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Analytical formula for the stopping power of low-energy ions in a free-electron gas

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HIGHLIGHTS

- The electronic stopping power of low-energy ions, calculated within the dielectric formalism and the Lindhard dielectric function, is revisited.
- A simple and accurate analytical formula for the electronic stopping power of low-energy bare ions is proposed.
- The new expression may be used together with the local-plasma approximation to predict stopping powers of ions in solids.

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ABSTRACT

The electronic stopping power of a slow heavy charged particle moving through a homogeneous free-electron gas is considered within the dielectric formalism and using the Lindhard dielectric function. A simple analytical formula is proposed that is more accurate than those employed hitherto, e.g. that of Lindhard and Winther, especially for small and intermediate electron densities.

1. Introduction

Swift charged particles moving through matter lose energy in inelastic collisions with the inhomogeneous electron gas that makes up the traversed medium. The electronic stopping power is the relevant magnitude that quantifies the rate at which these energy-loss processes take place. Perturbative and non-perturbative formalisms have been devised over the years to describe the dependence of the electronic stopping power on the projectile charge and velocity, and the properties of the medium (see e.g. Echenique et al., 1990; Sigmund, 2006).

The dielectric formalism is a perturbative (i.e. linear) theoretical framework that is extensively used to model the energy loss of charged particles in condensed matter. It furnishes a compact expression for the electronic stopping power that involves the complex dielectric function of the considered substance. Unfortunately, most often the complete (i.e. wave number and angular frequency dependent) dielectric function is not accessible experimentally, and ab initio calculations are also difficult to carry out. The local-plasma approximation (LPA) provides an elegant way to model the spatially varying electron density that the projectile encounters along its trajectory in real-life systems. To do so, every volume element in the medium is assumed to respond to the perturbation caused by the passing ion as if it was a homogeneous free-electron gas (FEG). The random-phase approximation yields a realistic description of the main properties of the FEG, viz. the production of electron–hole pairs and the possibility of collective (plasmon) excitations (Lindhard, 1954; Lindhard and Winther, 1964).

The LPA lacks a rigorous foundation (Johnson and Inokuti, 1983) but it is conceptually appealing and performs quite well when compared to other theoretical approaches (Mikkelsen et al., 1992; Sarasola et al., 2001). Thus, it has been adopted in many calculations of stopping powers and related quantities. In spite of being a first-order theory, the LPA implemented with the dielectric formalism and the Lindhard dielectric function (without local-field correction) is able to describe quite successfully the energy loss of ions at random incidence (Bonderup, 1967; Rousseau et al., 1971; Ziegler and Chu, 1974; Chu et al., 1975; Gertner et al., 1978, 1980; Iafrate et al., 1980; Ascolani and Arista, 1986; Arista, 1986), in channeling conditions (van Dijk et al., 1994) and even in grazing collisions on surfaces (Sarasola et al., 2003). Furthermore, this type

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of approach also predicts reasonable mean free paths and stopping powers of electrons and positrons in solids (Tung et al., 1979; Mayol et al., 1991).

The computation of electronic stopping powers based on the LPA requires, besides the double integral over wave number and angular frequency inherent to the stopping power of a FEG within the dielectric formalism, an additional integration over the spatial coordinates. Even in the favourable case of a spherically-symmetrical electron density, a triple integral has to be done. To facilitate the numerical calculations, which was a pressing need in the days of limited computing resources, many authors introduced approximations that render analytical formulas for the low- and high-energy stopping power of the FEG (Bonderup, 1967; Rousseau et al., 1971; Ziegler and Chu, 1974; Chu et al., 1975; Gertner et al., 1978, 1980; Ascolani and Arista, 1986; Arista, 1986).

In this context, the purpose of the present work is to briefly revisit the existing analytical expressions for the stopping power of a low-energy heavy charged particle in a FEG of constant density and to propose a simple analytical formula that is in much better agreement with the exact result than those commonly employed.

2. Theory

2.1. Stopping power in the dielectric formalism

Within the dielectric formalism, the electronic stopping power of a bare ion of mass $M \gg m_e$ and charge $Z_1 e$ (m_e and e are the electron mass and the elementary charge, respectively) moving with velocity v is given by (see e.g. Sigmund, 2006; Nersisyan and Das, 2008)

$$S(v) = \frac{2Z_1^2 e^2}{\pi v^2} \int_0^\infty \mathrm{d}k \, \frac{1}{k} \int_0^{kv} \mathrm{d}\omega \, \omega \, \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right], \tag{1}$$

where $\epsilon(k,\omega)$ is the complex dielectric function of the medium which depends on the wave number k and angular frequency ω of the electromagnetic disturbance caused by the passing projectile. The proportionality of S with Z_1^2 is a signature of linear-response theories.

