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*Stopping power and phase shift for slow ions in an electron gas*

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*الخلاصة:-*

إن نتائج قدرة الإيقاف وفرق الطور عند مستوي فيرمي قد بينت للايونات ( $v < v_f$ ). البطيئة المتحركة بسرعة اقل من سرعة فيرمي في الغاز الالكتروني لقد تم إجراء الحسابات بالاعتماد على نظرية الكثافة اللاخطية. فللايونات البطيئة يحصل تفاعل الايون مع إلكترون الغاز بواسطة الاستطارة عند سطح فيرمي والذي يمكن إن ينسق باستخدام فرق الطور عند طاقة فيرمي مؤديا إلى حساب المقطع العرضي للاستطارة والطاقة المفقودة. كذلك تم حساب فرق الطور باستخدام دالة الموجة لجسيم منفرد الذي ينشأ من دالة الكثافة والتي تستخدم في حساب كثافة الالكترونات للمستوي الأرضي. إن نتائج فرق الطور قد تم حسابها من النظرية اللاخطية باستخدام الميكانيك الكمي والكلاسيكي مع الأخذ بعين الاعتبار تأثير الشحنة الفعالة.

**Abstract**

The results of the stopping power and the Fermi – level phase shifts are presented for slow ions moving with velocity smaller than Fermi velocity  $v < v_f$  in an electron gas. The calculations are made based on nonlinear density functional theory (DFT). For slow ion the interaction of the ion – electron gas occurs via scattering at the Fermi surface and can be codified in phase shifts at the Fermi energy leading to scattering cross sections and energy loss. The phase shift was computed using the single particle wave functions using the density functional method. The single particle wave functions are used to calculate the ground – state density of the electron. Further, nonlinear – phase shift results of stopping power are also calculated in classical and quantum mechanics taking into consideration the effective charge  $Z_1^*$ .

**1. Introduction**

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The stopping power of matter for charged particles is an important physical quantity in various applications. It is a subject of great importance in numerous areas of fundamental and applied physics[<sup>1</sup>]. The interaction of charged particles with matter has been a subject of great interest both for the advance of the knowledge of the basic interaction processes, as well as for a multitude of practical applications[<sup>2</sup>].

The study of non – linear effects in the energy loss is a powerful approach to test and improve the precision of various theoretical models aiming to describe the interaction process[<sup>3</sup>].

The problem of energy losses suffered by charged particles moving in matter is of continuous interest in physics. When the ion velocity is greater than the average velocity of valence electrons in solids, a good description of the loss can be achieved using a linear response theory in which the screened potential is treated to the lowest order to calculate the loss due to the valence – band electrons with atomic type calculations due to core – electron excitations. However, at low velocities, the importance of screening nonlinearities was demonstrated by using a scattering theory approach to the stopping power and density – functional theory[<sup>4</sup>].

**1. Z<sub>1</sub> Structure: Application of Friedel Sum Rule**

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The extended sum rule for a particle with velocity  $v$  and charge  $z_1 e$  may be written as follow[1]

$$\frac{2}{\pi} \sum_{l=0}^{\infty} (2l+1) G_l(v, v_f) = Z_1 \quad (1)$$

Where  $v_f$  is the Fermi velocity of the solid. The function  $G_l(v, v_f)$  represents the contribution of each  $l$  – wave component to the screening charge, and may be expressed as an integral over a displaced Fermi sphere(DFS) of the corresponding phase – shift contribution, as follows:

$$G_l(v, v_f) = \frac{1}{4\pi} \int_{DFS} \left[ \frac{d\delta_l(k)}{dk} \right] d\Omega dk \quad (2)$$

$$= \int_{k_{min}}^{k_{max}} \left[ \frac{d\delta_l(k)}{dk} \right] g(k, v) dk \quad (3)$$

where  $k_{min} = \max\{0, v - v_f\}$  and  $k_{max} = v + v_f$ . The function  $g(k, v)$  takes into account the angular part of the integration over DFS, and the expression for the cases  $v < v_f$  and  $v > v_f$ .  $\delta_l(k)$  is the phase shift of the electron wave function, and  $k$  is the wave vector corresponding to the relative electron – ion motion ( $k = mv_r/\hbar$ , where  $v_r = v_e - v$ ). The derivative  $[d\delta_l(k)/dk]$  give e the contribution of each  $l$  – wave component to the accumulation of screening charge around the intruder

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charge. From these expression one may retrieve the usual Friedel sum rule in the low – velocity limit ( $v \ll v_f$ ), and a perturbative form of the sum rule for high velocities ( $v \gg v_f$ ) [3].

