

# Approximate Formulas for the Stopping Power of Charged Particles in an Electron Gas

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## Abstract

The aim of the work, a survey is presented on calculating the energy loss of charged particles within the linear response theory from the knowledge of the dielectric function of a free electron gas model that evaluated the electronic stopping power in the local density approximation (LDA). The basic idea for energy loss including excitation and ionization of the couple (projectile – target) system for both ( $C$  and  $N$ ) as a projectile and a number of atoms as a target by taking the value of  $r_s$  for each one. Approximate results for the electronic stopping power at high ( $v > v_f$ ) and low ( $v < v_f$ ) velocity are obtained. At low velocities, the stopping power is proportional to particle velocity, while at high velocities the stopping power is found familiar to the logarithmic dependence on velocity. The analytical results are compared with accurate numerical calculations.

## 1. Introduction

An vigorous field is presented about the interaction of charged particles with solids in theoretical and applied physics[1]. The valence electron response of a solid is well expressed by a free electron gas model which is a practical approximation for the passage of charged particle through it[2].

In the random – phase approximation(RPA), Lindhard obtained a wavevector – and frequency – dependent longitudinal dielectric function of interacting free electrons[1]. The Lindhard dielectric response has been utilized for calculation of the valence electron contribution to stopping power[2]. The energy losses of charged particles may be got by using linear response theory if the velocity of projectile is greater than the velocity of valence electrons in the targets[3]. In linear theory, the energy loss is proportional to the square of projectile charge and deals with the perturbing potential to the lowest order. While the energy losses which are proportional to the square of ion charge are resulted from the lowest – perturbation theory, the energy loss of positive and negative particles displays a reliance on the sign of the charge[4].

The Perturbative and non – perturbative formalisms explain the reliance of electronic stopping power on the properties of the medium, and the ion charge and velocity[5]. In Lindhard's stopping power theory, the perturbation due to a charged particle may be considered intruding into a free electron gas and the columbic force due to the cloud of screening electrons may also be calculated. When the particle moves at high speed, the cloud of screening electrons is unable to keep up with the particle, giving rise to a retarding force which relies on the effective charge of the particle[6]. The magnitude of the retarding fore is proportional to the speed of the ion at velocities well below the Bohr velocity( $v_0 = e^2/\hbar$ ) within a free electron gas and the approximations of linear response[6].

Lindhard stopping power theories treat the electron gas as translationally invariant. The band structure which includes the atomic structure of the system used to construct the dielectric function[6].

In the nonlinear calculation of the electronic stopping power of an electron gas at low velocity limit, the scattering theory approach to the stopping theory was used with the scattering cross sections[1]. The density – functional theory(DFT) was used to find out a statically screened potential which was helpful to evaluate the scattering cross sections[7]. The density functional theory (DFT) have been used to perform non – linear stopping power calculations of slow ion by considering the free electron gas as a target[6].

## 2. Local density approximation

The deposited energy in a collision of a fast charged particle with one of the target atoms is equally to the electronic energy loss of the particle[8]. In order to calculate the average energy loss and the energy straggling, i.e., the average square fluctuation of the energy deposition (or straggling) we use the well – known model suggested by Lindhard and Scharff[9], the so – called local plasma approximation (LPA).

In this model each volume of the target atom at position  $r$  is considered to be an independent plasma of uniform density  $\rho = \rho(r)$ , which is equal to the electron charge density of the atom. We normalized the density to the total number of electrons in the atom  $\int dr \rho(r) = Z_2$

The electronic energy loss of a particle of charge  $Z_1 e$  moving with velocity  $v$  in an electron gas of density  $\rho(r)$  is [10]

$$-\frac{dE}{dx}(r) = \frac{4\pi Z_1^2}{v^2} \rho(r) L(\rho(r), v) \quad (1)$$

Where  $L(\rho(r), v)$  is the usually stopping number. Hence, we can write the energy transferred to the atomic electrons  $Q(b)$  in a collision as a line integral which is taken along the particle trajectory  $r = r(l)$  with impact parameter  $b$

$$Q(b) = \int dl \left[ -\frac{dE}{dx}(r) \right] |_{r=r(l)} \quad (2)$$

We will use the straight – line approximation and will consider the particle moving in  $(z - axis)$

$$Q(b) = \frac{8\pi Z_1^2}{v^2} \int_0^\infty dz \rho(r) L(\rho(r), v) \quad (3)$$

In order to evaluate  $L(\rho(r), v)$  which becomes in this case as a function of ion velocity  $v$ , Fermi velocity  $v_f$  and medium plasma frequency  $\omega_p$ , we need convenient approximation[8].

$$L = C_1(\chi^2) \left( \frac{v}{v_f} \right)^3 \quad \text{for } v < v_f \quad (4)$$

$$L = \ln \frac{2mv^2}{\hbar\omega_p} - \frac{3}{5} \left( \frac{v}{v_f} \right)^2 \quad \text{for } v > v_f \quad (5)$$

Where  $C_1(\chi^2)$  is the density function, the value of Fermi velocity  $v_f$  will be taken as the point of intersection of the low – velocity and high – velocity approximation, eq.(4) and eq.(5).

### 3. Stopping power in the dielectric formalism of the homogenous free electron gas (FEG)

For swift heavy particles of low charge, the stopping power of a free electron gas is of considerable interest to actual slowing-down problems, therefore it is convenient to write the resulting stopping formula for an electron gas of density  $n$  electrons per unit volume in the form[11]

$$-\frac{dE}{dX} = \frac{4\pi e^4 Z_1^2}{mv^2} nL \quad (6)$$

Where  $m$  and  $e$  are the electron mass and charge, and  $L$  is the stopping number (dimensionless quantity). In dielectric formalism, it may written as

$$L = \frac{i}{\pi\omega_p^2} \int_0^\infty \frac{dk}{k} \int_{-kv}^{kv} \omega d\omega \left( \frac{1}{\epsilon(k,\omega)} - 1 \right) \quad (7)$$

