Nonequilibrium Effects on the Ionisation Energies in Dense Plasmas

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1 Introduction

Electrostatic potentials in dense plasmas are screened by the presence of free charge carriers. Screening alters the strength and shape of the potential and therefore modifies, among other properties, the wavefunctions and binding energies of bound states in the plasma [1]. The screening of the electron-core potential typically leads to a lowering of the ionisation energy known as continuum lowering or as ionisation potential depression (IPD) and can greatly affect the ionisation state of partially ionised plasmas. Consequently, IPD may also strongly influence a wide variety of plasma properties [2].

Models to describe screening by electrons and ions in local equilibrium have been developed for many years [3]. One of the most popular model was proposed by Stewart and Pyatt [4] and interpolates between the high-temperature, low-density Debye limit [3] and the low-temperature, high-density limit of the ion sphere model [5]. Of course, these easy screening models have been challenged by more elaborate theories (see e.g., Ref. [6]) however only recent contradictory experimental results [7, 8] have posed serious questions about the applicability of these models.

The use of high-power, short-pulse laser systems and free electron lasers in the VUV and X-ray domain (XFELs) allow highly excited, solid-density materials to be created and probed on femto and picosecond timescales. Experimental results [9] and simulations [10, 11] suggest the presence of a considerable non-equilibrium component to electron populations in such strongly driven systems. A well-founded theoretical approach for continuum lowering in plasmas with non-equilibrium electron distributions is therefore needed if we are to correctly analyse such materials. Such a generalised theory might also shine new light on the contradiction of recent experiments.

2 Theory

Using the linear approximation for the density response, the response of the free electrons to an imposed potential can be described by the dielectric function

$$V^S(\mathbf{q},\omega) = \frac{V}{|\varepsilon(\mathbf{q},\omega)|} \,. \qquad (1)$$

For a Coulomb potential in the static long wavelength limit, i.e., $\mathbf{q} \to 0$, $\omega \to 0$, the Debye potential with a screening length κ is obtained

$$V^D(\mathbf{q}) = V^S(\mathbf{q},0) = -\frac{1}{\varepsilon_0}\frac{e^2}{(q/\hbar)^2+\kappa^2} \qquad (2)$$

and by comparison, we obtain for the screening length

$$\kappa^2 = [\varepsilon(0,0)-1]\,(q/\hbar)^2 \;. \qquad (3)$$

For weakly coupled plasma components, the random phase approximation can be applied and the dielectric

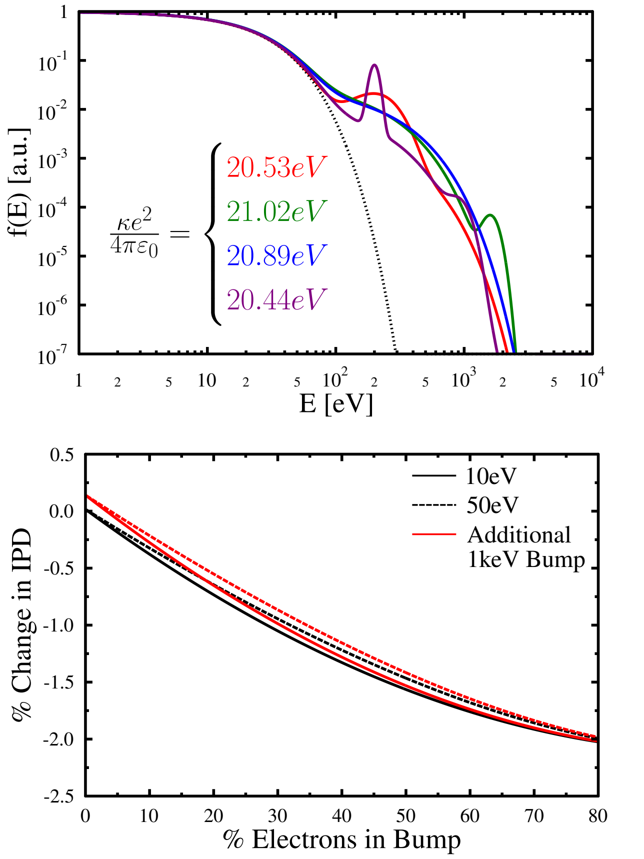

Figure 1: a) Example distribution functions and corresponding values for ΔI. The cold part of the distribution function (shown in black) and the total energy are the same in all cases. b) Calculated change in ionization potential depression as an increasing number of electrons are moved from a Boltzmann-like hot tail to Gaussian shaped features.