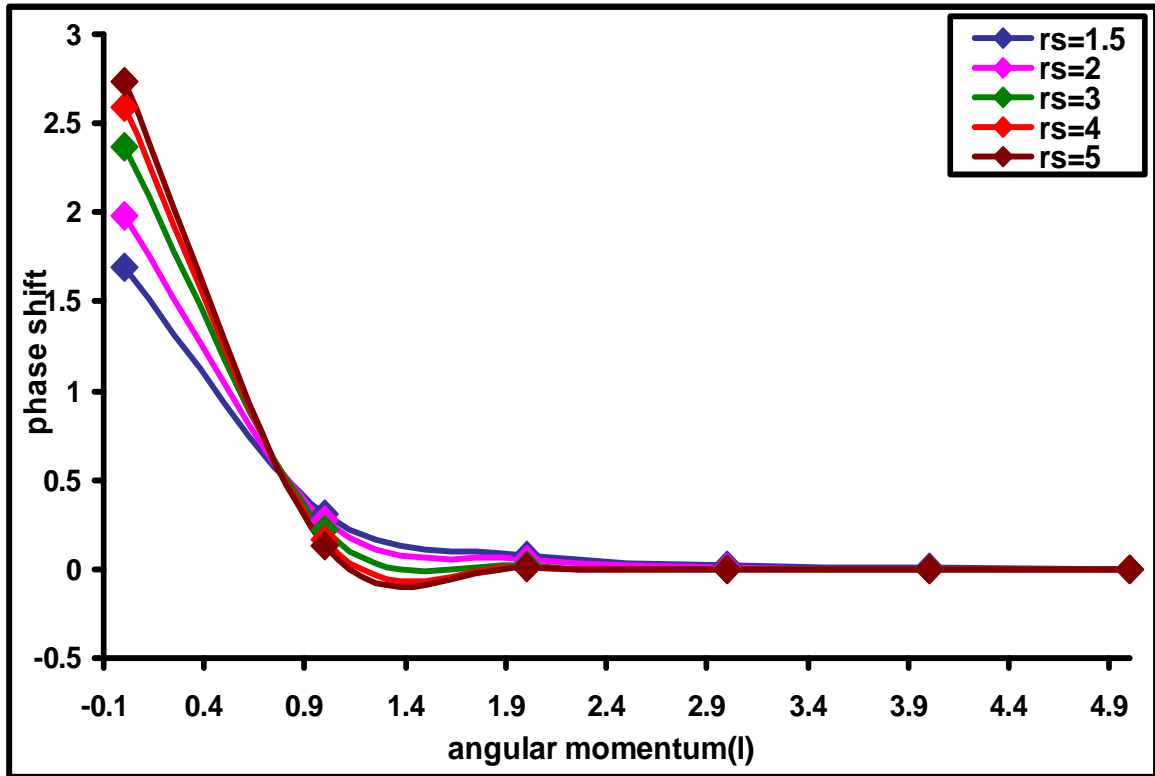
### 4. Phase shifts

At low projectile speed, the cross section is governed by contribution from small values of  $l$  and the scattering phase shifts at the Fermi energy due to the complete screening of the nuclear charge will satisfy the Friedel sum rule [4].

Figure (1) shows the phase shifts at Fermi level  $\delta_l(E_f)$  for atoms embedded in an electron gas as a function of angular momentum  $l$  by using the extended Friedel Sum Rule eq.(1) with projectile charge (a)  $Z_1 = (Z)$  and (b)  $Z_1 = (Z^*)$  and different target of density parameter ( $r_s = 1.5, 2, 3, 4, 5$ ). The phase shift will decrease when the angular momentum increase because the density of electrons  $n$  increases.

