\hbar\omega = E' - E$.

The choice of a cut-off Coulomb potential, mathematically represented as

$$U_H(r) = \begin{cases} -\frac{e^2}{r} + \frac{e^2}{r_c} & : \quad 0 < r \le r_c \\ 0 & : \quad r_c < r \end{cases}, \quad (8)$$

for the potential that describes the behavior of dense hydrogen plasma is made because of several reasons. In the equation (8) r_c stands for cut-off radius. The influence of a plasma is averaged in temporal and spatial domain, so it is possible to study only the quantum system consisting of a single atom and a potential of the rest of the plasma. With the averaging lot of processes are neglected in this figure, but they could be additionally introduced. The form of potential led us to dissolution on radial and spherical space with adequate wave function dissolution, i.e.

$$|\Psi(r,\theta,\varphi)\rangle = |R(r)\rangle \otimes |Y_l^m(\theta,\varphi)\rangle, \quad (9)$$

here $|\Psi(r,\theta,\varphi)\rangle$ is a complete wave function for a statical Schrödinger equation, $|Y_l^m(\theta,\varphi)\rangle$ is the spherical part which has well known solutions, and the radial part $|R(r)\rangle$. The radial part of a wave function has all the information on plasma influence on atom.

The additional effects are introduced by the use of a perturbation method. If the potential $\hat{V}$ generates the perturbation of the known system, i.e.

$$\hat{H}|\Psi\rangle + \lambda\hat{V}|\Psi\rangle = E|\Psi\rangle,$$

where λ is a small parameter, the solution $|\Psi\rangle$ and the energy E, for the first order approximation, are presented by the

$$|\Psi\rangle = |\Psi^{(0)}\rangle, \qquad E = E^{(0)} + \lambda E^{(1)}.$$

Here $|\Psi^{(0)}\rangle$ and $E^{(0)}$ are the solutions for the unperturbed Hamiltonian.

In the results shown here the spreading and the shifting of the bond states are introduced. Those effects are related to the Stark effect induced by the closest neighbor ions in plasma. The spreading is modeled as a Lorenz distribution

$$\rho_E(E_{nl},\gamma;E) = \frac{1}{\pi} \frac{\gamma/2}{(E_{nl}-E)^2 + \gamma^2/4}, \quad (10)$$

and for the cross section calculated with the introduced spreading yields equation

$$\widetilde{\sigma}(nl;E) = \int_{-E_{h\nu}}^{0} \sigma^*(nl;E_{h\nu}-E) \rho_E(E_{nl},\gamma;E)dE. \quad (11)$$

Here $\sigma^*(nl;E_{h\nu}-E)$ is a cross section for the photo absorption from the lower energy level, with the energy E and width dE, and with the energy density $\rho_E(E_{nl},\gamma;E)$ spread in the vicinity of the energy of nonperturbed state

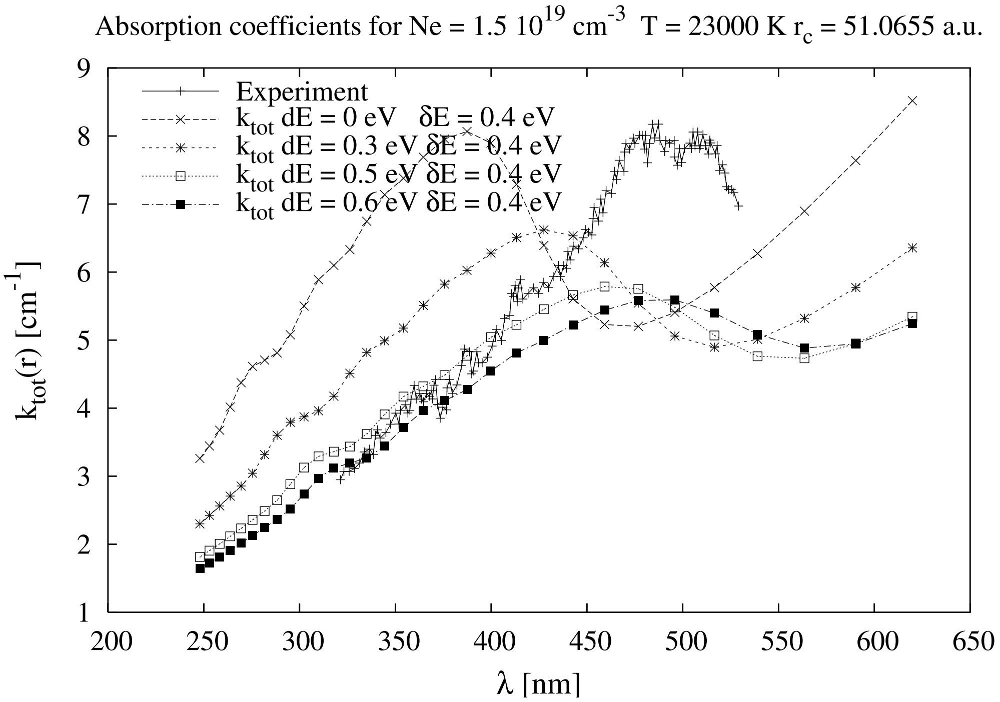

Fig. 1. Absorption spectra of dense hydrogen plasma, theoretical calculations and experimental data. $N_e = 1.5 \cdot 10^{19}$, $T = 23000K$, $r_c = 51.0655a.u.$.

E_{nl}. The wave function, in the first approximation, for this state is $|nl\rangle$.

With this approach the exact solutions for the wave functions are obtained. Because they are mathematically defined special functions the calculation for the free-free cross section is simplified and it is exact without any additional mathematical or numerical approximation.

The cut off radius r_c and the spreading of the wave function γ are the external parameters of the theory

2. Results

In the figure 1 an example of the comparison between the experimental and the calculated values for the dense plasma is given. Results presented here are taken from Vitel et al. (2003). The method presented here gave us possibility to adopt the adequate values for the external parameters r_c and energy level shifting dE and broadening δE to fit the experimental data. Figure here presents the possibility of adjustment of the energy level shift dE and presents a good illustration of external parameter fitting of the experimental results (same procedure is used for r_c and δE).

3. Conclusions

The modelling of an optical spectra of dense non-ideal plasma is a very difficult problem. Unlike the dynamical characteristics of a dense plasma, in the case of the optical properties there is no good model that could describe the behavior of a dense plasma, see for example Kobzev et al. (1995a,b). Disadvantage of previously used methods for description of optical properties of dense plasma was either complicated numerical procedure or the application of a physical model for ideal or moderately non ideal plasma in the area of dense, highly non ideal plasma. In both cases the result was not easy applicable in practice. The model presented here has three major advantages over other methods. As first, all of the approximations of this model are introduced with the physical definition of the model itself, this means that there are no additional approximation in the mathematical procedure. The second advantage is that the calculation of a free-free part of continuous spectra is completely done without any additional mathematical or numerical simplifications. And the third advantage is that this method is a complete quantum calculation with the analytical functions for the solution of bound as well as free states. Because of that there is a possibility to include additional effects.

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