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DEPARTMENT OF PHYSICS
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NORFOLK, VIRGINIA

TECHNICAL REPORT NO. PTR-83-5

A STUDY OF PHYSICAL PROCESSES FOR SPACE RADIATION PROTECTION

By

G.S. Khandelwal

and

Y.J. Xu

Progress Report
For the period ending December 1983

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

Under
Research Grant NCCI-42
Dr. Lawrence W. Townsend, Technical Monitor
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Submitted by the
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Norfolk, Virginia 23508

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A STUDY OF PHYSICAL PROCESSES FOR SPACE RADIATION PROTECTION

By

G.S. Khandelwal[1] and Y.J. Xu[2]

The performance on the above project, during this period, can best be described by the following three items (two research papers and one dissertation), which are described in detail in the papers attached with this report.

1. Intermediate Energy Proton Stopping Power for Hydrogen Molecules and Monoatomic Helium Gas, Physics Lett. A (in press).

2. Low-energy proton stopping power of N_2, O_2, and water vapor (Revised for publication in the Physical Review.)

3. A theoretical model for calculating molecular stopping power, Y.J. Xu's dissertation, to be submitted to the faculty in partial fulfillment of the requirement of the Ph.D. degree in Applied Physics.

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Intermediate Energy Proton Stopping Power for Hydrogen Molecules and Monoatomic Helium Gas

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ABSTRACT

Stopping power in the intermediate energy region (100 keV to 1 MeV) has been investigated, based on the work of Lindhard and Winther, and on the local plasma model. The theory is applied to calculate stopping power of hydrogen molecules and helium gas for protons of energy ranging from 100 keV to 2.5 MeV. Agreement with the experimental data is found to be within 10 percent.

Recent investigations suggest the usefulness of the local plasma model of Lindhard and Scharff [1] in calculating the mean excitation energies [2-5] of various systems. As is known, such calculations of mean excitation energy help in readily obtaining stopping power for high energy incident particles. On the other hand, the so called intermediate energy region (100 keV to 1 MeV in the context of this paper) is of considerable interest. Unfortunately, the theoretical calculations in this energy region are hindered, primarily due to the complexity of the problem. Bonderup's [6] theoretical calculations of stopping power for some elements, however, seem to be in good agreement with experimental results for incident proton energy above 500 keV.

In this letter, we present calculations of stopping power based on the work of Lindhard and Winther [7], and on the local plasma model of Lindhard and Scharff. The theory is expected to cover the intermediate energy region while retaining its applicability for the high energy case. The method should be easily applicable for calculating stopping power of different materials composed of molecules such as H_2 and N_2 gases, water vapor, and many other chemical systems of interest. The method first establishes a stopping number function L, based on Lindhard and Winther's formulas. Next, the Gordon-Kim model [8] for density function of a H_2 molecule is used to calculate its stopping power in the energy region from 100 keV to 2.5 MeV. Calculations are also performed for the monoatomic Helium gas.

The celebrated stopping power formula for an energetic charged particle of charge ze and velocity v, traversing matter of charge number Z is given by:

$$- \frac{dE}{dx} = \frac{4\pi z^2 e^4}{mv^2} NZL \qquad (1)$$

where m is the mass of an electron, and N is the number of atoms per unit volume of the medium.

The stopping number L of Eq. (1) has been a topic of considerable study. Most interest, however, has usually been centered on the high energy case for which L attains a simple formula, $L = \ln \frac{2mv^2}{I}$. In this situation, only one parameter I, the mean excitation energy of the medium, determines the stopping power. Lindhard and Winther have investigated the function L for a free electron gas in the regions of low and high energy incident charged particles. These authors [6, 7] give for the high energy case, the expression for L to order $\frac{1}{v^2}$ as:

$$L = \ln Y - \frac{\langle T \rangle}{\frac{1}{2} mv^2} \qquad (2)$$

where, $Y = \frac{2mv^2}{h\omega_p}$, the classical plasma frequency $\omega_p{}^2 = \frac{4\pi\rho e^2}{m}$, ρ the electron density, and < T >, the average kinetic energy is given by

$$\langle T \rangle = (\frac{3}{10})\ mv_F{}^2,$$

where v_F is the Fermi velocity.

For the low energy case, they give:

$$L = (\frac{\chi^2}{3})^{3/4}\ Y^{3/2}\ C_1(\chi) \qquad (3)$$

where,

$$C_1\ (\chi) \quad \frac{1}{2\ (1 - \frac{\chi^2}{3})^2} \left(\log \frac{1 + \frac{2}{3}\chi^2}{\chi^2} - \frac{1 - \frac{1}{3}\chi^2}{1 + \frac{2}{3}\chi^2} \right)$$

with

$$\chi^2 = \frac{e^2}{\pi h v_F}$$

The calculational procedure in this paper proceeds with the exploitation of Eqs. (2) and (3) with the following modifications in mind. First, as shown in a previous reference in context with the calculations of mean excitation energy, due to the Pine correction, one should replace ω_p by $\gamma\omega_p$ in the equations for L function where, γ is given by [2, 9]

