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Energy loss straggling for slow ions in an electron gas

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الخلاصة:-

إن تطوح الطاقة للايونات بسرعة اقل من سرعة فيرمي $(v \ll v_f)$ باستخدام نموذج الغاز الالكتروني قد تم ايجادة من فرق الطور الذي يمكن أن يحسب من دالة الكثافة اللاخطية. النتائج قد وضحت إن هناك تذبذبات في مقدار تطوح الطاقة بازدياد الشحنة النووية والذي قد صحح باستخدام خواص الاستطارة للإلكترون عند مستوي فيرمي. إن التصرف الخطي بالنسبة للطاقة المفقودة للجسيم مع سرعته تم الحصول علية إما باستخدام نموذج الغاز الالكتروني ودالة الكثافة اللاخطية أو صيغة العزل الخطية.

Abstract:-

Energy – loss straggling of ions with velocity small than Fermi velocity $v \ll v_f$ in an electron gas has been evaluated from phase shifts which are determined from nonlinear, density – functional calculations. The results show oscillations in straggling with increasing nuclear charge are correlated with the scattering properties of electrons at Fermi level. The linear behavior of the energy loss with the ion velocity is obtained under the free electron gas (FEG) in the frame of nonlinear density functional theory (DFT) or linear dielectric formalism.

١. Introduction:-

Due to the statistical nature of atomic collisions, the energy loss of originally monoenergetic particles while passing through matter fluctuates around an average energy loss($\overline{-\Delta E}$). This is known as energy loss straggling[١].

Energy straggling results from the statistical nature of the energy – loss processes a particle experiences as it penetrates matter. If $f(E)$ denotes the energy distribution function at some depth of an initially monoenergetic beam, then energy straggling Ω is defined as the standard deviation of $f(E)$ with respect to the average[٢]. This distribution function, in general, is rather complicated and nonsymmetrical with respect to the mean[٣]. However, $f(E)$ has been measured for thin targets and in this case found to be approximately a Gaussian function of energy[٤]. The backscattering spectrometry has been remarkably successful as a microanalytical tool for sensing mass, resolving depth, and perceiving monocrystalline structure in solids[٥]. Energy straggling of the incident beam as it penetrates the target limits the ultimate ability to resolve depth. To estimate these limits, the magnitude of the energy straggling must be known. Energy straggling depends on target material, beam energy , and incident particle.

The characterization of the distribution of energy losses suffered by energetic charged particles in their interaction with matter requires in the simplest case, two quantities the stopping power and the energy – loss straggling parameter. Knowledge of these quantities is relevant in depth the profiling and surface analytical techniques as well as in fusion and astrophysical studies. The straggling parameter is expressed in terms of scattering of electrons at the Fermi energy by a self – consistent, effective potential evaluated within the density – functional formalism[٦].

٢. *Energy loss straggling in an electron gas:-*

At low projectile velocities, calculation using the electron gas model can be used to describe the energy loss straggling[١].

The energy – straggling of a projectile traversing a pathlengh Δx in an electron gas of density n is defined by[٧]

$$\Omega^2 = \langle(\Delta E - \langle\Delta E\rangle)^2\rangle = n\Delta x W \qquad (١)$$

Where W ,the straggling parameter, is given by

$$W = \int d\sigma\, T^2 \qquad (٢)$$

$$= \int d\sigma\, (1 - \cos\theta)^2 \qquad (٣)$$

$d\sigma$ is the differential scattering cross section obtained also from the phase shifts $\delta_l(n)$ for energy loss T in the interval T to dT. For a projectile moving with speed v small compared with the magnitude of the Fermi velocity v_f with the Pauli exclusion principle taken into account, the energy loss straggling is given by[٨]

$$\Omega^2 = 3nv^2 v_f^2 \Delta x \int d\sigma_0(n,\theta) sin^3(\theta/2) \qquad (٤)$$

Where σ_0 is the scattering cross section and θ the scattering angle in the centre – of – mass system. For $v \ll v_f$, the interaction of an ion with an electron gas occurs via scattering of electrons near the Fermi surface[٩].