$\omega_p$  is the plasma frequency of uniform electron gas

$$\omega_p = \left( \frac{4\pi ne^2}{m} \right)^{1/2} \quad (8)$$

The electronic stopping power for ion of charge  $Z_1 e$  and mass  $m$  moving with velocity  $v$  in a medium of density  $n$ , by substituting eqs.(7,8) into eq.(6) to get the electronic stopping power[5]

$$-\frac{dE}{dX} = \frac{2e^2 Z_1^2}{v^2} \int_0^\infty \frac{dk}{k} \int_0^{kv} \omega d\omega \text{Im} \left( \frac{-1}{\epsilon(k,\omega)} \right) \quad (9)$$

$\epsilon(k, \omega)$  is the longitudinal dielectric function of the medium depending on the wave number  $k$  and angular frequency  $\omega$  of the electromagnetic disturbance caused by the passing projectile. Lindhard obtained dielectric constant for a free electron gas within first - order perturbation theory as[11]

$$\epsilon(k, \omega) = 1 + \frac{8\pi me^2}{\hbar^2 k^2} \sum_n f(E_n) \left( \frac{1}{k^2 + 2k.k_n - (2m/\hbar^2)(\omega + i\gamma)} + \frac{1}{k^2 - 2k.k_n + (2m/\hbar^2)(\omega + i\gamma)} \right) \quad (10)$$

here  $E_n$  is the energy and  $k_n$  is the wave number of the electron in  $n$  state,  $\gamma$  is a positive infinitesimal damping constant, and  $f(E_n)$  is the distribution function which is an even function of  $k_n$  and normalized to  $N$ , the total number of electrons

$$\sum_n f(E_n) = N \quad (11)$$

$$f(E_n) = 1 \quad E_n < E_f \quad (12)$$

$$f(E_n) = 0 \quad E_n > E_f \quad (13)$$

In the case of a degenerate electron gas with Fermi energy  $E_f$  which is related to density  $n$  of the gas

$$E_f = \frac{1}{2} m v_f^2 = \frac{\hbar^2 k_f^2}{2m} = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \quad (14)$$

The result of summation in eq.(10) is

$$\epsilon(u, z) = 1 + \frac{\chi^2}{z^2} \{ f_1(u, z) + i f_2(u, z) \} \quad (15)$$

$$f_1(u, z) = \frac{1}{2} + \frac{1}{8z} [1 - (z - u)^2] \ln \left| \frac{z - u + 1}{z - u - 1} \right| + \frac{1}{8z} [1 - (z + u)^2] \ln \left| \frac{z + u + 1}{z + u - 1} \right| \quad (16)$$

$$f_2(u, z) = \begin{cases} \frac{\pi}{2} u & \text{for } z + u < 1 \\ \frac{\pi}{8z} [1 - (z - u)^2] & \text{for } z - u < 1 < z + u \\ 0 & \text{for } z - u > 1 \end{cases} \quad (17)$$

The variables  $k$  and  $\omega$  are replaced by dimensionless variables  $u = (\omega/k v_f)$  and  $z = (k/2 k_f)$ ,  $\chi$  is the density parameter and  $\chi^2$  is a measure of the ration between the potential energy of two neighboring particles and their kinetic energy. This indicates that free particle is for small values of  $\chi^2$ . Dielectric function is based on the

first order perturbation and started from free electrons. In higher order, account can be taken of the circumstance that the electrons are not free when  $\chi^2 > 1$ , i.e. at low gas densities[11].

$$\chi^2 = \frac{v_0}{\pi v_f} \quad \text{With } v_0 = \frac{e^2}{\hbar} \text{ is the Bohr velocity} \quad (18)$$

$$\chi^2 = \frac{e^2}{\pi \hbar v_f} \quad (19)$$

when atomic units (a. u.),  $e^2 = \hbar = m = 1$  are used throughout

$$\chi^2 = \frac{1}{\pi v_f} \quad (20)$$

The dielectric function given in eq.(15) is substituted in eq.(7), one get[11]

$$L = \frac{-6}{\pi \chi^2} \int_0^{v/v_f} u du \int_0^\infty z dz \text{Im} \left( \frac{1}{\epsilon(u,z)} \right) \quad (21)$$

$$L = \frac{6}{\pi} \int_0^{v/v_f} u du \int_0^\infty dz \frac{z^3 f_2(u,z)}{[z^2 + \chi^2 f_1(u,z)]^2 + [\chi^2 f_2(u,z)]^2} \quad (22)$$

The integral in eq.(22) receives contribution from the  $|u - z| < 1$  where  $f_2(u, z) \neq 0$  and from  $u > z + 1$  for which  $\epsilon(u, z) = 0$ , i.e.  $z^2 + \chi^2 f_1(u, z) = 0$  we must done a series on  $f_1(u, z)$  by assuming  $z - u > 1$  to be large compared to unity and taking the dispersion relation  $\epsilon(u, z) = 0$

$$f_1(u, z) = \frac{1}{3(z^2 - u^2)} + \frac{z^2 + 3u^2}{15(z^2 - u^2)^3} \quad (23)$$

$$u^2 = \frac{\chi^2}{3z^2} + \frac{3}{5} + \dots \quad \omega = \omega_p + \frac{3v_f^2}{10\omega_p} k^2 + \dots \quad (24)$$

For large value of  $u$ , the dispersion relation eq.(24) approaches the hyperbola[11]

$$u \cdot z = \chi/\sqrt{3} \quad \omega = \omega_p \quad (25)$$

In eq.(22), the velocity is measured in Fermi velocity and the variable  $y$  measures the velocity in unit  $(\hbar\omega_p/2m)^{1/2}$  defined by the plasma frequency.

$$y = \frac{2mv^2}{\hbar\omega_p} = \frac{\sqrt{3}}{\chi} \left( \frac{v}{v_f} \right)^2 \quad (26)$$

### 3.1 Low velocities $v < v_f$

For low particle velocities, we find from eqs.(16, 17 and 23) that the stopping number is proportional to  $v^3$  and from eqs.(4 and 26)[11]

$$L = C_1(\chi^2) \left( \frac{v}{v_f} \right)^3 = C_1(\chi^2) y^{3/2} \frac{\chi^{3/2}}{3^{3/4}} = C_1(\chi^2) y^{3/2} \left( \frac{\chi^2}{3} \right)^{3/4} \quad (27)$$