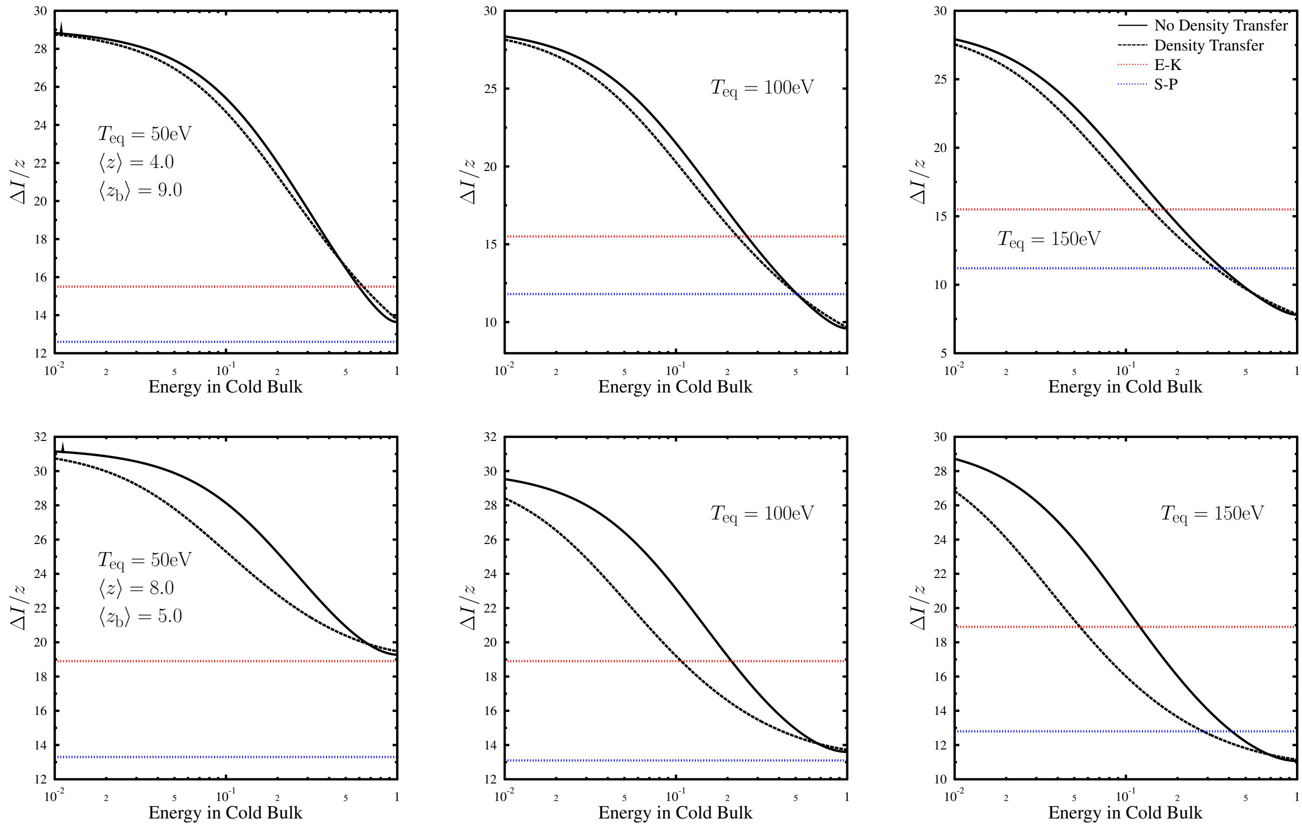

Figure 2: Calculated IPD for transitions in Aluminium at two ionization levels. The ion density is the solid state value $n_i = 6.0 \times 10^{22}\mathrm{cm}^{-3}$. The temperatures shown are for the limiting equilibrium distribution, obtained as the energy in the bulk reaches 1. For comparison, values calculated according to the Stewart-Pyatt [4] and Ecker-Kröll [13] models are shown.

function is given by [2]

$$\varepsilon(\mathbf{q},\omega) = 1+\frac{\hbar^2 e^2}{\varepsilon_0 q^2}\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{f_e(\mathbf{p}+\mathbf{q})-f_e(\mathbf{p})}{\hbar\omega - E(\mathbf{p}+\mathbf{q})+E(\mathbf{p})+i\epsilon}\,. \tag{4}$$

This approximation is valid for the electrons in many dense plasmas and warm dense matter systems as either the thermal energy $k_B T_e$ or the Fermi energy dominates the correlation energy.

The static long wavelength limit of the RPA dielectric function now leads to an explicit form for the screening length

$$\kappa^2(t) = \frac{e^2}{\varepsilon_0}\cdot 4\pi m_e \int_0^\infty \frac{dp}{(2\pi\hbar)^3} f_e(p,t)\,, \tag{5}$$

which is given in terms of the (nonequilibrium) electron distribution function.

Assuming strongly localised bound states, we expand the screened potential around $r = 0$

$$-\frac{ze^2}{4\pi\varepsilon_0 r}e^{-\kappa r} \approx -\frac{ze^2}{4\pi\varepsilon_0 r} + \frac{z\kappa e^2}{4\pi\varepsilon_0} + \mathcal{O}(r) \tag{6}$$

and obtain for the reduction in ionization potential

$$\Delta I = \frac{z\kappa e^2}{4\pi\varepsilon_0}\,. \tag{7}$$

Via the generalised form of the screening length, the IPD is now related to the electron distribution which may take any nonequilibrium form.

