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Analytical Potential for Core and Single Excited Configurations Including Plasma Effects to Obtain Atomic Properties for Ions in Dense and Hot Plasmas

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1. Introduction

The first stage in the radiation modelling of hot plasmas involve the determination of the atomic data for all the ions immersed into the plasma, which are able to be both in ground configuration and excited configurations. This fact implies to deal with an enormous amount of atomic data. Although there are some computer codes [1-3] based on numerical solution of Schrödinger or Dirac equations for highly ionized atoms currently available to calculate those atomic data by using self-consistent methods, they mean a considerable increase in computing time. A possible solution to this problem, in this kind of models, is to limit the number of excited configurations to include per ion. Nevertheless, care must be taken in selecting level structure adequate to describe the main ion abundance in the density regime where the model is to be applied since excited configurations have a large effect on ion abundance in all regimes of densities. An interesting alternative to self-consistent models is based on models including analytical expressions for the effective potential avoiding the iterative procedures. Thus, these models will allow us to include more excited configurations in atomic calculations improving ion abundance calculations.

2. Analytical potential for non isolated ions in excited configurations

In this work we present an expression for an analytical potential to model non isolated ions in excited configurations. This potential has been built up from analytical potentials developed by us for both isolated ions in excited configurations [4] and non isolated ions in ground configuration [5] (denoted in the following by *EIP* and *GNIP*, respectively) and its general expression, for an ion of nuclear charge *Z* and *N* bound electrons, is given by

$$U^{ENIP}(r) = -\frac{1}{r}\left\{(N-1)(\phi^{EIP}(r) - \eta^{EIP}(r)) + \left[Z - N + (N-1)\eta^{EIP}(0)\right]e^{-ar} + 1\right\} \tag{1}$$

being ϕ^{EIP} (the screening function for isolated ions in excited configurations)

$$\phi^{EIP}(r) = \phi^{GIP}(r) + \delta\phi^{EIP}(r) \quad ; \quad \delta\phi^{EIP}(r) = -\frac{1}{N-1} r\delta U^{EIP}(r) \tag{2}$$

where $\phi^{GIP}(r)$ is the screening function of the analytical potential for isolated ions in ground state (denoted as *GIP* in the following) [6]

$$\phi^{GIP}(r) = \begin{cases} e^{-a_1 r^{a_3}} & \text{if } N \geq 12 \\ (1-a_2 r) & \text{if } 8 \leq N \leq 11 \text{ or } N = 2,3 \\ e^{-a_1 r} & \text{if } 4 \leq N \leq 7 \end{cases} \tag{3}$$

and δU^{EIP} is the term which corrects this potential including the excitation configuration effects [4]

$$\begin{aligned} \delta U^{EIP}(r) = -\sum_{l=0, l\,even}^{2l_k} D(l,l_k) \cdot \left[\frac{1}{r^{l+1}} \int_0^r A_k^*(r_k) A_k(r_k) r_k^l dr_k + r^l \int_r^\infty A_k^*(r_k) A_k(r_k) \frac{1}{r_k^{l+1}} dr_k \right] - \\ \sum_{l=0, l\,even}^{2l_k'} D(l,l_k') \cdot \left[\frac{1}{r^{l+1}} \int_0^r B_k^*(r_k) B_k(r_k) r_k^l dr_k + r^l \int_r^\infty B_k^*(r_k) B_k(r_k) \frac{1}{r_k^{l+1}} dr_k \right] + \\ \sum_{l=0, l\,even}^{2l_{k'}} D(l,l_{k'}) \cdot \left[\frac{1}{r^{l+1}} \int_0^r A_{k'}^*(r_{k'}) A_{k'}(r_{k'}) r_{k'}^l dr_{k'} + r^l \int_r^\infty A_{k'}^*(r_{k'}) A_{k'}(r_{k'}) \frac{1}{r_{k'}^{l+1}} dr_{k'} \right] + \\ \sum_{l=0, l\,even}^{2l_{k'}'} D(l,l_{k'}') \cdot \left[\frac{1}{r^{l+1}} \int_0^r B_{k'}^*(r_{k'}) B_{k'}(r_{r'}) r_{k'}^l dr_{k'} + r^l \int_r^\infty B_{k'}^*(r_{r'}) B_u(r_{k'}) \frac{1}{r_{k'}^{l+1}} dr_{k'} \right] \end{aligned} \tag{4}$$