We must substitute the value of stopping number given in eq.(27) into eq.(6) in order to obtain the stopping power at low velocities[5]

$$-\frac{dE}{dX} = \frac{4\pi e^2 z_1^2}{mv^2} n C_1(\chi^2) \left( \frac{v}{v_f} \right)^3 \quad (28)$$

$$v_f = \frac{\hbar}{m} (3\pi^2 n)^{1/3} \quad (29)$$

Where  $v_f$  is the Fermi velocity which substituted in eq.(28) to get the stopping power

$$-\frac{dE}{dX} = \frac{4\pi e^2 z_1^2}{mv^2} n C_1(\chi^2) \frac{v^3 m^3}{3\pi^2 n \hbar^3} = \frac{4}{3\pi} \frac{m^2 e^4}{\hbar^3} Z_1^2 v C_1(\chi^2) \quad (30)$$

$$-\frac{dE}{dX} = \frac{4}{3\pi} Z_1^2 v C_1(\chi^2) \quad \text{in (a. u.)} \quad (31)$$

$$C_1(\chi^2) = \int_0^\infty \frac{z^3}{[z^2 + \chi^2 f_1(u,z)]^2} dz \quad (32)$$

$$f_1(z, 0) = \frac{1}{2} + \frac{1-z^2}{4z} \ln \left| \frac{z+1}{z-1} \right| \quad (33)$$

Hence, the stopping power proportional to velocity  $(-\frac{dE}{dX} \propto v)$  at low velocities. Also the dependence of stopping power on the density of free electron gas FEG appears exclusively in the factor  $C_1(\chi^2)$  which may be evaluated either exactly by solving numerically the integral (32) or approximately[5].

#### 3.1.1 Approximate expressions for $C_1(\chi^2)$

An approximate expression for the  $C_1(\chi^2)$  can be achieved by setting  $f_1(z, 0) \approx f_1(0,0) = 1$ . In the definition of  $C_1(\chi^2)$ , it follows that

$$C_1^{(R1)}(\chi^2) = \frac{1}{2} \left[ \ln \left( \frac{1+\chi^2}{\chi^2} \right) - \frac{1}{1+\chi^2} \right] \quad (34)$$

This equation connects between linear and non – linear formalisms in which the stopping power of a fast ion is proportional to the transport cross section.  $C_1^{(R1)}(\chi^2)$  is also proportional to the transport cross section. In linear – response theory, the stopping power can be calculated only in the higher – electron density limit which is equivalent to the use of the first – order Born approximation for the scattering cross section of Yukawa potential[12].

In figures (1, 2, 3, 4, and 5), the calculations of linear stopping power ( $\frac{1}{v} \frac{dE}{dx}$ ) in a. u. as a function of  $r_s$  for projectiles of atomic number  $Z_1 = 6$  and 7 have been fulfilled at low velocities. It is found that the enhancement of stopping power for  $Z_1 = 7$  is larger than for  $Z_1 = 6$ . The enhancement can be ascribed to dependence of stopping power on projectile atomic number. It is also noted that for the same projectile the stopping power values vary when changing the formula of density function because the stopping power also relies on the electrons density that become visible in the density function  $C_1(\chi^2)$ . In the limit of high density,  $r_s \ll 1$ , the stopping power increasing with decreasing  $r_s$  because for large electron gas densities, the projectile screening is brawny and the screened potential leads to scatter the electrons. In the local density approximation, the density of electrons is inhomogeneous and  $r_s$  changes according to local electron density.

$$n = \frac{3}{4\pi r_s^3} \quad (35)$$

Where  $r_s$  is the Wigner – Seitz radius. We substitute eq.(35) and taken in atomic units and the value of  $\alpha = (4/9\pi)^{1/3}$  into the eq.(29) to get the Fermi velocity

$$v_f = \frac{1}{\alpha r_s} = \frac{1.92}{r_s} \quad (36)$$

By substituting eq.(36) into eq.(20), the density parameter becomes  $\chi^2$

$$\chi^2 = \frac{\alpha r_s}{\pi} = 0.166 r_s \quad (37)$$

By taking the value of density parameter given in eq.(37), the eq.(34) in terms of  $r_s$  becomes

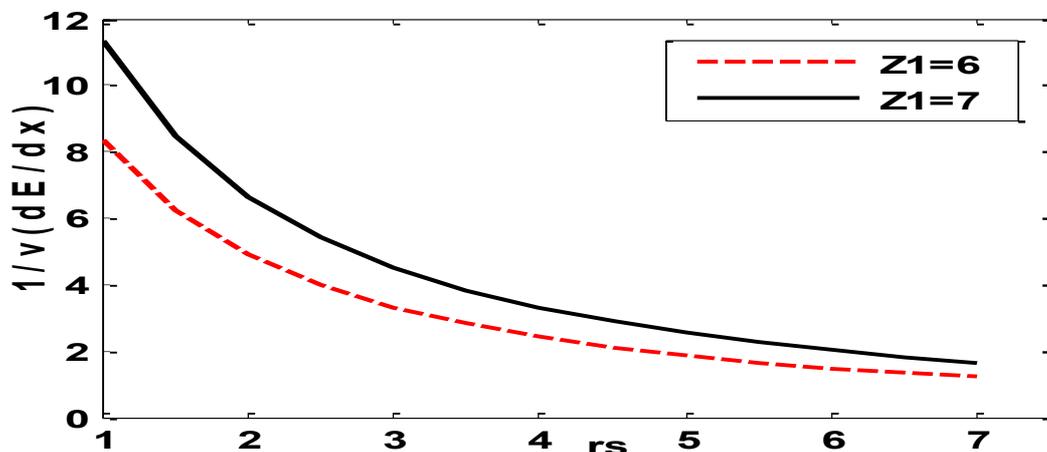
$$C_1^{(R1)}(\chi^2) = \frac{1}{2} \left[ \ln \left( 1 + \frac{1}{\alpha r_s/\pi} \right) - \frac{1}{1 + \alpha r_s/\pi} \right] \quad (38)$$

And the stopping power corresponding to  $C_1^{(R1)}(\chi^2)$  is

$$-\frac{dE}{dX} = \frac{2}{3\pi} \frac{m^2 e^4}{\hbar^3} Z_1^2 v \left[ \ln \left( 1 + \frac{1}{\alpha r_s/\pi} \right) - \frac{1}{1 + \alpha r_s/\pi} \right] \quad (39)$$

$$-\frac{dE}{dX} = \frac{2}{3\pi} Z_1^2 v \left[ \ln \left( 1 + \frac{1}{\alpha r_s/\pi} \right) - \frac{1}{1 + \alpha r_s/\pi} \right] \quad \text{in (a. u.)} \quad (40)$$

Ferrell and Ritchie apparently published this formula for the first time[13]. After the pioneering work of Fermi and Teller within the framework of linear – response theory, an improvement over the Fermi – Teller formula was done by using the random – phase approximation(RPA) at low velocities ( $v \ll v_f$ ) for small  $\omega$  and  $k \leq k_f$ . This is equivalent to assuming that the density fluctuations in the electron gas screen exponentially the potential around an ion.