By using the equivalence $(1-\cos\theta) = 2sin^2(\theta/2)$, eq.(٣) may be written as

$$W = \int d\sigma\,\left(2sin^2(\theta/2)\right)^2 \quad (٥)$$

$$W = \int_0^{\pi}\left(2sin^2(\theta/2)\right)^2 \sigma_s(\theta, v_f) 2\pi \sin\theta\, d\theta\,. \quad (٦)$$

$$\sigma_s(\theta, v_f) = \frac{Z_1 e^4}{4m^2 v_f^2} \frac{1}{\left[sin^2\frac{\theta}{2} + \left(\frac{\lambda^2}{2a}\right)^2\right]^2} \quad (٧)$$

Where σ_s is the scattering cross section, a is the atomic radius, and $\lambda = \frac{\hbar}{m v_f}$ is the Fermi wave length[١٠]. By substituting eq.(٧) into eq.(٦) , we can get on the equation

$$W = 2\pi \int_0^{\pi}\left(2sin^2(\theta/2)\right)^2 \sin\theta\, d\theta \frac{Z_1 e^4}{4m^2 v_f^2} \frac{1}{\left[sin^2\frac{\theta}{2} + \left(\frac{\lambda^2}{2a}\right)^2\right]^2} \quad (٨)$$

By using the quantum formalism and depended on the spherical symmetric potential and Legendre polynomials, the straggling parameter for scattering of electrons by the screened potential of the ion may be expressed in terms of phase shifts δ and leads to[٦]

$$W = \frac{3\pi^2}{4\sqrt{2}} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} (2l+1)(2m+1)\{1 - cos(2\delta_l) - cos(2\delta_m) + cos[2(\delta_l - \delta_m)]\} J_{lm}$$

(٩)

Where $\delta_l \equiv \delta_l(E_F)$ are the phase shifts for scattering of electrons at the Fermi energy. The quantity J_{lm} is defined by

$$J_{lm} = \int_{-1}^{1} d\mu (1-\mu)^{3/2} P_l(\mu) P_m(\mu) \quad (١٠)$$

Where the $P_l's$ are Legendre polynomials. This integral can be expressed as a generalized hypergeometric series which reduced to[٦]

$$J_{lm}=\frac{2^{5/2}\Gamma\left(\frac{5}{2}\right)\Gamma\left(m-\frac{3}{2}\right)}{\Gamma\left(-\frac{3}{2}\right)\Gamma\left(m-\frac{7}{2}\right)}*\sum_{k=0}^{l}\frac{(-1)_k(l+1)_k\left[\left(\frac{5}{2}\right)_k\right]^2}{\left(\frac{7}{2}+m\right)_k\left(\frac{5}{2}-m\right)_k(k!)^2} \qquad (١١)$$

By using the quantum formalism and depended on the spherical symmetric potential, eq.(٩) are written as[١١]

$$W=\frac{4\pi}{k_f^2}\sum_{l=0}(l+1)\left[2\sin^2(\delta_{l+1}-\delta_l)-\frac{l+2}{2l+3}\sin^2(\delta_{l+2}-\delta_l)\right] \qquad (١٢)$$

$$\frac{d\Omega^2}{dx}=nZ_2m^2v^2v_f^2W \qquad (١٣)$$

k_f is the Fermi wave vector and the results will be presented in atomic units(a.u.) which (e=m=ħ=١) and ($v_f=k_f$)

By substituting eq.(١٢) into eq.(١٣), we get

$$\frac{1}{v^2}\frac{d\Omega^2}{dx}=4\pi\, n\, Z_2\sum_{l=0}(l+1)\left[2\sin^2(\delta_{l+1}-\delta_l)-\frac{l+2}{2l+3}\sin^2(\delta_{l+2}-\delta_l)\right] \qquad (١٤)$$

Phase shifts for scattering of an electrons at the Fermi energy from the spherically symmetric, self – consistent potential of a static ion have been evaluated by Puska and Nieminen using nonlinear, density – functional calculations. For comparison we show the predictions of linear theory in the random – phase approximation and using the dielectric function (RPA)[١١,١٢]

$$W=6\pi Z_1^2\left(v/v_f\right)^2C_2(\chi) \qquad (١٥)$$

Where

$$C_2(\chi)=\int_0^1\frac{dZ_1Z_1^4}{\left(Z_1^2+\chi^2f_1\right)^2} \qquad (١٦)$$

$$f_1\equiv\frac{1}{2}+\frac{1}{4Z_1}\left(1-Z_1^2\right)\ln\left[\frac{1+Z_1}{1-Z_1}\right] \qquad (١٧)$$

