New formula for the electronic stopping power of ions in an electron gas system

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Synopsis A formula [1] for determining the electronic stopping power and the transport cross section in electron-ion binary collisions is derived from the induced density for spherically symmetric potentials using the partial-wave expansion. In contrast to the previous one found in many textbooks, the present formula converges to the Bethe and Bloch stopping-power formulas at high ion velocities and agrees rather well with experimental stopping-power data

The energy transfer between electrons and ions in binary collisions has been studied for more than 100 years and was a subject of interest for many prominent scientists, such as Bohr, Landau and Lindhard, who first established the underlying physics. The stopping power or force (dE/dz) is connected to the transport cross-section by the following:

$$\frac{dE}{dz} = n_0 m_e \left\langle \frac{|\vec{v}_e - \vec{v}|}{v} \vec{v}.(\vec{v} - \vec{v}_e)\sigma_{tr}(|\vec{v}_e - \vec{v}|) \right\rangle_{\vec{v}_e}, \tag{1}$$

where m_e is the electron mass, $\langle ... \rangle$ stands for the average over the electron velocities $\vec{v}_e$, $\vec{v}$ is the ion velocity, and n_0 is the undisturbed electron density. Atomic units (a.u) and non-relativistic expressions will be used throughout, unless stated otherwise.

Usually, calculations of the transport cross-section σ_{tr} assume a central potential for the electron scattering at the ion and therefore make use of the partial-wave expansion. Thus, $\sigma_{tr}(k)$ can be expressed by phase shifts δ_ℓ at the relative speed v', according to

$$\sigma_{tr}(v') = \frac{4\pi}{v'^2} \sum_{\ell=0}^{\infty} (\ell+1) \sin^2(\delta_\ell - \delta_{\ell+1}). \tag{2}$$

However, the weakest point of the use this formula with Yukawa potential is the asymptotic high-velocity limit : it does not give the well-established Bethe Formula

$$\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \ln\left(\frac{2v^2}{\omega_p}\right), \tag{3}$$

but instead results in

$$\frac{dE}{dz} = Z^2 \frac{\omega_p^2}{v^2} \left(\ln\left(\frac{2v^2}{\omega_p}\right) - \frac{1}{2}\right). \tag{4}$$

In this work, I demonstrate that a central potential (as the Yukawa potential) and the corresponding partial-wave analysis can still be used by replacing Eq.(2) with the following one :

$$\sigma_{tr}^{eff}(v') = \frac{2\pi Z}{v'^3} \sum_{\ell=0}^{\infty} \sin\left(2(\delta_\ell(v') - \delta_{\ell+1}(v'))\right), \tag{5}$$

which is not derived from the definition of transport cross-section (from the momentum-transfer cross-section) but rather from the retarding force acting on the ion due to the induced charge density. The resulting stopping force gives the correct Bethe limit according to Eq.(3) and, in addition, is consistent with the full non-perturbative Bloch formula.

References

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