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Analytical potential for determining atomic properties of ions in plasmas for a wide range of plasma coupling parameters. An application to calculate total photoionization cross section.

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1.- Introduction.

To calculate optical properties of plasmas the atomic data have to be obtained for all the ions immersed into the plasma, which are able to be in ground configuration and in a large number of excited configurations as well. For medium and high density the atomic properties must be corrected for each plasma condition taking into account the influence of the plasma surrounding into atomic potential. These facts mean that the amount of atomic data to handle with is huge and sometimes it is necessary, in order to reduce the complexity of the problem and the computing time, to resort to some more simple models that provide these data in a quite accurate manner, such as the effective analytical potentials.

In this work we propose a model for obtaining an effective atomic potential which includes interaction of the bound electron of the ion with the plasma surrounding, for a wide range of plasma coupling parameters. The potential has been developed considering free electrons charge distribution in the neighbourhood of the ion, linearized Boltzmann charge distribution for free electron and ions at medium and large distances of the nucleus and the reaction of the plasma-charge density to the optical electron in a relativistic quantum state (nlj). An analytical expresion for this non isolated potential is proposed.

Our objetive is to obtain a simple non isolated effective analytical potential to correct the isolated atomic data as for example energy levels, energy transitions and the continuum lowering. This will allow us to carry out more realistic calculation of LTE and non-LTE ionic populations. Finally, this model is used to make some comments aboutobt the total photoionization cross sections for a wide range of the plasma coupling parameters.

2.- The non isolated atomic potential.

Consider a ion with nuclear charge Z, which consist of a point nucleus at the origen and N bound electrons, in a sea of electrons and point ions. The effective time-averaged electrostatic potential is determinated by the Poisson equation

$$\frac{1}{r}\frac{d^2\left(rU_{eff}(r)\right)}{dr^2}=\frac{1}{r}\frac{d^2\left(rU_{N\text{-}1}(r)\right)}{dr^2}+4\pi e\left(n_{fe}(r)-\sum_{i=1}^{Z}Z_i n_i(r)\right) \tag{1}$$

where we have assumed that the electrostatic potential is spherically symetric, $U_{eff}(r)$ is the non isolated effective potential, $U_{N\text{-}1}(\vec{r})$ is the potential generated by the *N-1* bound electrons, n_{fe} is the free electron density and n_i is the ion density of ions with net charge Z_i $(=Z-i,\ i=0,1,\ldots\ldots,Z)$. Moreover, the potential $U_{N\text{-}1}(r)$ is determined by a funtional of the bound electron density which is calculated with the relativistic wave funtions obtained from Dirac equation given by

$$\left[-i\vec{\alpha}\cdot\vec{\nabla}+\beta mc^2+U_{eff}(r)\right]\varphi_k(r)=\varepsilon_k\varphi_k(r) \tag{2}$$

where p_{i} and φ_i are the occupation number and relativistic bound wave funtions respectively. Selecting an appropiated free electron and ion densities, this set of equations define a self-consistent procedure to obtain the total and effective electrostatic potentials in a similar way that other models studied by differents authors. Our objetive is focused in the effective electrostatic potential.

First of all, we consider the zero order approximation for the *N-1* bound electrons, i.e., we consider $U_{N-1}\approx U^{\mathrm{o}}_{N\text{-}1}$, being $U^{\mathrm{o}}_{N\text{-}1}$ the isolated potential of the bound electrons. This one can be a self-consistent isolated potential or one of the analytical expressions available in the bibliography for isolated ions.

We distinguish three regions. In the first one there are not free electrons and it is defined by the sphere of radious R_N which contains *N-1* bound electrons. The second region., is characterized by a constant free electrons density. Finally, in the third region it is found free electrons and ions being their densities approached by the Debye-Hückel linealized approximation.

$$U_{\mathrm{eff}}(r)=\begin{cases}U^{o}_{N\text{-}1}(r)+C_1+C_2/r & 0<r<R_N\\ U^{o}_{N\text{-}1}(r)-(2/3)\pi N_e r^2+B_1+B_2/r & R_N<r<R_T\\ U^{o}_{N\text{-}1}(r)-(A_1/r)e^{-r/R_D}+((N-1)/2rR_D)+(Z-N)/r+C_2/r & R_T<r\end{cases} \tag{3}$$

where the constans in the last expression are given by

$C_1=2\pi\pi_e\left(R_T^2-R_N^2\right)+(4/3)\pi N_e\left(R_N^3-R_T^3\right)+((Z-N)/2R_D)+((N-1)/2)(1-(R_T/R_D)+(1/R_D))$,

$C_2=0$, $B_1=C_1+2\pi\pi_e R_N^2$, $B_2=-(4/3)\pi N_e R_N^3$ and

$$A_1=\frac{R_D}{(R_D+R_T)}\left[(Z-N)+(4/3)\pi N_e\left(R_N^3-R_T^3\right)++((N-1)/2)(1-(R_T/R_D))\right]e^{R_T/R_D}$$

These constants have been determined, after some straightforward manipulations, assuming that the behaviour of the effective potential near of the origin must be $rU_{eff}(r) \rightarrow -Z$ and requiring continuity of the effective potential and their derivate. The parameter R_T is determined requiring continuity of the plasma-charge density in this point. In the present work we have used for U^{o}_{N-1} the self-consistent isolated potential provided by code DAVID developed by David Liberman *et al* [1].

