Complete description of the energy loss of particles in dense matter and plasmas through dielectric formalism

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Introduction

For the last few decades, the interaction of ion beams and charged particles with plasmas has been an issue widely studied. Free electrons can be described by the dielectric well known formalism [1]. Recent experiments have shown that for a variety of plasma conditions of interest for plasma physics bound electrons contribution to stopping power is relatively important [2, 3]. Historically, there has been mainly two ways to consider the bound electrons in the stopping theories; either by a Bethe-like expression with mean ionization potential, as in [2, 3] or with complex Average Atom Local Density Approximation theories [4, 5]. In this work a model is developed to consider both free and bound electrons via the dielectric formalism and the Shellwise Local Plasma Approximation [6]. Atomic units (a.u.), $e == m_e = 1$, are used through all the work, unless other units are stated.

Dielectric Formalism

In the dielectric formalism, the electron response of an isotropic and homogeneous material to a perturbation produced by an external charge is contained in the dielectric function, $\varepsilon(r,t)$ of the medium [7]. In this formalism, the expression of the electronic stopping power is

$$S = \frac{2Z^2}{\pi v^2} \int_0^\infty \frac{dk}{k} \int_0^{kv} d\omega\omega \mathrm{Im}\left[\frac{-1}{\varepsilon(k,\omega)}\right] \tag{1}$$

where Z is the atomic number of the projectile, ω is the frequency, k the wave number and v is the projectile velocity. $\varepsilon(k,\omega)$ is the Fourier transform of the target dielectric function and $\mathrm{Im}\left[\frac{-1}{\varepsilon(k,\omega)}\right]$ is called the energy loss function. The energy loss in partially ionized matter can be estimated through two contributions, free and bound electrons being the total stopping $S_{free} + S_{bound}$

Free electrons: The dielectric function of a free electron gas was calculated first by Lindhard [1] in the RPA. The RPA is valid at high projectile energies and when electron collisions are not significant in the gas. But, as we want to consider plasmas in a wide variety of degeneracy states, the dielectric function developed in [8] is more appropriate as it is valid for an electron gas at any temperature [9]

$$\varepsilon(k,\omega) = 1 + (\frac{1}{\pi k})^2 \int d^3k' \frac{\hat{f}(\vec{k}+\vec{k}') - \hat{f}(\vec{k}')}{\omega + i\delta - (E_{\vec{k}+\vec{k}'} - E_{\vec{k}'})} \tag{2}$$

where $E_k = k^2/2m$, δ is the collision frequency between electrons. The temperature dependence is introduced by $f(k)$, which is the Fermi-Dirac function. The imaginary part of the dielectric function can be obtained by direct integration for $\delta \to 0$.

$$\text{Im}\varepsilon_A = \frac{\pi\chi_0^2}{8Z^3}\theta ln\left(\frac{1+exp[\eta - D(u-z)^2]}{1+exp[\eta - D(u+z)^2]}\right) \tag{3}$$

where $\chi_0^2 = 1/\pi k_F$ is the coupling parameter for degenerated plasmas, $\theta = 1/D = k_B T/E_F$ is the reduced temperature, $\eta = \beta\mu$, $u = \omega/kv_F$, $z = k/2k_F$ are the common dimensionless variables, being $E_F =^2 k_F^2/2m$ the Fermi energy and $k_F = (3\pi^2 n_e)^{1/3}$ the corresponding wave number, with n_e being the free electron density. When T tends to 0, Arista dielectric function is equivalent to Lindhard function [8]. The real part of this dielectric function may be obtained from Imε_A using the Kramers-Kronig relations,

$$\text{Re}\varepsilon_A(k,\omega) = 1 + \frac{\chi_0^2}{4Z^3}[g(u+z) - g(u-z)] \tag{4}$$

where the function $g(x)$ is given by $g(x) = \int_0^\infty \frac{ydy}{e^{Dy^2-\eta}+1} ln\left|\frac{x+y}{x-y}\right|$.

Bound electrons: In partially ionized plasmas, the stopping power of the electrons still bound to the target plasma ions must be taken into account. In order to include the binding energy we use the Levine-Louie dielectric function [10]

$$\text{Im}\varepsilon_{LL}(k,\omega) = \begin{cases} \text{Im}\varepsilon_L(k,\omega_g) & \text{if } |\omega| > \omega_m \\ 0 & \text{if } |\omega| < \omega_m \end{cases} \tag{5}$$

with ω_m being the binding energy, $\omega_g = \sqrt{\omega^2 - \omega_m^2}$, and ε_L being the Lindhard dielectric function as defined before. If no binding energy is considered, $\omega_m = 0$ the usual expression for the dielectric function, Eq.4 and Eq.3 are recovered.