Figure(1) Stopping power calculated from linear theory eq.(40) for  $Z_1 = 6$  and 7 at low velocity  $v < v_f$

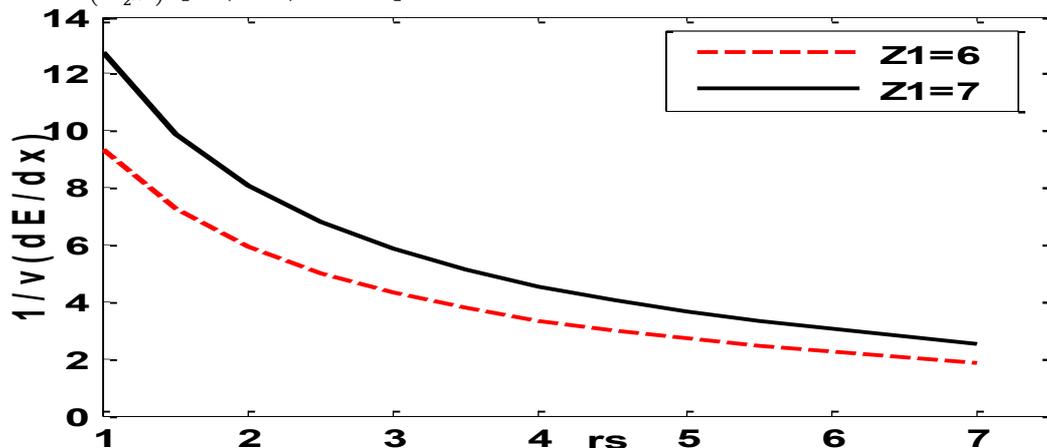
Ritchie proposed another analytical expression for  $C_1(\chi^2)$  making the substitution  $f_1(z, 0) = 1 - \frac{1}{2}z^2$ , in the definition of  $C_1(\chi^2)$ , it leads to[14]

$$C_1^{(R2)}(\chi^2) = \frac{1}{2(1-\frac{1}{2}\chi^2)^2} \left[ \ln \left( \frac{1-\frac{1}{2}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{2}\chi^2}{1+\frac{1}{2}\chi^2} \right] \quad (41)$$

And the stopping power corresponding to  $C_1^{(R2)}(\chi^2)$  is

$$-\frac{dE}{dX} = \frac{2}{3\pi} \frac{m^2 e^4}{\hbar^3} Z_1^2 v \frac{1}{(1-\frac{1}{2}\chi^2)^2} \left[ \ln \left( \frac{1-\frac{1}{2}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{2}\chi^2}{1+\frac{1}{2}\chi^2} \right] \quad (42)$$

$$-\frac{dE}{dX} = \frac{2}{3\pi} Z_1^2 v \frac{1}{(1-\frac{1}{2}\chi^2)^2} \left[ \ln \left( \frac{1+\frac{1}{2}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{2}\chi^2}{1+\frac{1}{2}\chi^2} \right] \quad \text{in (a. u.)} \quad (43)$$



Figure(2) Stopping power calculated from linear theory eq.(43) for  $Z_1 = 6$  and  $7$  at low velocity  $v < v_f$

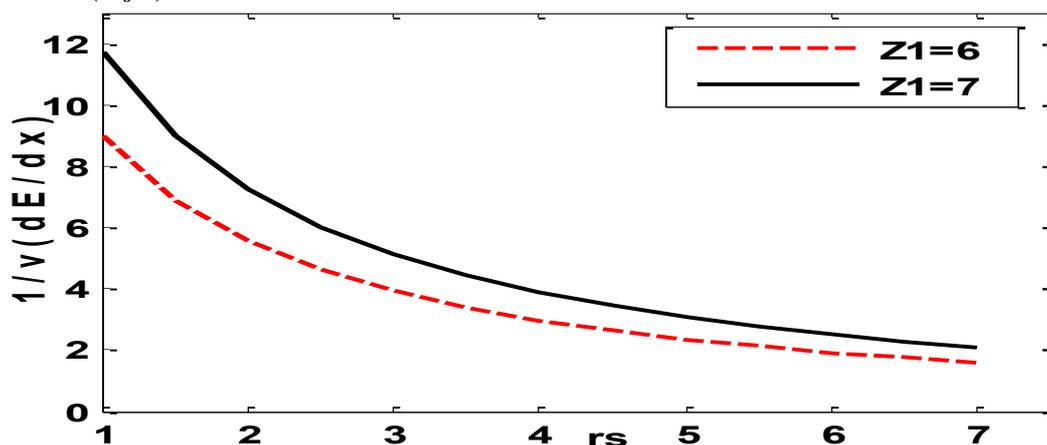
Lindhard and Winter (L – W) extended the original work of Lindhard[11]. They obtained an analytic expression for the stopping power in high and low ion velocity limit comparative to Fermi velocity of an electron gas. The mean ionization potential and shell correction in Bethe stopping power were obtained in the high velocity limit in which the linear stopping power depended on the velocity of projectile in the limit of low velocity.  $C_1(\chi^2)$  can be approximated by substituting  $f_1(z, 0) = 1 - \frac{1}{3}z^2$ , the first two terms in the Taylor expansion in power of  $z^2$

$$C_1^{(LW)}(\chi^2) = \frac{1}{2(1-\frac{1}{3}\chi^2)^2} \left[ \ln \left( \frac{1-\frac{2}{3}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{3}\chi^2}{1+\frac{2}{3}\chi^2} \right] \quad (44)$$

