Reduction of the ionization energy for 1s-electrons in dense aluminum plasmas

C Lin¹, H Reinholz¹,² and G Röpke¹
¹ Universität Rostock, Institut für Physik, 18051 Rostock, Germany
² The University of Western Australia, School of Physics, WA 6009 Crawley, Australia
E-mail: chengliang.lin@uni-rostock.de

Abstract. The properties of a bound multi-electron system immersed in a plasma environment are strongly modified by the surrounding plasma. In particular, the modification of the ionization energy is described by the electronic self-energy within the framework of the quantum statistical theory. We present the energy shift of the eigenstates and the lowering of the continuum edge of free electrons in a plasma. The reduction of the ionization potential is determined by their difference. This ionization potential depression for the 1s-levels in dense aluminum plasmas is calculated. Comparisons with other theories and the experimental data are shown for aluminum plasma at solid density 2.7 g/cm³.

1. Introduction
The controversy in the interpretation of two recent measurements on dense aluminum plasma [1,2] renews the interest on a better theoretical description of the ionization potential depression (IPD) in dense plasmas. Neither the generally accepted Stewart-Pyatt (SP) model [3] nor the Ecker-Kröll (EK) model [4] is able to explain both experiments. In this communication, a quantum-statistical approach [5,6] is used to calculate the reduction of the ionization energy for the 1s-electron in dense aluminum plasma. We consider atoms or ions as (N+1)-particle clusters, consisting of a nucleus with Z protons and N bound electrons (N ≤ Z), as separate species. An effective two-particle description is introduced within this chemical model.

2. Quantum-statistical approach
To investigate the reduction of the ionization energy, two different effects should be mentioned. Firstly, the continuum edge of free electrons in plasmas is modified due to screening. Secondly, the energy levels of the bound electrons are shifted because of the plasma microfield. Within the Green’s function method, both effects are described by the change of self-energies in plasma.

In the following, we only discuss the electronic contribution to the self-energies. The self-energy of free electrons in plasma is given in the Montroll-Ward approximation [6] as

\[
\Delta_{MW} = -\frac{e^2}{8\pi \epsilon_0} \left( \frac{n_e e^2}{\epsilon_0 k_B T_e} + \frac{m_e e^4}{8 \epsilon_0^2 (2\pi \hbar)^2} \right) \left\{ \frac{\sqrt{2\pi^2} e^4 n_e \lambda_e}{8 (4\pi \epsilon_0)^2 (k_B T_e)^2} - \frac{n_e \lambda_e^2}{8\sqrt{2}} + \frac{e^2 n_e \lambda_e^2}{4 (4\pi \epsilon_0)^2 k_B T_e} \right\}
\]

with the electron density \( n_e \) and the electron temperature \( T_e \). \( \lambda_e = \sqrt{2\pi \hbar^2/(m_e k_B T_e)} \) denotes the thermal wavelength.
The correction of the eigenenergy of the electron in level $|\nu\rangle$ due to the plasma microfield is determined by the self-energy $\Sigma_\nu$, which can be generally splitted into an electronic and an ionic part $\Sigma_\nu = \Sigma_\nu^{el} + \Sigma_\nu^{ion}$ because of their different mobilities. The electronic contribution $\Sigma_\nu^{el}$ is expressed in the dynamically screened Born approximation as

$$\Sigma_\nu^{el} = \frac{1}{e^2} \int \frac{d^3q}{(2\pi \hbar)^3} V(q) \sum_{\nu'} |M_{\nu\nu'}(q)|^2 \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \left[ 1 + n_{\nu}(\omega) \right] \frac{\text{Im} \epsilon^{-1}(q, \omega + i0)}{E_\nu - E_{\nu'} + (\hbar \omega + i0)},$$

with the interaction potential $V(q)$ between an electron in eigenstate $E_\nu$ and the plasma electrons. $n_{\nu}(\omega)$ and $\epsilon(q, \omega + i0)$ are the Bose-Einstein distribution and the dielectric function of the plasmas, respectively. The summation over virtual states $|\nu\rangle$ should include both bound and scattering states. In other words, three different contributions need to be considered: the elastic scattering channel, the bound-bound transition, and the bound-free transition.