Shellwise Local Plasma Approximation

The SLPA formulation considers the contribution to the stopping power of each *nl* sub-shell of target electrons independently [6]. The stopping power for a given *nl* sub-shell is calculated as in Eq.1, where each ε is replaced by a Levine-Louie dielectric function ε_{nl}. The total stopping of the bound electrons will be the addition of the sub-shell contributions $S_t = \sum_{nl} S_{nl}$. The

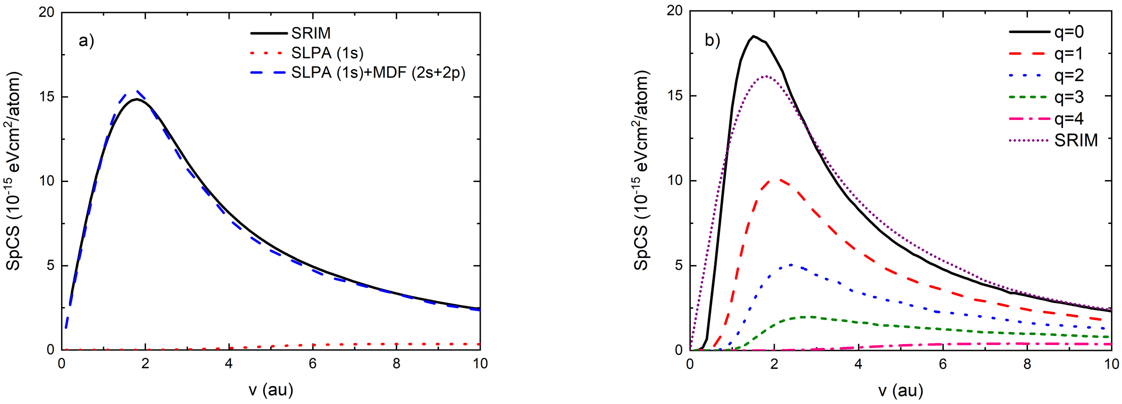

Figure 1: Stopping cross section of protons as a function of projectile velocity. a) Solid carbon target b) Bound electrons of a carbon gas target at different ionizations q.

Local Plasma Approximation (LPA) extends the dielectric formalism to deal with atomic bound electrons as a free-electron gas of local density, ρ_{nl}. The new energy loss function is calculated as

$$\mathrm{Im}\left[\frac{-1}{\varepsilon_{nl}(k,\omega)}\right] = \int 4\pi r^2 \mathrm{Im}\left[\frac{-1}{\varepsilon_{LLnl}(k,\omega,\rho_{nl}(r))}\right] dr \qquad (6)$$

Theoretical Results

Plasma response to a traversing charged particle depends mainly on the plasma temperature and the ionization state. First, as a basic test for the model, solid carbon and carbon gas targets at $T = 0$ are studied in Fig.1. Both cases are compared with SRIM code [11]. For the solid case, only $1s$ sub-shell is calculated with SLPA, while valence shells, $2s$ and $2p$, are calculated with the Mermin dielectric function using a collision frequency $\delta = 0.69$ [6]. Both comparisons offer an excellent fit to SRIM experimental data. Further, in the ionized cases of Fig.1b, as the ionization increases, due to the consideration of the binding energies, the bound contribution decreases quickly and the stopping is shifted to higher projectile velocities.

Now, to study the effect of temperature in our model, in Fig.2a ionization is kept constant at $q = 4$ and comparison is made with a recent model, UWPM [12], which is based on Kaneko dielectric function. Both models agree fairly well and minor differences are found at the medium velocities, which is the most sensitive region for stopping theories.

Finally, to model a realistic plasma, temperature and ionization are considered simultaneously in Fig.2b for a carbon plasma at different states. Notice that for the temperature range considered in Fig.2a, considering ionization as a constant is fairly correct in this case. However, this could change at lower densities or with heavier atoms targets.

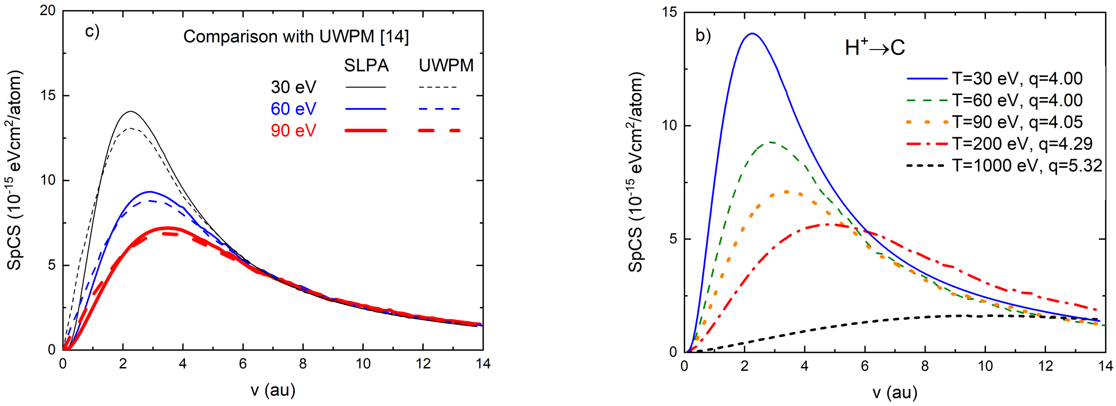

Figure 2: Stopping cross section of protons in a carbon plasma target at normal solid density as a function of projectile velocity at different temperatures; a) Constant ionization $q = 4$. b) SLPA model with ionization varying with temperature.

Conclusions

SLPA offers an excellent description of the stopping of bound electrons as can be seen in the results of [6] and in the comparisons of Fig.1. Furthermore, the response of the model to ionization and temperature effects is correct, so in principle, more precise results of stopping for partially ionized matter are expected with respect to mean ionization Bethe-like models, which are restricted in their ranges of validity. To model a realistic plasma ionization and temperature must be accounted simultaneously, but results here obtained can be further improved considering the distribution of ionization states in the plasma, and ionization potential depression effects. In the case here studied, bound electrons represent at most a 20% of the total stopping, so this considerations will not change the results significantly, but could be relevant in other cases.

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