And the stopping power corresponding to  $C_1^{(LW)}(\chi^2)$  is

$$-\frac{dE}{dX} = \frac{2}{3\pi} \frac{m^2 e^4}{h^3} Z_1^2 v \frac{1}{(1-\frac{1}{3}\chi^2)^2} \left[ \ln \left( \frac{1-\frac{2}{3}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{3}\chi^2}{1+\frac{2}{3}\chi^2} \right] \quad (45)$$

$$-\frac{dE}{dX} = \frac{2}{3\pi} Z_1^2 v \frac{1}{(1-\frac{1}{3}\chi^2)^2} \left[ \ln \left( \frac{1+\frac{2}{3}\chi^2}{\chi^2} \right) - \frac{1-\frac{1}{3}\chi^2}{1+\frac{2}{3}\chi^2} \right] \quad \text{in (a. u.)} \quad (46)$$



Figure(3) Stopping power calculated from linear theory eq.(46) for  $Z_1 = 6$  and  $7$  at low velocity  $v < v_f$

L–W expansion was utilized by Bonderup to incorporate the local density approximation (LDA) of Lindhard and Scharff (L–S) in order to extract the mean ionization potential and shell corrections [9]. Each volume element of the solid is considered to be an independent plasma of uniform density in the local density approximation therefore, by spatially averaging a specific stopping power over the target electron charge distribution, we can get the total electronic stopping power.

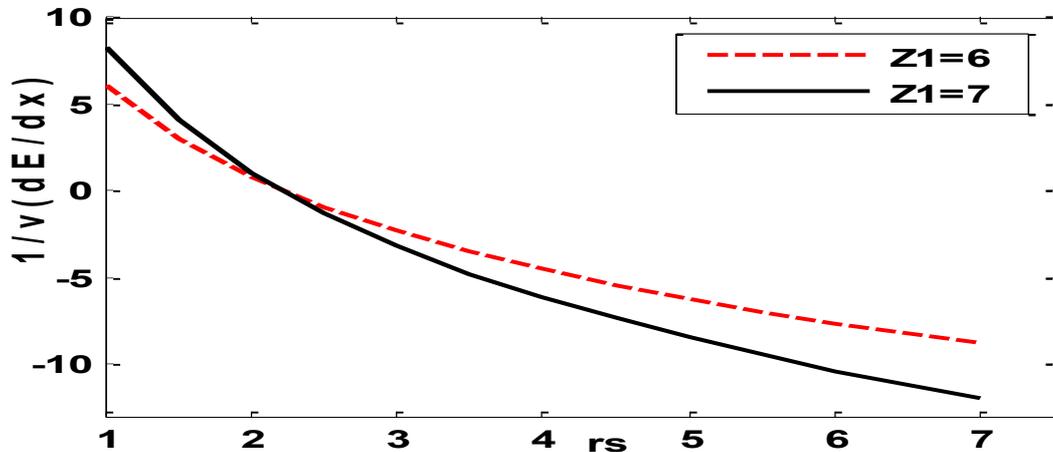
Bonderup employed the Lenz – Jensen to describe the target electrons Lenz charge distribution and used a simplified version of  $C_1^{(LW)}(\chi^2)$  or  $C_1^{(R2)}(\chi^2)$ , namely[15]

$$C_1^{(B)}(\chi^2) = \frac{1}{2} \left[ \ln \left( \frac{1}{\chi^2} \right) - 1 \right] \quad (47)$$

$C_1^{(B)}(\chi^2)$  becomes negative when  $\chi^2 > e^{-1} \approx 0.368$ . The stopping power corresponding to  $C_1^{(B)}(\chi^2)$  is

$$-\frac{dE}{dX} = \frac{2}{3\pi} \frac{m^2 e^4}{\hbar^3} Z_1^2 v \left[ \ln\left(\frac{1}{\chi^2}\right) - 1 \right] \quad (48)$$

$$-\frac{dE}{dX} = \frac{2}{3\pi} Z_1^2 v \left[ \ln\left(\frac{1}{\chi^2}\right) - 1 \right] \quad \text{in (a. u.)} \quad (49)$$



Figure(4) Stopping power calculated from linear theory eq.(49) for  $Z_1 = 6$  and  $7$  at low velocity  $v < v_f$

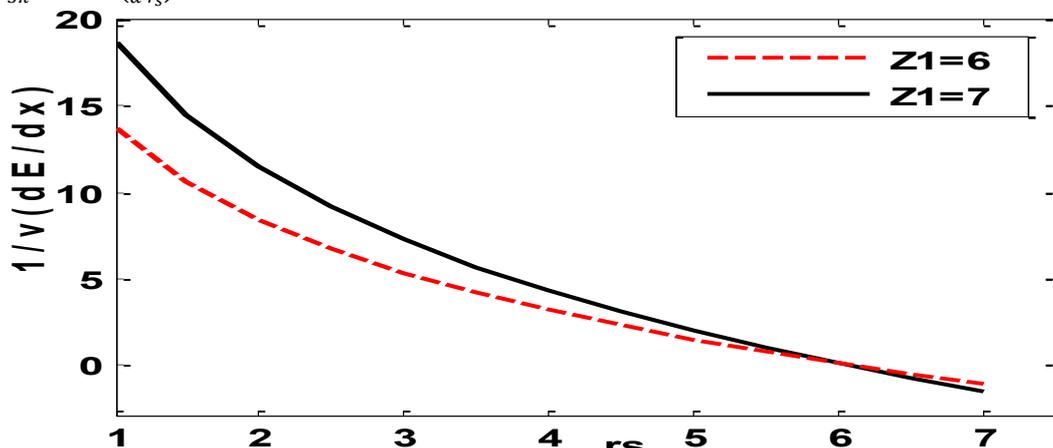
Fermi and Teller were the first to evaluate the stopping power of a charged particle moving with velocity small compared to the Fermi velocity ( $v \ll v_f$ ) [16]. They were interesting in estimating the time required for a muon with ( $v \ll v_f$ ) to be stopped in various solids. According to exclusion principle only electrons within a small velocity ( $v \ll v_f$ ) will participate in the loss process. In the limit of high density (dense FEG,  $n \gg 1$ , and  $\chi^2 \ll 1$ ), eqs.(34, 41, 44, and 47) reduce to

$$C_1^{(FT)}(\chi^2) = \frac{1}{2} \ln\left(\frac{1}{\chi^2}\right) = \frac{1}{2} \ln\left(\frac{\pi}{\alpha r_s}\right) \quad (50)$$