where *A* and *B* are the large and the small components of the electron wave-function, respectively, and *k* and *k'* denote the quantum numbers of the mono-electronic levels involved in the excitation. Finally, $\eta^{EIP}(r)$, which is called plasma structural screening function [5], is given by

$$\eta^{EIP}(r) = \frac{1}{2} a \int_0^\infty e^{-a|s-r|} \phi^{EIP}(s) ds \tag{5}$$

being *a* the inverse of the Debye radius.

3. Results

In table 1 we have listed the excited configurations considered in this study, and also the conditions for aluminium plasma and the abundances of these configurations. The ion selected is Al XI since for these conditions of density and temperature the average ionization is approximately 11.2. The abundance has been obtained in non-local thermodynamic equilibrium solving the rate equations [7] without coupling the radiation. As we can see from the table, the abundance of each excited configuration is nearby of the ground state one, so they will be relevant in the calculation of the ion abundance.

Table 1. Excited configurations and their abundances at two aluminium plasma conditions

	$T_e = 400$ eV, $n_e = 10^{20}$ cm^{-3}	$T_e = 400$ eV, $n_e = 10^{22}$ cm^{-3}
Electronic Conf.	**Abundance**	**Abundance**
$1s^2 4f^1_{7/2}$ (Exc. Conf. 1)	0.2912×10^{-4}	0.1414×10^{-2}
$1s^2 6h^1_{11/2}$ (Exc. Conf. 2)	0.2914×10^{-4}	0.1836×10^{-2}
$1s^2 7f^1_{7/2}$ (Exc. Conf. 3)	0.1831×10^{-4}	0.1188×10^{-2}
$1s^2 2s^1$ (Ground State)	0.9258×10^{-3}	0.2162×10^{-2}

In figure 1 it is shown the behaviour of each potential for the excited configuration 1 for the density of 10^{22} cm^{-3}. From the figure, three regions can be distinguished: the first one is next to the nucleus, wherein the asymptotic behaviour of all the potentials is the same, i.e. the nuclear charge *Z*. The second region involves long distances from the nucleus; in this case the conduct both of *GIP* and *EIP* tends to $Z-N-1$, whereas the *ENIP* potential is mainly ruled by the behaviour of the *GNIP*, having a tendency to -1 due to the correction of the optical electron. Finally, the third region is corresponded to the core (intermediate distances). In this region the behaviour of *ENIP* depends on both *EIP* and *GNIP*, and we have focused this work in this region.

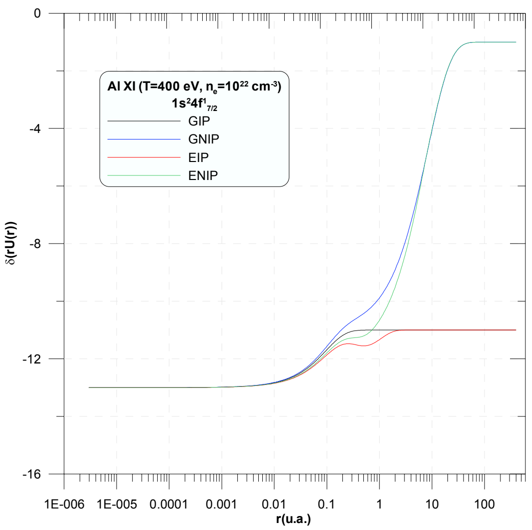

Figure 1. Behavior of the potentials.