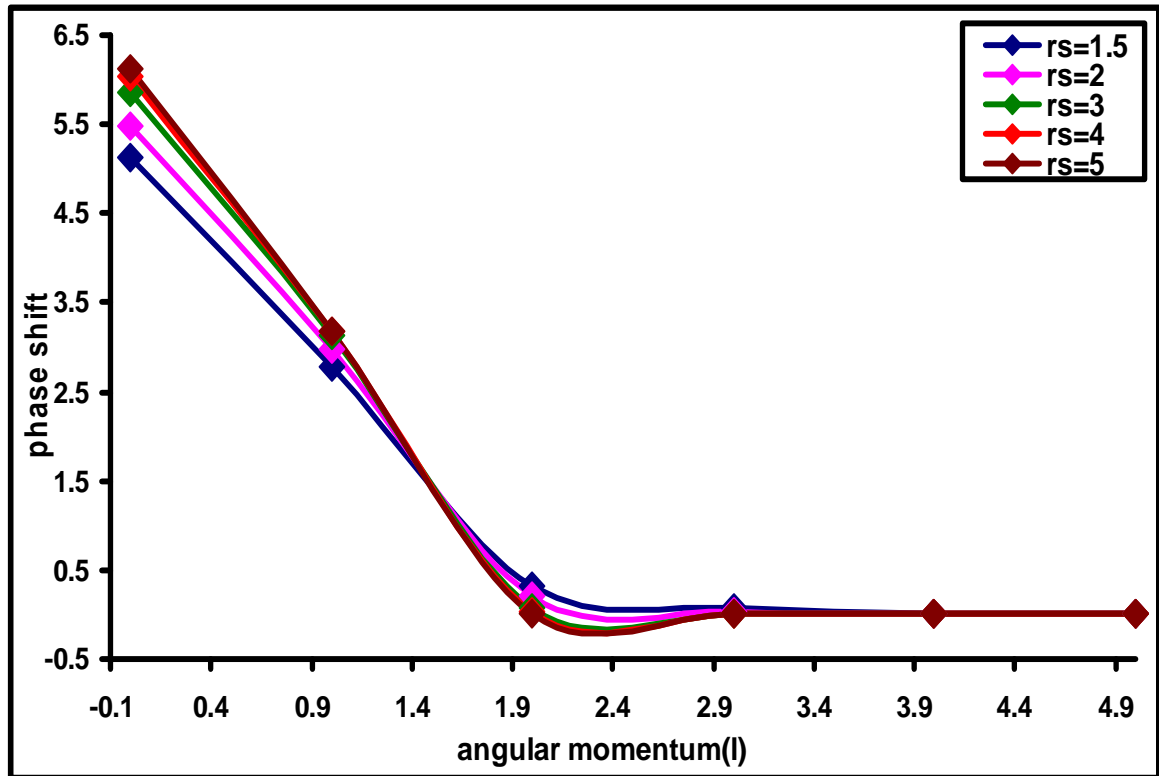
Figure (2) shows the phase shifts at Fermi level  $\delta_l(E_f)$  for atoms embedded in an electron gas as a function of density parameter  $r_s$  by using the extended Friedel Sum Rule eq.(1) with projectile charge (a)  $Z_1 = (Z)$  and (b)  $Z_1 = (Z^*)$  and different angular momentum  $l = (0, 1, 2, 3, 4, 5)$ . For  $Z_1 = Z$ , at angular momentum  $l < Z$  there is a direct relation between the phase shift and density parameter  $r_s$  but at  $Z \leq l \leq 2Z$  the phase shift increases with decreasing the angular momentum  $l$  and there is no effect of the density at  $l > 2Z$ . For  $Z_1 = Z^*$ , at angular momentum  $l < Z$  there is a direct relation between the phase shift and density parameter  $r_s$  but at  $Z \leq l \leq 2Z$  the phase shift increases with decreasing the angular momentum  $l$  and there is no effect of the density at  $l > 2Z$ .