The stopping power corresponding to  $C_1^{(FT)}(\chi^2)$  is

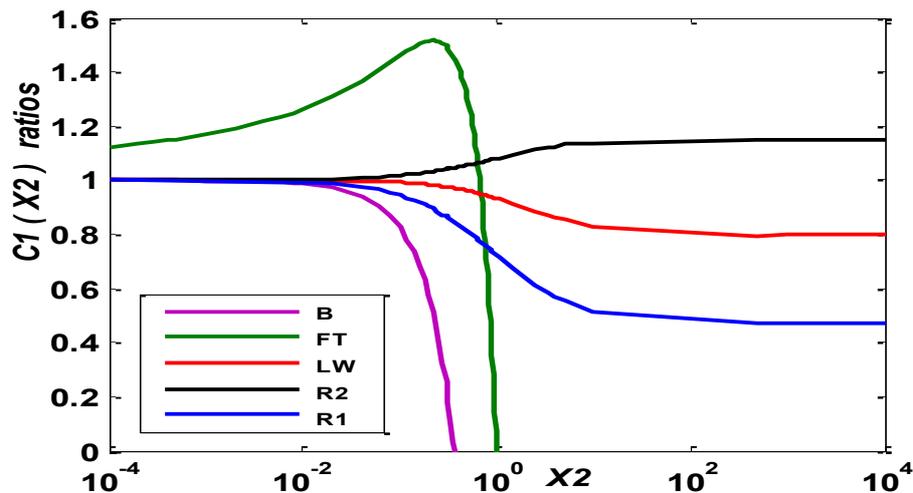
$$-\frac{dE}{dX} = \frac{2}{3\pi} \frac{m^2 e^4}{\hbar^3} Z_1^2 v \ln\left(\frac{\pi}{\alpha r_s}\right) \quad (51)$$

$$-\frac{dE}{dX} = \frac{2}{3\pi} Z_1^2 v \ln\left(\frac{\pi}{\alpha r_s}\right) \quad \text{in (a. u.)} \quad (52)$$



Figure(5) Stopping power calculated from linear theory eq.(52) for  $Z_1 = 6$  and  $7$  at low velocity  $v < v_f$

Figure (6) explains the ratios of density function  $C_1(\chi^2)$  evaluated from analytical expressions eqs.(34, 41, 44, 48, and 50) to the numerical result eq.(32) as a function of density parameter  $\chi^2$ . It is noted that all the curves merge into the numerical result at high FEG density and low  $\chi^2$ , in other words the analytical approach the numerical results except  $C_1$  that calculated from Fermi – Teller. Also at low density and high  $\chi^2$ ,  $C_1$  obtained from Fermi – Teller and Bonderup become unphysical but that  $C_1^{(R1)}(\chi^2)$ ,  $C_1^{(R2)}(\chi^2)$ , and  $C_1^{(LW)}(\chi^2)$  differ according to the chosen formula of  $f_1(z, 0)$  and the value of  $c$ .  $C_1^{(R1)}$  with  $c = 0$  has lower values than that of  $C_1^{(LW)}$  of  $c = 1/3$  (both the numerical results have larger values than analytical results) which undervalue  $C_1^{(R2)}$  with  $c = 1/2$  (the analytical results have larger values than numerical results).



Figure(6) Ratios of  $C_1$  evaluated from analytical to numerical result

### 3.1.2 Improved approximate expressions for $C_1(\chi^2)$

It is noted that  $C_1^{(R1)}(\chi^2)$ ,  $C_1^{(R2)}(\chi^2)$ , and  $C_1^{(LW)}(\chi^2)$  rely on the substitution  $f_1(z, 0) = 1 - cz^2$  and differ in the choice of the constant  $c$ . The same mathematical steps are followed in order to lead eqs.(34, 41, and 44) [5]

$$C_1(\chi^2) = \frac{1}{(1-c\chi^2)^2} \left[ \ln \left( \frac{1+(1-c)\chi^2}{\chi^2} \right) - \frac{1-c\chi^2}{1+(1-c)\chi^2} \right] \quad (53)$$

In the high – density limit,  $\chi^2 \rightarrow 0$ , eq.(53) tends to exact  $C_1(\chi^2)$  function eq.(32) not considering the value of  $c$ . In the low – density limit,  $\chi^2 \rightarrow \infty$ , the exact  $C_1(\chi^2)$  function eq.(32) reduced to[5]

$$C_1(\chi^2) \sim \left\{ \int_0^\infty \frac{z^3}{[f_1(u,z)]^2} dz \right\} \chi^{-4} \quad (54)$$

$$\int_0^\infty \frac{z^3}{[f_1(u,z)]^2} dz = 0.52827848933 \quad (55)$$

The integration is solved numerically by using various quadrature methods. In the same the low – density limit,  $\chi^2 \rightarrow \infty$ , eq.(53) becomes[5]

$$C_1(\chi^2) \sim \frac{1}{2c^2} \left[ \ln(1-c) + \frac{c}{1-c} \right] \chi^{-4} \quad (56)$$

Eq.(56 and 54) are equal

$$\frac{1}{2c^2} \left[ \ln(1-c) + \frac{c}{1-c} \right] = \int_0^\infty \frac{z^3}{[f_1(u,z)]^2} dz = 0.52827848933 \quad (57)$$

The solution of the above equation leads to the value of  $c = 0.44$  to ensure the correct behavior of eq.(53) for  $\chi^2 \rightarrow \infty$ .