We are interested in the level shift of bound electrons, which is obtained from the real part

$$\Delta_\nu^{el} = \text{Re} \Sigma_\nu^{el} = -\frac{2}{\Omega^2} \mathcal{P} \left\{ \sum_{p,q,\nu'} V^2(q) f_p(E_p) \cdot \frac{|M_{\nu\nu'}(q)|^2}{E_\nu - E_{\nu'} + E_p - E_{p+q}} \right\},$$

see [7], with the Fermi-Dirac distribution $f_p(E_p)$ which can be replaced by the Maxwell-Boltzmann distribution in the non-degenerate limit. The essentially important quantity is the transition matrix element $M_{\nu\nu'}(q)$. In the Green’s function technique, a generalized matrix element $M_{\nu\nu'}(q)$ for a $(N + 1)$-particle bound state should be considered [6]. Within the mean-field approximation, the independent-particle approximation is usually performed. An effective two-particle description can be introduced by decomposing the bound cluster into two parts: an involved electron in subshell $|\nu\rangle = |n_{\nu}l_{\nu}\rangle$ that is defined as the “transition electron” and is assumed to move in an effective mean field induced by the remaining $N$-particle ion core $|\beta\rangle$.

The effective charge, seen by the transition electron in the subshell $|\nu\rangle$, is given by [8]

$$Z_\nu = Z - \sum_{\nu'}^{\nu_{\text{max}}} \sigma_{\nu\nu'} \cdot (g_{\nu'} - \delta_{\nu\nu'}),$$

where $\nu_{\text{max}}$ denotes the highest occupied subshell. The constant $\sigma_{\nu\nu'}$ represents the screening of an electron in the subshell $|\nu\rangle$ by the electron in another subshell $|\nu'\rangle$ [8]. This phenomenological approach is now generalized to take into account the spatial distribution of bound electrons through expressing the effective charge via a charge distribution

$$Z_\nu(q) = Z - \sum_{\nu'}^{\nu_{\text{max}}} \sigma_{\nu\nu'} \cdot (g_{\nu'} - \delta_{\nu\nu'}) \cdot F_{\nu\nu'}(q),$$

with the diagonal element of the atomic form factor $F_{\nu\nu'}(q) = \int d^3r e^{iqr} \psi_{\nu'}(r) \psi_{\nu}(r)$. It is expressed via the hydrogenic wave function $\psi_{\nu}(r) = R_{n_{\nu}l_{\nu}}(r)Y_{l_{\nu}m_{\nu}}(\Omega_r)$. The total transition matrix element can be derived from the general vertex function [6] and is given by

$$M_{\nu\nu'}(q) = S_\beta(q) \cdot \left\{ Z_\nu(q) \delta_{\nu\nu'} - F_{\nu\nu'}(q) \right\}$$

with a screening function $S_\beta(q)$ resulting from the ion core $|\beta\rangle$, which is expressed as

$$S_\beta(q) = 1 - \frac{1}{Z} \sum_{\nu'}^{\nu_{\text{max}}} F_{\nu\nu'}(q) \cdot (g_{\nu'} - \delta_{\nu\nu'}).$$

With the aforementioned effective two-particle description (6) of the matrix element, the expression (3) for the level shift is determined for the multi-electron bound system. Then the IPD of individual energy levels can be calculated by

$$\Delta_\nu^{\text{IPD}} = \Delta_\nu^{el} - \Delta_\nu^{\text{MW}}.$$
3. Results and Conclusions

Exemplarily, the IPD of the 1s-electron in a laser induced Al-plasma [1] in comparison to different theoretical models is shown in Figure 1. In experiment, the local plasma conditions for each charge state are different as shown in [9]. Within our calculation, only the elastic scattering channel (\(|\nu'\rangle = |\nu\rangle\)) is considered. Because of the phase occupation by other bound electrons and the strong coupling between the 1s-electron and the nucleus, the bound-bound and bound-free transitions only give small contributions to the IPD. Furthermore, the IPDs are evaluated only for the ground state of each charge state. Our results are larger than the experimental data and the results estimated by the SP and EK model, since no ionic correlation effect is considered and only the electronic Debye screening in the interaction potential \(V(q)\) is used. The ionic correlation has strong influence on the IPD and should be reflected in the boundary condition of the confined atoms in plasmas. In the SP model, the IPD is determined by the Wigner-Seitz radius \(R_{WS} = \sqrt{3}/(4\pi n_{ion})\) and the Debye length including both ions and electrons. However, in the EK model, the characteristic length determining the IPD is calculated by the radius \(R_{EK} = \sqrt{3}/(4\pi (n_{ion} + n_e))\) where both the electron density \(n_e\) and ion density \(n_{ion}\) are considered. Comparing the two models with the experimental data, it shows the necessity of a deeper understanding of the concept “IPD”.

We have presented an effective two-particle description within the framework of the thermodynamic Green’s function technique to investigate the level shift of a bound system in dense plasmas. The inclusion of an ionic microfield and the application of our approach to \(K_\alpha\) spectral lines [10] will be discussed in a forthcoming paper. Furthermore, the dependence of the IPD on the atomic configurations, e.g. excited states, also deserves further discussion.

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