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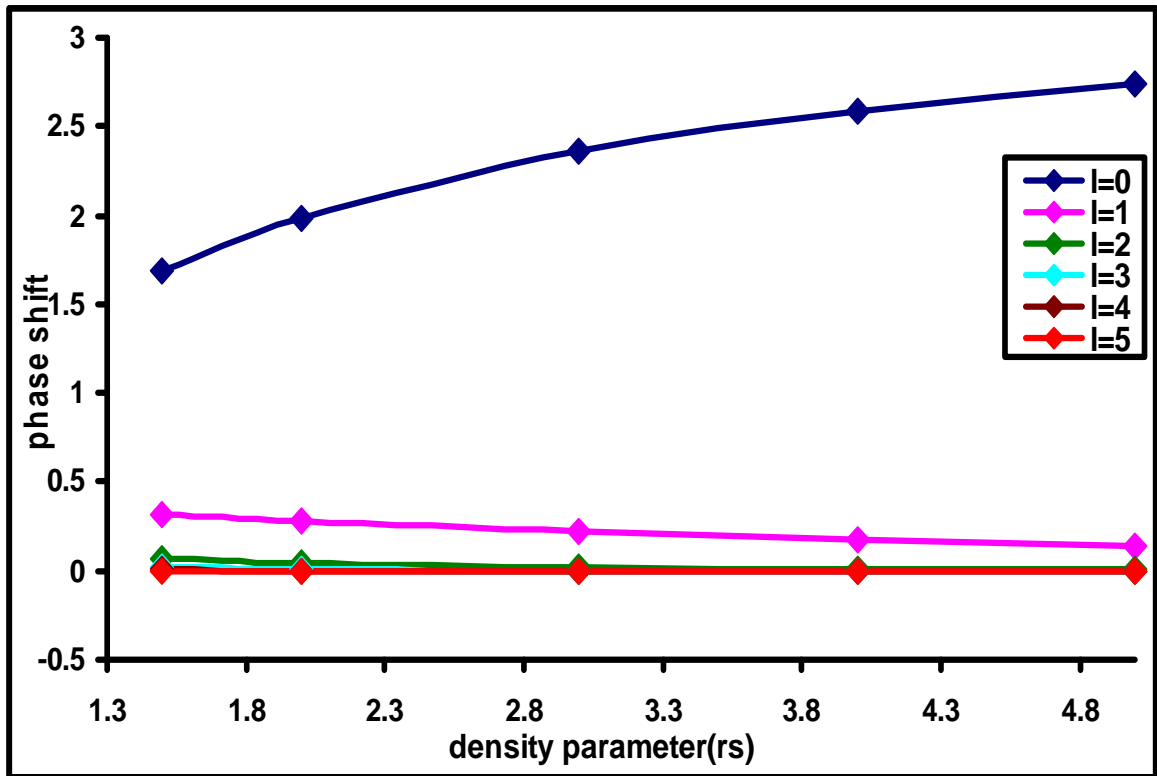
*Fig.( 1-a) Phase shift at Fermi for projectile of atomic number ( $Z_1 = Z$ ) which is calculated from the extended Friedel Sum Rule for atoms embedded in an electron gas with density parameter ( $r_s = 1.0, 2, 3, 4, 5$ ).*

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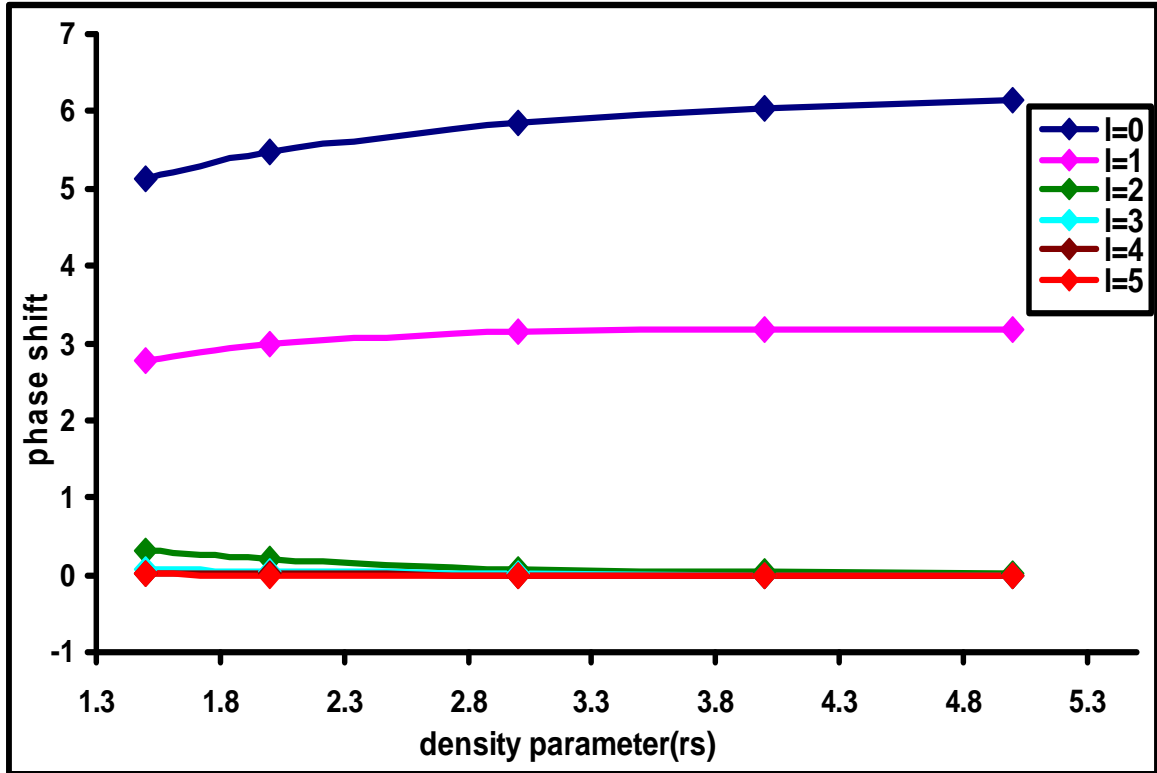