Figure (7) shows the ratios of density function  $C_1(\chi^2)$  evaluated from analytical expressions eqs.(41, 44, and 53) to the numerical result eq.(32) as a function of density parameter  $\chi^2$ . In LW curve, the analytical results of  $C_1^{(LW)}$  with  $c = 1/3$  have smaller values than that of numerical but in  $R_2$  curve, the analytical results of  $C_1^{(R2)}$  with  $c = 1/2$  possess larger values than numerical results. In curve with  $c = 0.44$  both the numerical and analytical results are the same except at  $\chi^2 = 1$  there is an error of about 2% and the analytical formula with  $c = 0.44$  which lies between  $c = (1/2 \text{ and } 1/3)$  satisfy the numerical (exact) result.

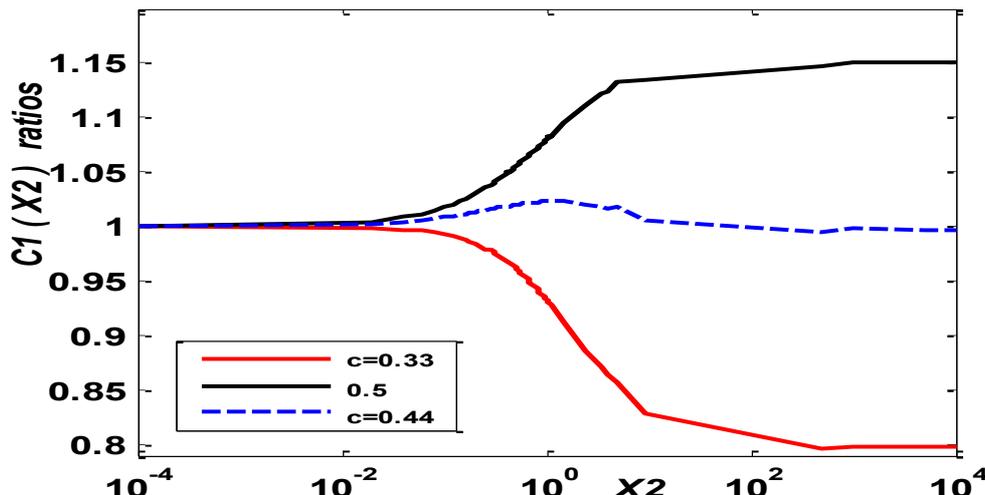


Figure (7) Ratios of  $C_1$  evaluated from analytical to numerical result

### 3.2 High velocities $v > v_f$

In the high velocity limit, the general formula for the stopping power eq.(6) is reduced to the simple Bethe – Bloch formula  $L = \ln(2mv^2/I)$ . In order to evaluate the stopping power and the mean excitation potential ( $I$ ) at high velocities, one must recourse to the Bethe sum rule for generalized oscillator strengths for a free electron gas[11]

$$\frac{1}{i\pi\omega_p^2} \int_{-\infty}^{\infty} \omega d\omega \frac{1}{\epsilon(k,\omega)} - 1 = 1 \quad (58)$$

At high velocities, there is an attempt for a series expansion in powers of  $1/v^2$ . We are concerned with stopping contributions from resonance absorption and close collisions for large values of  $u$ . In the equipartition rule, the change in the stopping number  $L$  with particle velocity receives exactly equal contribution from the resonance absorption and close collisions. The increase in  $L$  between two velocities  $v_1$  and  $v_2$  is twice the contribution from the resonance absorption[11]

$$L(v_1) - L(v_2) = 2 \int_{z_r(v_2/v_f)}^{z_r(v_1/v_f)} \frac{dz}{z} F_r(z) \quad (59)$$

Where  $F_r(z)$  is the oscillator strength of the resonance absorption as a function of  $z$ ,  $z_r(u)$  indicates to the value of  $z$  on the resonance as a function of the variable  $u$ , i.e.[11]

$$z_r^2(u) = -\chi^2 f_1(u, z_r(u)) \quad (60)$$

$$F_r(z) = \frac{-6}{\pi\chi^2} \int u du z^2 \text{Im} \left( \frac{1}{\epsilon(u,z)} - 1 \right) \quad (61)$$

$$F_r(z) = \frac{6z^4}{\chi^4 \left( \frac{\partial f_1(u,z)}{u \partial u} \right)_r} \quad (62)$$

Where the quantity  $(f_1(u, z)/u \partial u)$  is the partial derivative for constant  $z$ .  $F_r(z)$  remains close to unity and may be found by series expansion in power of  $u^{-2}$

$$F_r = 1 - \frac{12}{175u^2} + O\left(\frac{1}{u^6}, \frac{\chi^2}{u^4}\right) \quad (63)$$

We noted that the absence of a term proportional to  $u^{-2}$ .  $L$  also can be written in eq.(59) in a series expansion as[11]

$$L(v_1) - L(v_2) = \frac{6}{\chi^2} \int_{v_2/v_f}^{v_1/v_f} \frac{z_r^2(u) u du}{1 + \frac{\chi^2}{2z_r} \left( \frac{\partial f_1(u,z)}{\partial z} \right)} \quad (64)$$

And neglecting terms of higher order in  $\chi^2$

$$L(v_1) - L(v_2) = \left\{ u^3 \ln \frac{u+1}{u-1} + \ln(u^2 - 1) - 2u^2 + O\left(\frac{\chi^2}{u^4}\right) \right\} \Bigg|_{v_2/v_f}^{v_1/v_f} \quad (65)$$

By combining the above equation with the equation of the mean excitation potential  $I = \hbar\omega_p$  and taking only the first terms in a series expansion in  $v_f^2/v^2$ [11]

$$L = \ln \frac{2mv^2}{\hbar\omega_p} - \frac{3v_f^2}{5v^2} - \dots + O\left(\frac{\chi^2 v_f^4}{v^4}\right) \quad (66)$$

By substituting eq.(26) into the above equation, it becomes

$$L = \ln y - \frac{3^{3/2}}{5\chi y} - \dots \quad (67)$$

In order to get the stopping power at high velocities, we must substitute eq.(66) into eq.(6)

$$-\frac{dE}{dX} = \frac{4\pi e^4 z_1^2}{mv^2} n \left[ \ln \left( \frac{2mv^2}{\hbar\omega_p} \right) - \frac{3v_f^2}{5v^2} \right] \quad (68)$$

From eq.(8), we can obtain the density of electrons  $n = m \omega_p^2 / 4\pi e^2$  and then substituted in eq.(68)

$$-\frac{dE}{dX} = e^2 z_1^2 \frac{\omega_p^2}{v^2} \left[ \ln \left( \frac{2mv^2}{h\omega_p} \right) - \frac{3v_f^2}{5v^2} \right] \quad (69)$$

$$-\frac{dE}{dX} = z_1^2 \frac{\omega_p^2}{v^2} \left[ \ln \left( \frac{2v^2}{\omega_p} \right) - \frac{3v_f^2}{5v^2} \right] \quad \text{in (a. u.)} \quad (70)$$

Every term in eq.(70) is contributed equally from the resonance and close collisions. Fano and Turner get the result for any atom in the case of resonance collision while Walske obtained it for both resonance and close collisions in hydrogen atom[11].