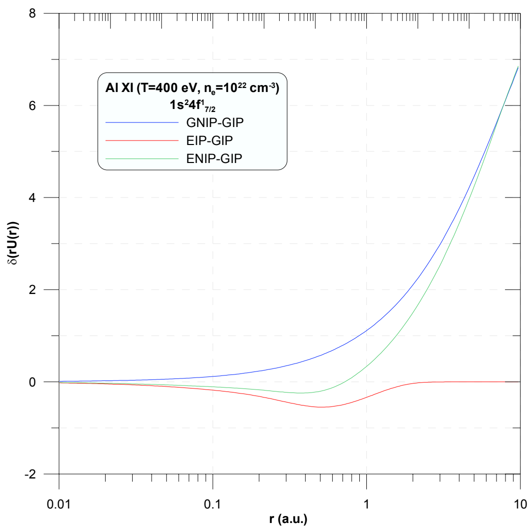

Figure 2. Differences with respect to GIP.

As it is known, the plasma and the excitation effects on the potential and the atomic magnitudes act in opposite sense. Thus, the main effect of the plasma is to screen the nuclear charge whereas the excited configurations imply a diminution of the screening. So the total correction of both effects on the ground state potential of the isolated ions will be always smaller than when they are included separately (see figure 2). In certain plasma conditions and some excited configurations both effects could even cancel one to another in the core area. Thus, we can see in figure 3 that for the higher density, as the effect of the plasma is larger than for the other density, the difference of *ENIP* with respect to *GIP* becomes smaller. Finally, in figure 4, we show the influence of the excited configuration selected in *ENIP*. As it is expected, for the same plasma conditions, as the final level of the excitation is more external, i.e. the ion is more excited, the *ENIP* tends to the behaviour of the *EIP* potential in the third region, i.e. in the core.

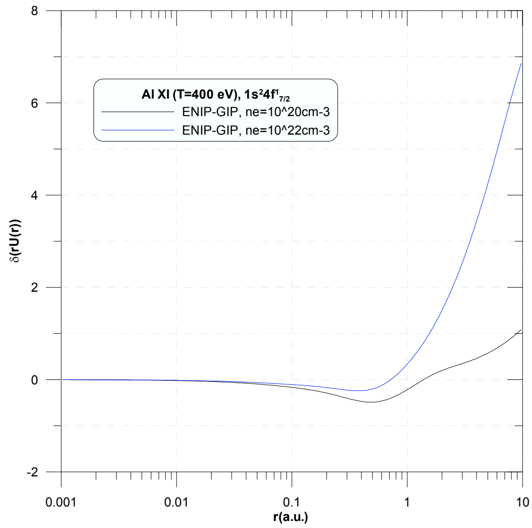

Figure 3. Difference between *ENIP* and *GIP* in the core region for two densities.

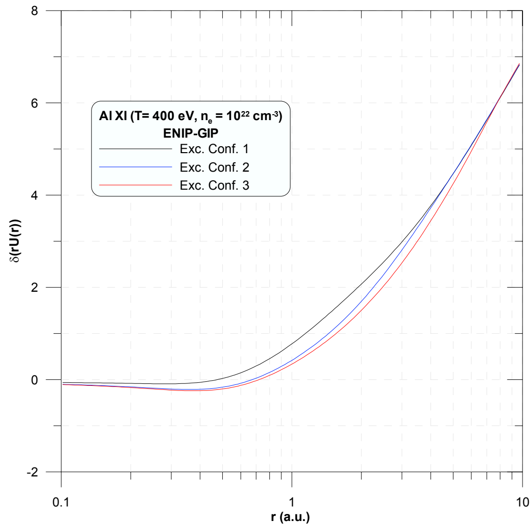

Figure 4. Difference between *ENIP* and *GIP* for three excited configurations.

Acknowledgments

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