*Fig.( 1-b) Phase shift at Fermi for projectile of atomic number ( $Z = 1$ ) which is calculated from the extended Friedel Sum Rule for atoms embedded in an electron gas with density parameter ( $r_s = 1.5, 2, 3, 4, 5$ ).*

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*Fig.( 1-a) Phase shift at Fermi for projectile of atomic number ( $Z_p = 1$ ) which is calculated from the extended Friedel Sum Rule for atoms embedded in an electron gas with angular momentum ( $l = 0, 1, 2, 3, 4, 5$ ).*



*Fig.( γ-b) Phase shift at Fermi for projectile of atomic number ( $Z = 10$ ) which is calculated from the extended Friedel Sum Rule for atoms embedded in an electron gas with angular momentum ( $l = 0, 1, 2, 3, 4, 5$ ).*

**ξ. Transport cross section**

An improvement over the linear – theory results can be achieved including the effect of the Pauli principle by restricting electron states to those outside the occupied Fermi sphere only in the last transition.

One find, at beam velocities small compared to the Fermi speed,  $v \ll v_f$ , the stopping cross section per target electron reduces to [°]:



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$$-\frac{dE}{dx} = n v v_f \sigma_{tr}(v_f) \quad (5)$$

where  $n$  is the electron density given by

$$n = \frac{3}{4\pi r_s^3} \quad (6)$$

Where  $r_s$  is the density parameter and  $\sigma_{tr}$  is the transport cross section which is defined by :-

$$\sigma_{tr} = \frac{4\pi}{k_f^2} \sum_{l=0}^{\infty} (l+1) \sin^2(\delta_l - \delta_{l+1}) \quad (7)$$

Where  $k_f$  is the Fermi wavevector,  $\delta_l$  is the phase shifts of the  $l$ th partial wave for scattering of electrons at the Fermi surface from the screened potential of the proton.

By substituting eqs.(6, 7) into eq.(5), with atomic units ( $e = m = \hbar$ ,  $v_f = k_f$ ) one can get the stopping power by using quantum mechanical [7]

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$$-\frac{1}{v} \frac{dE}{dx} = \frac{3}{k_f r_s^3} \sum_{l=0}^{\infty} (l+1) \sin^2 [\delta_l(k, v) - \delta_{l+1}(k, v)]$$

(٧)

$$\sin^2(\delta_l - \delta_{l+1}) = \frac{K^2/4}{(l+1)^2 + K^2/4}$$

(٨)

$$K = \frac{2Z_1 v_0}{v}$$

is the Bohr parameter

(٩)

$$v_0 = \frac{e^2}{h}$$

is the Bohr velocity

(١٠)

the stopping power of incident charged particles from using the classical mechanical is obtained by substituting eqs.(٨) and (٩) into eq.(٧) we get

$$-\frac{1}{v} \frac{dE}{dx} = \frac{3}{k_f r_s^3} \sum_{l=0}^{\infty} (l+1) \frac{(Z_1 v_0/v)^2}{(l+1)^2 + (Z_1 v_0/v)^2}$$

(١١)

$$-\frac{1}{v} \frac{dE}{dx} = \frac{3}{k_f r_s^3} (Z_1 v_0/v)^2 \sum_{l=0}^{\infty} \frac{(l+1)}{(l+1)^2 + (Z_1 v_0/v)^2}$$

(١٢)

And by using the effective charge  $Z_1'$ , eq.(١٢) becomes

$$-\frac{1}{v} \frac{dE}{dx} = \frac{3}{k_f r_s^3} (Z_1' v_0/v)^2 \sum_{l=0}^{\infty} \frac{(l+1)}{(l+1)^2 + (Z_1' v_0/v)^2}$$

(١٣)

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$$Z_1^* = Z_1 \left( 1 - e^{-0.92/z_1^{2/3} v_0} \right)$$

(14)

For a more quantitative picture, we need a more reliable potential function. To this end, we have studied two trial functions containing an adjustable parameter which has been chosen to satisfy the Friedel Sum Rule[4].

In addition to the Yukawa potential with a free screening parameter  $\alpha$  we also studied the potential of a hydrogen – like atom[4],

$$V(r) = -Z_1 e^2 \left( \frac{1}{2\alpha} + \frac{1}{r} \right) e^{-r/\alpha}$$

(15)

Phase shifts are calculated here from the semi classical expression(1). After the values of  $\alpha$  were determined by adjustment according to eq. (1), the transport cross section was calculated from eq.(6).