Where Z_1 is the atomic number of projectile. By integration the eq.(١٦) we get on the following equation

$$C_2(\chi) = 1 - 2\chi^2 \left[\ln\frac{1+\chi^2}{\chi^2} + \frac{\chi^2}{1+\chi^2}\right] \qquad (١٨)$$

$\chi^2 = 0.166\, r_s$ is the density parameter

$v_f = 1.92/\, r_s$ is the Fermi velocity

Figure (١) shows the results of the energy loss – straggling $\Omega/v\sqrt{\Delta x}$ as a function of density parameter r_s which are calculated from the nonlinear density – functional eq.(١٤) results with the experimental data at low velocity. The straggling are for six materials for (a) proton $Z_1 = 1$ and (b) helium $Z_1 = 2$ and the electron – gas densities corresponding to the materials are determined from effective values of r_s. Comparison of experimental data with the results of calculation for straggling show quite weak agreement for some cases but differ by a factor of ٢ for others. With the exception of Se, for which the straggling fall below the theoretical estimates, and Ge for $Z_1 = 1$, the calculated straggling gives results smaller than the data.

Figure (٢) shows the results of the straggling for (a) proton $Z_1 = 1$ and (b) helium $Z_1 = 2$ which are obtain from the nonlinear theory(phase shift and density function) eq.(١٤) and those calculated from linear (random phase approximation and dielectric function) eq.(١٥) as a function of density parameter r_s in an electron gas at low velocities $v \ll v_f$. The results obtained from the nonlinear decrease with increasing the density parameter but the values calculated from the random phase approximation increase with increasing the density parameter. At large electron – gas densities n screening of the ion is very strong and predictions based on the nonlinear tend toward agreement with those of the linear of the linear theory. This requires values of r_s much smaller than in the figure and the straggling for a helium nucleus becomes less than that for an equal velocity proton for $r_s \geq 2.8$ because the straggling is proportional inversely with the atomic number Z_1. There is an improvement in the results of linear theory by using the phase shift in the nonlinear theory of calculating the energy loss straggling.

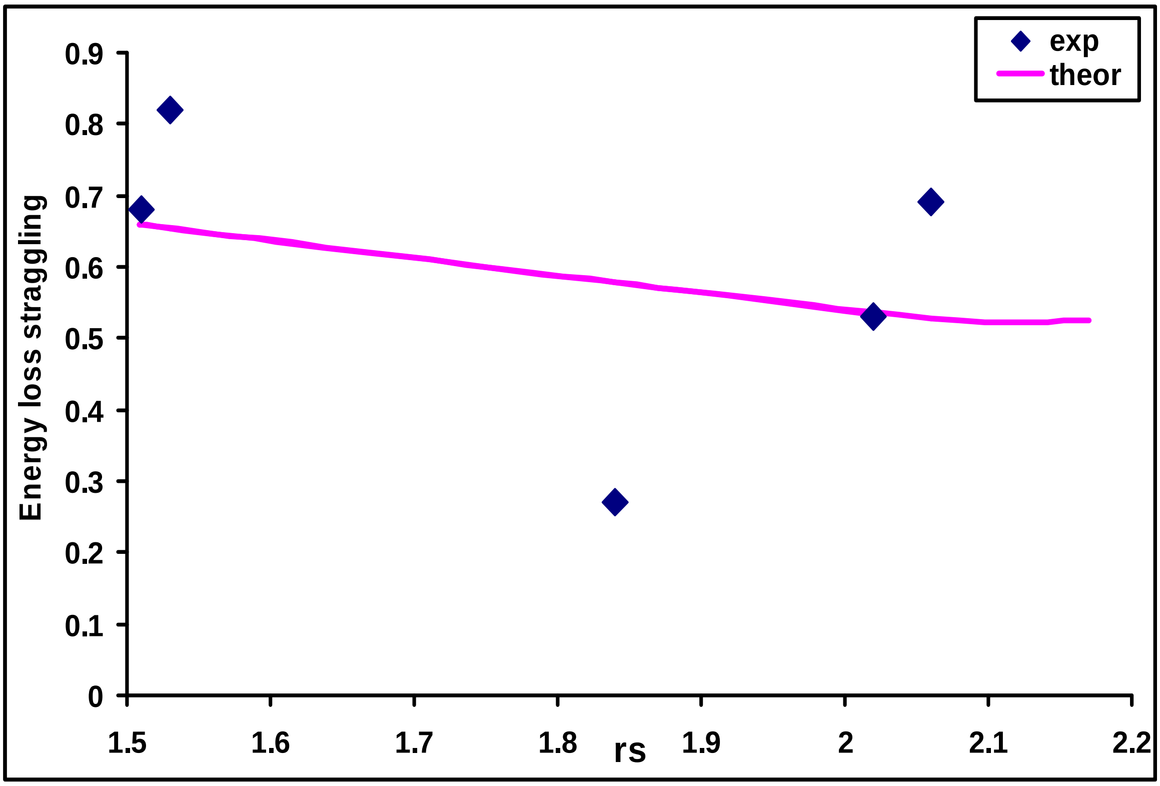
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Fig.(١-a) Energy loss straggling of proton (Z_1=١) which is calculated from density functional with experimental data as a function of density parameter r_s