3.- Results.

For ions with a small ionization it has been observed that the R_T radius becomes smaller than R_N and then the potential given in equation 3 is reduced to an effective potential divided only into two regions, vanishing the region where the plasma surrounding was only described by a uniform free electrons density. On the other hand, for highly ionized ions, R_N is much smaller than R_T which implies that the effective potential is mainly ruled by the second and third regions of the potential.

In this work it has been focused the study of the potential in the determination of the continuum lowering, i.e. the plasma potential in points nearby to the origin which is given by the constant denoted as C_1 in this work. The analysis has been done for aluminum plasmas in a wide range of densities (10^{18} – 10^{25} cm^{-3}) and temperatures (50 – 300 eV). The results have been compared with the continuum lowering provided by Stewart and Pyatt (SP) [2] and whith those given by the ion-sphere model (IS). This can be seen in table 1 where it has been listed some samples of the results and also in figure 1 in which it has been plotted.

Table 1. *Continuum lowering (eV) for H-like and He-like aluminum plasma at 300 eV and several free elertron densities*

	H-like Al			He-like Al		
N_e (cm^{-3})	SP	This work	IS	SP	This work	IS
10^{18}	0.45	0.46	1.93	0.46	0.42	1.83
10^{19}	1.54	1.43	4.15	1.43	1.31	3.93
10^{20}	4.63	4.31	8.94	4.30	3.97	8.47
10^{21}	12.99	12.22	19.25	12.12	11.32	18.25
10^{22}	33.40	32.07	41.47	31.36	29.90	39.32
10^{23}	79.76	79.12	89.35	75.20	73.93	84.71
10^{24}	181.57	189.97	192.50	171.63	177.66	182.50

As it can be seen the agreement found with respect to the results of SP is excelent for medium and high ionization states in all the cases studied. However, some discrepancies are observed for the opposite degrees of ionization.

Finally, in a previous work we calculated de photoionization cross section in a relativistic contex and in the approximation of the independent particle model by using two differents non isolated effective analytical potentials: one based in the Debye-Hückel approximation which is valid at low free electron densities and other based in the ion esphere aproximation which is valid at very high density. These models does not give an apropppiated description of the continuum lowering as it can be seen in figura 1 for the ion sphere model.

This fact is specially important for computing the photoionization cross section because the threshold energy is dominated by this effect. As it has been proved in this work the new potential describes it with a better accuracy being competitive to be used in photoionization cross section calculation.

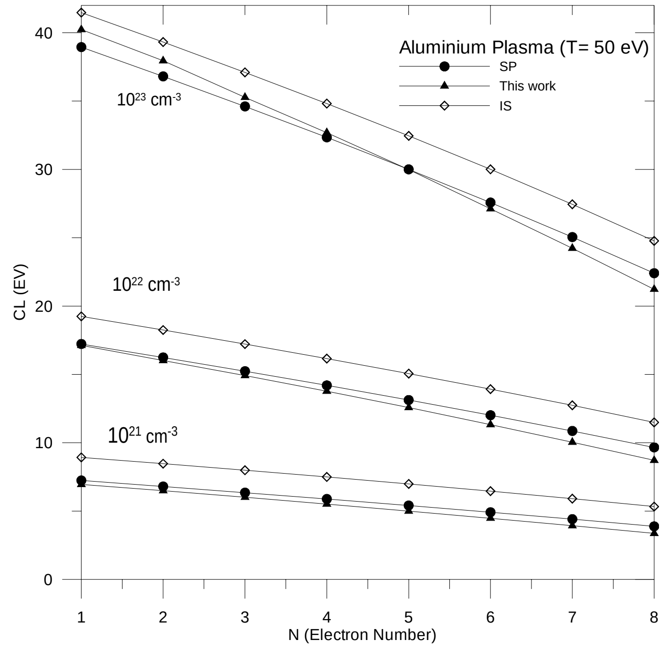

Figure 1. Continuum lowering for aluminium plasma at 50 eV and several free electron

4.- Summary and conclusions.

In this work it has been presented a new effective potential which includes plasma effects in a very simple way. This potential is, in general, divided in three regions which depend on the plasma-charge density.

The set of equations presented can provide a selfconsistent effective potential though in this work we have limited ourselves to the zero order approximation.

This potential has been used to obtain the continuum lowering for aluminum plasmas in a wide range of conditions, and the results have been checked with others obtained using method available in the bibliography, obtaining good agreements for medium and high ionizations.

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