Figure (7) shows the values of  $\left( \frac{1}{v} \frac{dE}{dx} \right)$  that were calculated from eq.(7) by using the extended Friedel Sum Rule in atomic units as a function of density parameter  $r_s$  with different incident ions of charge ( $Z_1 = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$ ). From this figure, the decrease of density parameter causes a strong increase in stopping power and a filling of the minima. Evidently, the increase of ionic radius, also, makes important slowing processes other than conduction- electron damping. The prominent feature of the curves is the oscillation as a function of  $Z_1$ . The origin of these is the filling of a resonance peak in the conduction

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band. The strong  $Z_1$  oscillations in stopping powers is due to variation in ion effective charge.

Figure (ξ) shows the comparison of stopping power ( $\frac{1}{v} dE/dx$ ) which are calculated from nonlinear phase shift by quantum mechanics eq.(Υ) to the results obtained by classical mechanics and using the effective charge instead of the atomic number eq.(Ψ) a function of density parameter  $r_s$  in an electron gas at low velocities for (a) proton  $Z_1 = 1$  and (b) helium  $Z_1 = 2$ . There is an improvement in the results by entering the phase shifts and effective charges. As  $r_s$  increase, the energy loss for proton and helium decrease more rapidly due to the fact that bound states of atomic character develop, thereby tending to screen out interaction with the electron gas. The energy loss of a helium nucleus at large  $r_s$  is smaller than that of a proton at the same velocity. This is qualitatively from any linear theory in which the energy loss scales as the square of the ionic charge can be easily understood in terms of the atomic character of the scattering process in a very dilute electron gas.