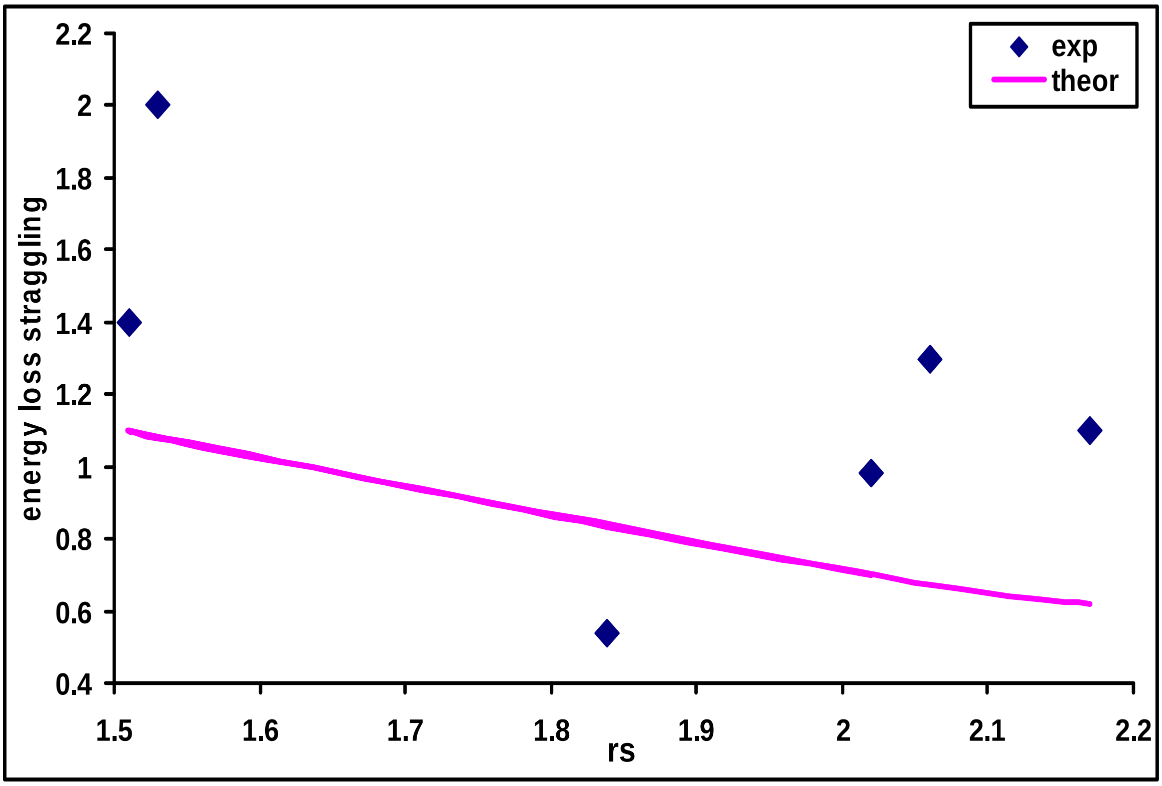

Fig.(١-b) Energy loss straggling of helium(Z١=٢) which is calculated from density functional with experimental data as a function of density parameter rs