Figures(8 and 9) explain the results of linear calculation of stopping number  $L$  obtained from eq.(67) at high velocities as a function of  $y$  for different density parameter  $\chi^2 = 0.02, 0.3, \text{ and } 1$ . It is seen in each curve that the stopping number increases with increasing the variable  $y$  (the velocity). Also we noted the enhancement of stopping number with increasing  $\chi^2$  at low  $y$  but at high  $y$  the values of stopping power are coincident because at high velocities all the ions are tracked by oscillation wake and all curves approach the straight line  $\ln y$  at high values of  $y$ .

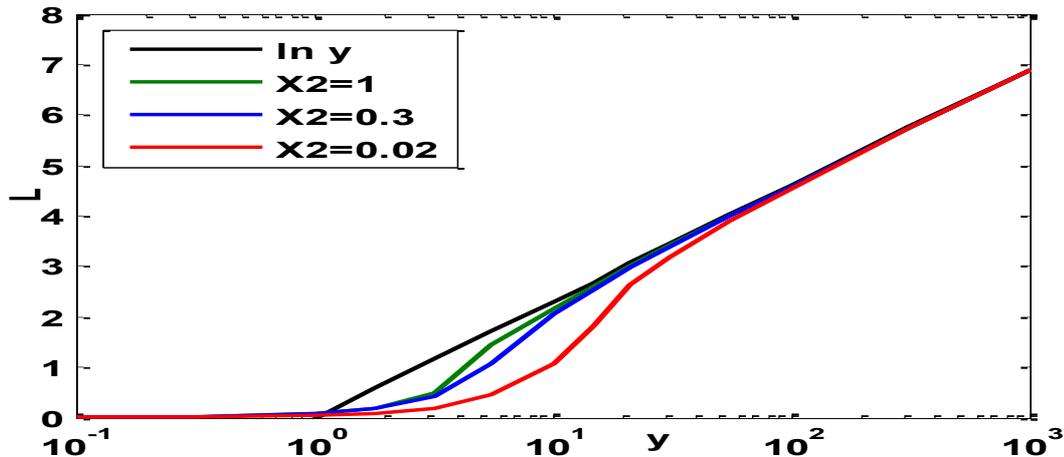


Figure (8) Stopping number  $L$  as a function of velocity parameter  $y$  for three electron gas densities  $\chi^2 = 1, 0.3, 0.02$ . Straight line refers to  $L = \ln y$

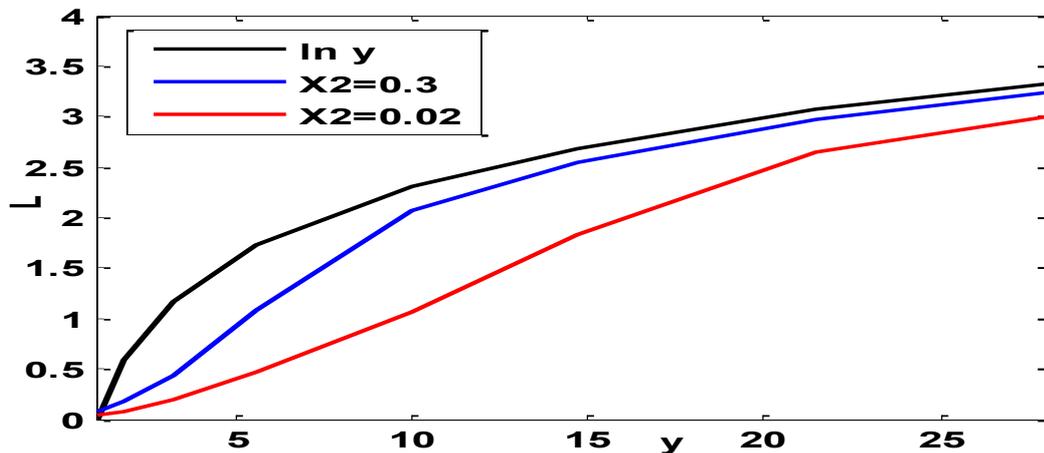


Figure (9) Stopping number  $L$  as a function of velocity parameter  $y$  for  $y < 25$  for two electron gas densities  $\chi^2 = 0.3, 0.02$ . The function  $L = \ln y$  is also referred

#### 4. Discussion

When a charged particle moves through matter, it loses energy to the medium through collisions with it and leads to a consequence of electronic excitation in the target. The excitation of target electrons may be depicted by the dielectric response and dielectric function which depends on the angular frequency and wave number.

In a free electron gas(FEG), at low velocities stopping powers of charged particles are due to valence electrons, therefore it is helpful to use the free electron gas model for this purpose because it is the best to show the contribution of conduction electrons not the bound core electrons in stopping power calculations. In a free electron gas if the density of valence electrons is inhomogeneous in the solid and are represented by the parameter

$n$ , parameter  $r_s$  changes due to the local electron density therefore the local density approximation are used within a free electron, for this reason the valence electrons stopping powers vary with its location according to  $r_s$  because of its inverse dependence on  $r_s$ .

The stopping power of a charged particles in linear response are proportional to the ion velocity and square of its charge  $Z_1^2$ . In the low velocity limit, the linear stopping power changes according to the chosen density function  $C_1(\chi^2)$  because of its dependence on it. There are a number of analytical expressions (*R1*, *R2*, *LW*, *B*, and *FT*) with results larger or smaller than that of a numerical (exact) formula for the  $C_1(\chi^2)$ .

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