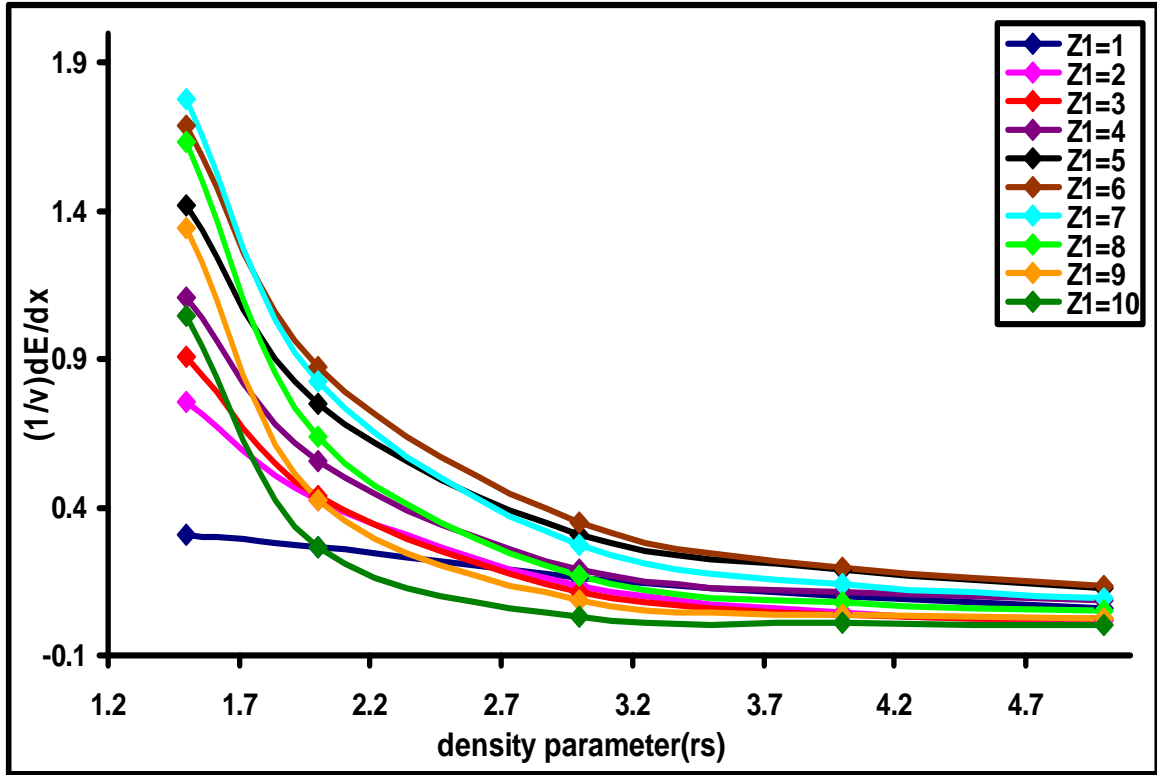
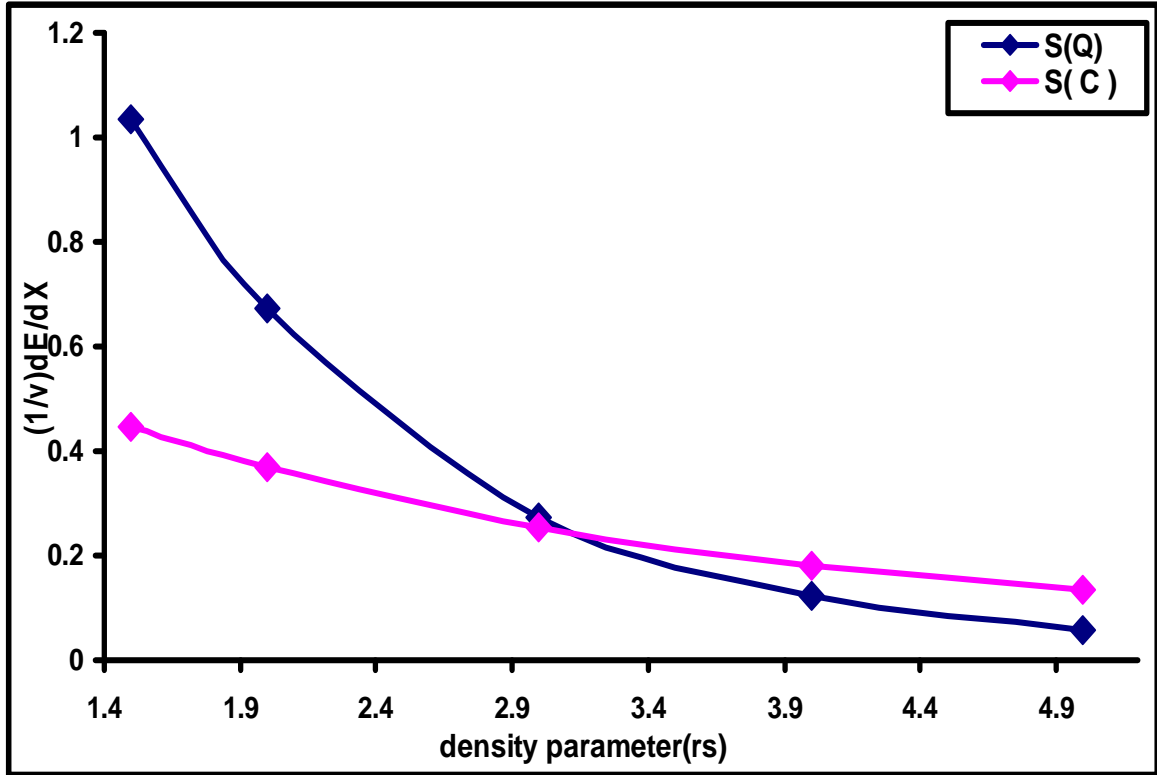