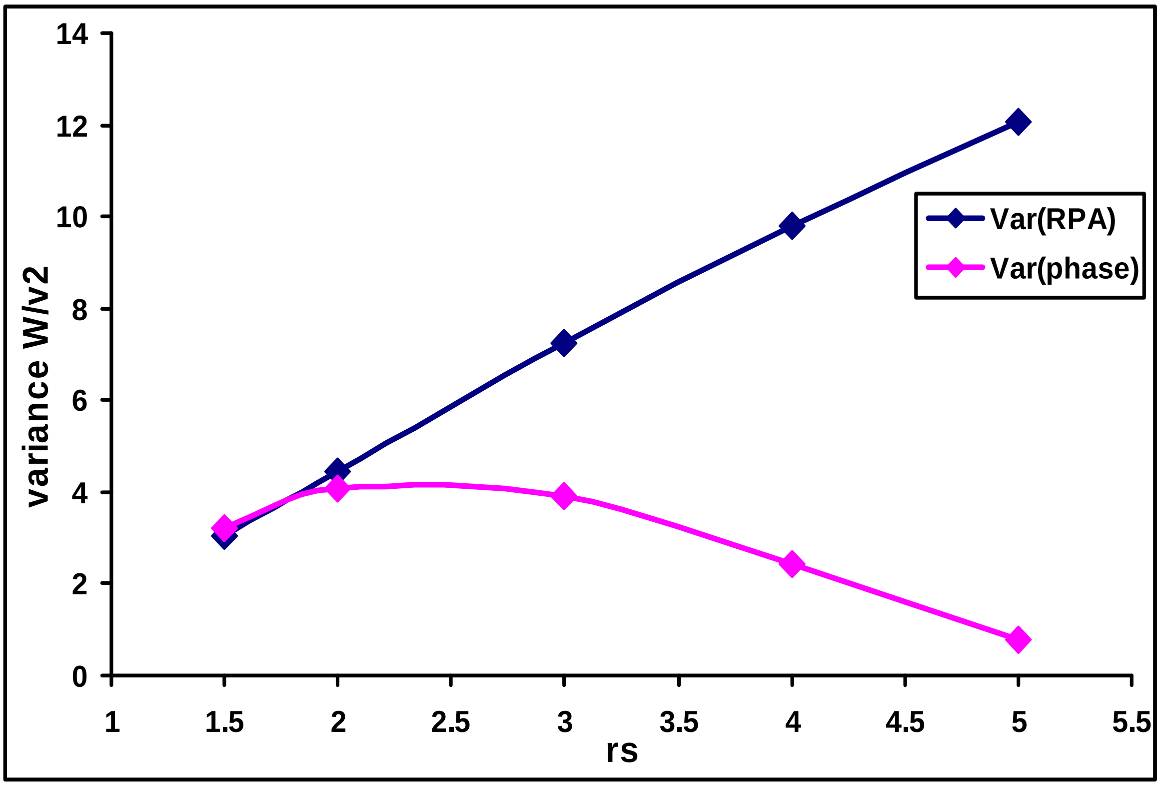

Fig.(٢-a) Comparison of variance of proton Z_1=١ which is calculated using nonlinear – phase shift theory to the linear RPA at low velocity $v \ll v_f$.