We approximate the distribution function by the form

$$f_e(p) = f_{\rm cold}(n_c, T_c) + f_{\rm hot}(n_h, T_h) + f_{\rm bump}(p_0, p_b, n_b)\,, \tag{8}$$

which combines two equilibrium distribution functions at different temperatures with a Gaussian bump with adjustable position and width. This form has been used previously in the study of Thomson scattering from nonequilibrium electrons [12] and roughly reproduces the features observed in simulations [11]. Gaussian bump features are typically produced at photoelectron and Auger electron energies. Ultra-fast relaxation of these bumps leads to a hot, Boltzmann-like tail, whilst pre-existing conduction band electrons remain relatively cold and are described by a Fermi distribution with T_c. Combining these three components makes it possible to produce distribution functions of almost arbitrary shape within this framework. For this model to remain a good approximation to a physical distribution, the hot tail must remain strongly non-degenerate. Otherwise, the model may yield occupation numbers greater than unity at low momenta.

3 Calculations

First we examined the sensitivity of continuum lowering to the shape of the high energy part of the distribution function ($f_{hot}+f_{bump}$). Due to their higher energy, these electrons should respond only weakly to any imposed potential, and should contribute little to the screening of the potential. Sensitivity to the exact distribution of high energy electrons should therefore be low.

The quantity ΔI was calculated for distributions with a hot tail and up to two Gaussian bumps, whilst the cold part of the distribution was kept fixed. All the distribution functions studied contained the same total energy. The IPD was indeed found to be insensitive to the particular shape of the high-energy part of the electron distribution function, with ΔI varying by only $\sim 3\%$ (see Fig. 1). Based on this finding, subsequent calculations applied a simplified two-temperature version of the electron distribution function, comprising the cold Fermi part and the hot Boltzmann tail only.

In a second step, we studied the effects of changing the shape of the nonequilibrium distribution function. For a fixed total energy, we varied the energy between the cold bulk and the hot tail and calculated the resulting IPD. Two possible models for the electron density were considered. In the first case, the density in each part is held fixed. The temperatures of the two distributions then relax towards each other as energy is moved from hot to cold. In the second case, electrons are added to the cold part in proportion to energy. This treatment gives a hot tail with constant temperature and equilibrium is reached as the energy and density in the tail approaches zero.

The results in Fig. 2 demonstrate a significant increase in IPD with the amount of energy in the hot tail of the distribution. The increased screening due to the lower temperature in the main part of the electron distribution (T_c) overcompensates for the reduction in screening by high energy electrons. The two models for density give qualitatively similar results, suggesting that the hot tail is most significant as an energy sink.

4 Conclusion

We have calculated continuum lowering or IPD due to nonequilibrium electron distributions within the linear response formalism. We find that the contribution to the screening length from high energy electrons is small and that the form of any hot tail does not significantly affect the ionization potential. In particular, the presence of Gaussian features in the tail does not alter continuum lowering when compared to a Boltzmann-like tail.

Although the high-energy electrons do not contribute significantly to screening, they do act as an energy sink, causing the remaining bulk part of electrons to be colder than in a case assuming an equilibrium distribution with the same total energy. A nonequilibrium distribution will therefore result in larger continuum lowering when compared to the equilibrium case. Depending on the fraction of energy contained in the high-energy part of the distribution function, changes in the IPD may be significant.

References

[1] M.S. Murillo and J.C. Weisheit, *Phys. Rep.,* **302,** 1 (1998).
[2] D. Kremp, M. Schlanges, and W.-D. Kraeft, *Quantum Statistics of Nonideal Plasmas*, (Springer, Berlin 2005).
[3] P. Debye and E. Hückel, *Z. f. Phys.,* **24,** 185 (1923).
[4] J.C. Stewart and K.D. Pyatt, Jr., *Astrophys. J.,* **144,** 1203 (1965).
[5] G. Zimmerman and R. More, *J. Quant. Spectrosc. Radiat. Transfer,* **27,** 345 (1980).
[6] S. Pankov and V. Dobrosavljevic, *Phys. Rev. Lett.* **94**, 046402 (2005).
[7] O. Ciricosta *et. al.*, *Phy. Rev. Lett.,* **109,** 065002 (2012).
[8] D.J. Hoarty *et. al.*, *Phys. Rev. Lett.* **110**, 265003(2011).
[9] F.N. Beg *et. al.*, *Phys. Plasmas,* **4,** 447 (1997).
[10] S.P. Hau-Riege, *Phys. Rev. E* **87**, 053102 (2013).
[11] N. Medvedev, U. Zastrau, E. Forster, D.O. Gericke and B. Rethfeld, *Phys. Rev. Lett.* **107**, 165003 (2011).
[12] D.A. Chapman and D.O. Gericke, *Phys. Rev. Lett.* **107**, 165004 (2011).
[13] G. Ecker and W. Kröll, *Phys. Fluids* **6**, 62 (1963).