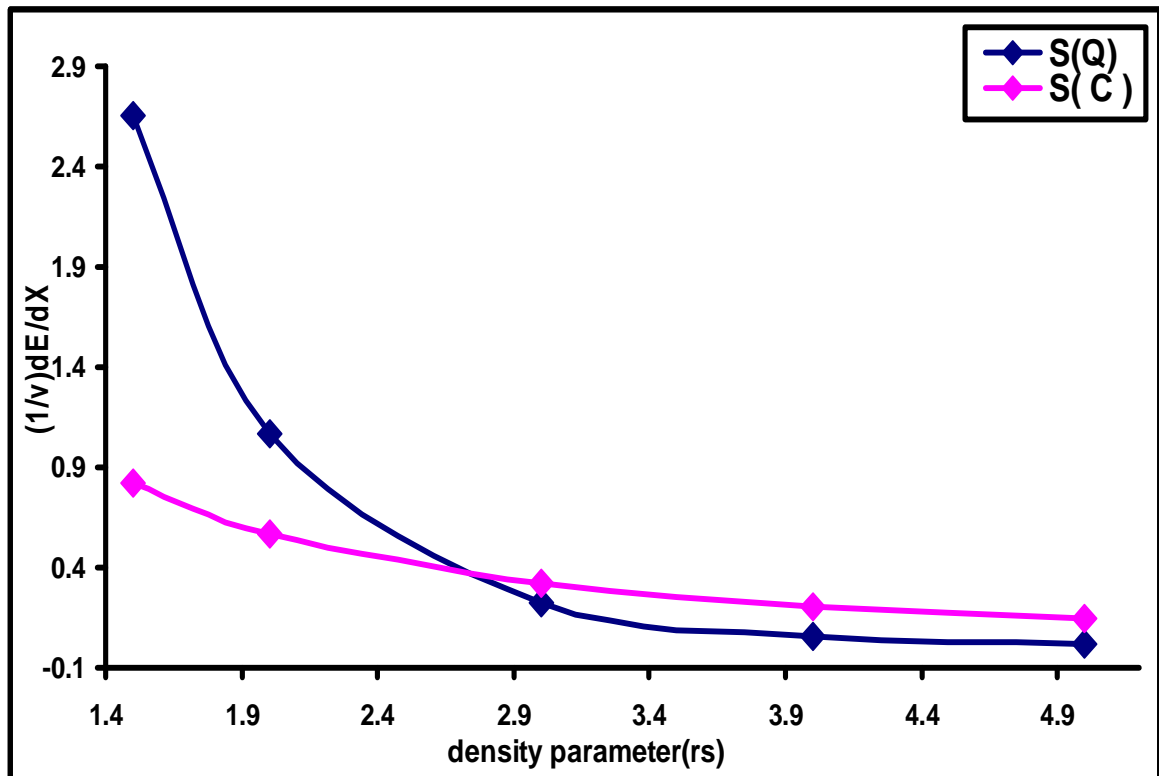
Fig.(۳) Stopping power at Fermi level for atoms embedded in an electron gas with projectile charge ( $Z_1 = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10$ ).

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*Fig.( 4-a) Comparison of the stopping power for proton with atomic number ( $Z_1=1$ ) which is calculated from the phase shift by using the classical and quantum mechanics at ( $v \ll v_f$ ).*

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*Fig.( 4-b) Comparison of the stopping power for helium with atomic number ( $Z=2$ ) which is calculated from the phase shift by using the classical and quantum mechanics at ( $v \ll v_f$ ).*

### *2. Conclusions*

The Extended Friedel Sum Rule (EFSR) model was used to represent the contribution to the stopping power due to valence electrons, which is usually the main contribution for low and intermediate energies. In that approach, the additional contribution from inner shells was incorporated using the harmonic oscillator model, including up to second – order terms in the perturbative expansion. The approach in this case hinges in two different models: the non – linear EFSR method and the second – order oscillator model. The Extended Friedel Sum Rule – Transport Cross

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Section (EFSR – TCS) method provides a closed approach to the study of non – linear effects in a wide range of velocities.

At low projectile speed one may expect a fundamental difference between excitation of free and bound electrons. Indeed, it is well known the excitation of bound electrons by slow heavy ions is influenced by electron promotion, a process very different from Coulomb excitation. This is not the case for a free – electron gas: While the plasma frequency takes the place of the binding frequency in the interaction with high – speed projectile, it loses relevance at low speed, where the Fermi speed becomes the important parameter.

The stopping cross section  $S$  which is calculated from eq.(V) is proportional inversely with the density parameter  $r_e$ . When  $r_e$  increases, the stopping cross section decrease because of the low density of electrons according to eq.( $\rho$ ) and there is an oscillation in stopping power due to atomic number  $Z_1$  but experimentally, the stopping power values tend to increase more rapidly as  $Z_1$  increase. The increase can be due to several effects. The ionic radius increases with  $Z_1$  and therefore heavier channeling ions see a larger effective electron density than the lighter ones. The density parameter  $r_e$  has an evident influence on the phase shift according to the value of the angular momentum  $l$  which also affects inversely on the phase shift and therefore any increase of it led to a strong decrease in phase shifts because of the low density of electrons. Both transport cross section and phase shift depend on the ion velocity because of the optimization of the screening potential.

We used the phase shift from angular momentum  $l = 0$  until  $l \leq 5$  because phase shifts for  $l > 5$  are very small.



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At  $r_s$  decreases toward values much less than  $\lambda$ , our results tend toward agreement with linear theory, that is, all stopping powers tend to be proportional to  $Z_1^2$ . This is easily visualized when one considers that for large electron – gas densities the screening of the ion is so strong that bound states can not exist; thus the electron are scattered essentially by an exponentially screened potential with screening length approaching zero as  $r_s$  goes to zero. At low velocities, we take into account the effective charge because the slowing of charged particles through the medium causes a change in its charge due to the loss or capture electrons from the medium.

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