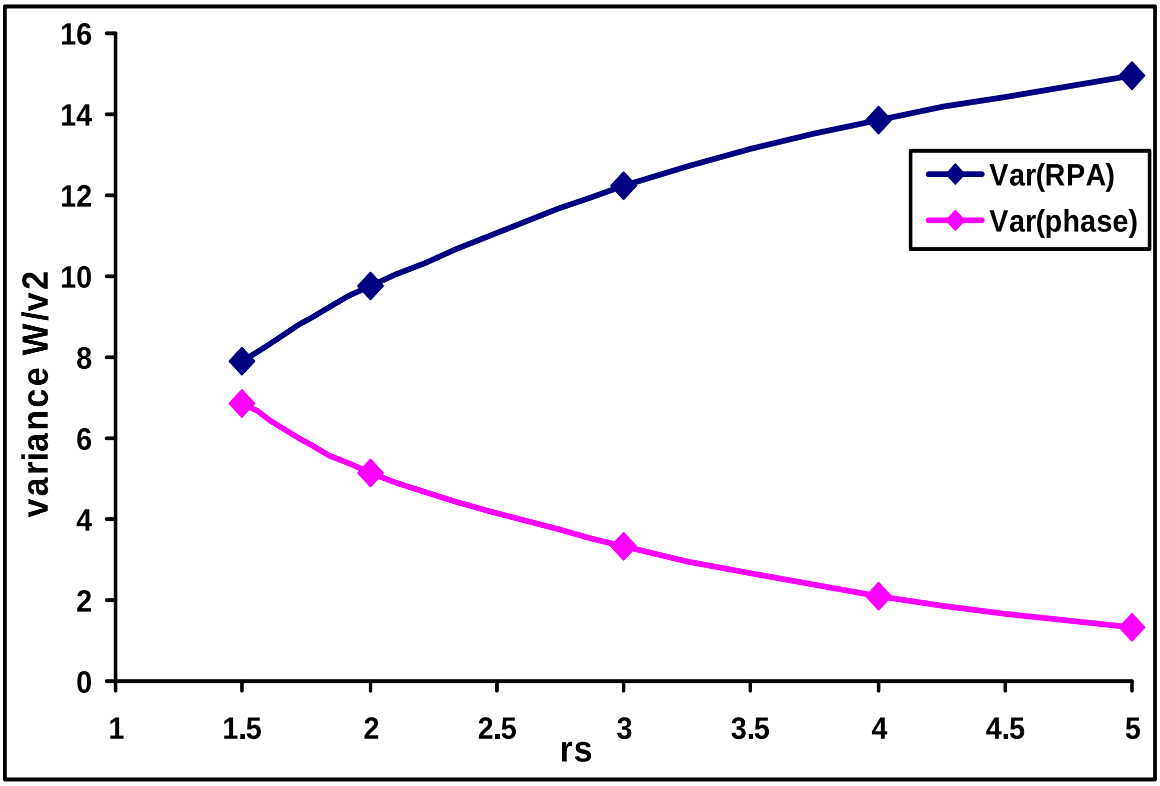

Fig.(٢-a) Comparison of variance of helium Z_1=٢ which is calculated using nonlinear – phase shift theory to the linear RPA at low velocity $v \ll v_f$.

٣.Conclusions:-

Energy loss straggling accounts for the fact electronic energy loss process is stochastic, two ions going through the same amount of matter not necessarily exciting the same levels or number of electrons and thus not loosing the same amount of energy. Except at high energy, the probability of exciting an electron depends strongly on their speed.

Straggling is a complex topic and has been much less studied than the energy loss. One reason is that straggling is not the only reason for observed broadening of an energy loss profile: non – uniform layer thickness and target in homogeneities may compete and sometimes become dominant, and separating these effects from straggling is by no means trivial.

In principle, all the factors binding, orbital motion (shell correction), Barkas – Andersen effect, projectile screening and excitation and relativity influence the stopping cross section also affect the straggling parameter

Th energy loss straggling has been calculated in density functional theory (DFT) and it is noted that the general improvements are due mainly to the correct phase shift determination. These calculations reflect the importance of screening nonlinearities. The response of the system remains linear to the external probe and this behavior is reflected in the determination of the available states for the density fluctuation near the Fermi level.

The results of the energy – loss straggling exhibit oscillations of them with the incident ion nuclear charge Z_1 and these oscillations are correlated with those in the obtained from stopping power. Z_1 oscillations appear naturally since they are related to the appearance of bound states which are taken into account in a natural way in our self – consistent calculation. A qualitative understanding of the main features of the oscillation can easily be achieved in terms of scattering theory and resonance levels in solids.

As r_s increases, the results of energy loss straggling obtained from nonlinear response theory for both helium and proton decrease more rapidly than predicted by linear theory due to the fact that bound states of atomic character develop, thereby tending to screen out interactions with the electron gas. Predictions for straggling from linear theory using the random – phase approximation(RPA) increase with density parameter r_s and the increase of density parameter $r_s$causes a strong increase in straggling and this is mathematically clear from eq.(١٥).

In the high density limit, $r_s \ll 1$, the results obtained from linear theory by using phase shift converge to those of the random phase approximation (RPA). The convergence of the results to those of the (both at high velocities and at high densities) provides a stringent test of the model. 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 electrons are scattered essentially by an exponentially screened potential with screening length approaching zero as r_s goes to zero.

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