2.2. Dielectric function of the homogeneous FEG

Consider a homogeneous FEG of density ρ and Fermi wave number

$$k_F = (3\pi^2\rho)^{1/3}. \tag{2}$$

Alternatively, the FEG can be characterized by the Lindhard parameter χ^2 or the one-electron radius r_s; these dimensionless quantities are connected to k_F through

$$\chi^2 = (\pi k_F a_0)^{-1} = \alpha r_s/\pi, \tag{3}$$

where $a_0 = \hbar^2/m_e e^2$ is the Bohr radius ($\hbar$ is the reduced Planck constant) and $\alpha = (4/9\pi)^{1/3}$. The dielectric function of the FEG was obtained, within the random-phase approximation, by Lindhard in his celebrated article from 1954 (Lindhard, 1954). He found it convenient to replace k and ω by the dimensionless variables

$$z \equiv \frac{1}{2}\frac{k}{k_F} \quad \text{and} \quad u \equiv \frac{\omega}{k v_F}, \tag{4}$$

where $v_F = \hbar k_F/m_e$ stands for the Fermi velocity, in terms of which the dielectric function can be written as (Lindhard, 1954; Lindhard and Winther, 1964)

$$\varepsilon_L(z,u) = 1 + \frac{\chi^2}{z^2}\,[f_1(z,u) + \mathrm{i} f_2(z,u)] \tag{5}$$

with

$$f_1(z,u) = \frac{1}{2} + \frac{1}{8z}[1-(z-u)^2] \ln\left|\frac{z-u+1}{z-u-1}\right| + \frac{1}{8z}[1-(z+u)^2] \ln\left|\frac{z+u+1}{z+u-1}\right| \tag{6}$$

and

$$f_2(z,u) = \begin{cases} \dfrac{\pi}{2}u & \text{if } z+u<1 \text{ (I)}, \\ \dfrac{\pi}{8z}[1-(z-u)^2] & \text{if } |z-u|<1<z+u \text{ (II)}, \\ 0 & \text{if } |z-u|>1 \text{ (III)}. \end{cases} \tag{7}$$

2.3. Stopping power of a homogeneous FEG at $v \ll v_F$

Introducing ε_L in Eq. (1) and changing to the (z,u) variables we get

$$S(v) = \frac{8}{\pi^2}\,\frac{m_e^2 e^4}{\hbar^3}\,\frac{Z_1^2 v_F^3}{v^2} \int_0^{v/v_F} \mathrm{d}u \, u \int_0^\infty \mathrm{d}z \times \frac{z^3 f_2(z,u)}{[z^2+\chi^2 f_1(z,u)]^2 + [\chi^2 f_2(z,u)]^2}. \tag{8}$$

At very low speed, $v \ll v_F$, only the narrow rectangular strip of region I defined by $u < v/v_F \ll 1$ and $z < 1$ contributes to the integral.[1] In this strip $f_1(z,u) \approx f_1(z,0)$ and $f_2(z,u) = (\pi/2)u$, so that the stopping power simplifies to (Lindhard and Winther, 1964)

$$S(v) = \frac{4}{3\pi}\,\frac{m_e^2 e^4}{\hbar^3}\, Z_1^2 C_1(\chi^2) v, \tag{9}$$

where

$$C_1(\chi^2) \equiv \int_0^1 \frac{z^3}{[z^2+\chi^2 f_1(z,0)]^2}\,\mathrm{d}z \tag{10}$$

and

$$f_1(z,0) = \frac{1}{2} + \frac{1-z^2}{4z} \ln\left|\frac{z+1}{z-1}\right|. \tag{11}$$

Hence, at low velocities $S(v) \propto v$. Moreover, the dependence of S on the density of the FEG appears exclusively in the factor C_1, which may be evaluated either exactly by solving numerically the integral (10) or resorting to any of the approximations described in the next section.

2.4. Approximate expressions for $C_1(\chi^2)$

A simple, approximate analytical expression for the C_1 coefficient can be achieved by setting

$$f_1(z,0) \approx f_1(0,0) = 1 \tag{12}$$

in the definition of $C_1(\chi^2)$. It follows that[2]

$$C_1^{(\mathrm{R1})}(\chi^2) = \frac{1}{2}\left[\ln\left(\frac{1+\chi^2}{\chi^2}\right) - \frac{1}{1+\chi^2}\right]. \tag{13}$$

Incidentally, this equation provides a link to non-linear formalisms where the electronic stopping power of a slow ion is proportional to the transport cross section (Echenique et al., 1990). Specifically, $C_1^{(\mathrm{R1})}$ is proportional to the transport cross section in the first-order Born approximation of the Yukawa potential, which is often used to model the stopping of low-energy ions in matter (Ferrell and Ritchie, 1977; Calera-Rubio et al., 1994). In terms of r_s, the

[1] The small contribution of region II is neglected.

[2] The change of variables $z^2 = t$ gives rise to an integral that can be solved by means of Eq. (2.113 2) in Gradshteyn and Ryzhik (1980).