$$\gamma = 1 + \frac{3}{2}\frac{\beta^2}{\lambda_s}\left(1 + \frac{3}{10}\beta^2\right) \tag{4}$$

where $\lambda_s = \frac{\gamma_s}{a_0}$ is the average distance between electrons in units of Bohr radius. The parameter β is determined by solving the following equation

$$0.076\ \beta^2 + \frac{2.598}{\lambda_s^{1/2}} - 0.916 = 0$$

The equation (2) for the L function warrants some discussion. First, one notes that the L function of Eqs. (2) and (3) are derived by Lindhard and Winther for a free electron system. Transition to an atomic system of the first term of Eq. (2), as studied widely, is accomplished under the so called local plasma model in which density $\rho(\vec{r})$ is evaluated by using Quantum mechanical wave functions. Such a Quantum mechanical analogue of the second term of Eq. (2) would be of interest. In this context, a result first derived by Brown [10] would prove to be useful. Brown studied the K-shell asymptotic stopping power of an Hydrogenic system (with 2 K-electrons) for a fast projectile, taking the maximum momentum transfer to a free electron appropriately equal to 2mv. He obtained for the second term in Eq. (2) for an Hydrogenic system, the quantity

$$\frac{1}{2}\ \frac{\langle T \rangle}{\frac{1}{2}mv^2}.$$

Thus, in order to make a transition to an atomic system consistant with the free electron model, we assume Brown's result and accordingly replace Eq. (2) by:

$$L = \ln Y - \frac{3^{1.5}}{10\chi} \frac{1}{Y} \qquad (5)$$

At this stage, we combine the low and high energy L functions to determine the appropriate dependence of stopping power on energy. To do this, we used equations (3), (4) and (5) for our desired results. Bonderup, in his calculations, had combined Eqs. (2) and (3) and assumed a constant value of γ equal to $\sqrt{2}$. Furthermore, we attempt to preserve continuity between $L_1(\underset{\rightarrow}{r}, v)$, the low energy stopping number function given by Eq. (3) and $L_2(\underset{\rightarrow}{r}, v)$, the high energy function given by Eq. (5), in the following way. Extensive numerical evaluations, using a computer program, of the functions L_1 and L_2 for various values of the variable Y, revealed that in most useful cases there were found two roots Y_1 and Y_2 of the equation $L_1 = L_2$ where $Y_1 < Y_2$. Furthermore, the slope M of the function L_2 for values of Y greater than Y_2 was always small. On the other hand, the slope of L_2 for Y values less than Y_1 was very steep. These observations, including the behavior of these functions (see the figure), led us to the following recipe to preserve the continuity consistant with the physics of the situation:

$$\begin{aligned} L &= L_2 && \text{when} \quad MY < L_2 \\ L &= \mathrm{Max}\,[L_1, L_2] && \text{when} \quad MY > L_2 \end{aligned} \qquad (6)$$

where, L_1 and L_2 are given by Eq. (3) and (5) respectively. Eq. (6) can now be used to obtain stopping number values for a system, given the velocity of the projectile and the density $\rho(\underset{\rightarrow}{r})$. For a molecule, Gordon-Kim give the density as:

$$\rho(\underset{\rightarrow}{r}) = \rho_1(\underset{\rightarrow}{r}) + \rho_2(\underset{\rightarrow}{r} - \underset{\rightarrow}{R}_{12}) \qquad (7)$$

where, $\rho_1(\underset{\rightarrow}{r})$ is given by the square of the ground state wave function of the hydrogen atom. R_{12} is the distance between two hydrogen atoms, which is known to be $1.4a_0$. Knowing the density by Eq. (7), stopping power was obtained by integrating Eq. (6) over $\underset{\rightarrow}{r}$, for protons of energy between 100 keV and 2.5 MeV, for both H_2 and monoatomic helium gas. For He atoms, Hartree-Fock wave functions [11] were employed. Table 1 lists the results of this paper, together with Anderson-Ziegler curve fitted results [12], and three sets of experimental data [13, 14, 15]. Good agreement, within 10 percent, is found with the experimental data. Calculations of the equations established by Bonderup were also undertaken by extending them to molecular systems. Table 1 lists these values for the H_2 molecule in the last column. These differ from our results in the low energy region. Table 2 lists the same physical quantities for helium gas [14-18]. The same trend is observed as in the case of the H_2 molecule.

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Summary of the stopping cross sections (in units of ev x 10^{-15} cm^2/molecule) for a Hydrogen molecule for various proton energies

E (Kev)	Theoretical Values of the Present Paper	Curve Fitted Values Anderson and Ziegler [12]	Best Available Experimental Results Reynolds et al.* [14]	 Langley [13]	 Bonderup and Hrelpland [15]	Theoretical Values Calculated from Bonderup's Work [6]
100	11.41	11.6	11.66		11.2	10.23
200	7.52	8.0	7.80		7.64	7.02
300	5.70	5.95	5.82	4.54 (311 kev)		5.39
400	4.63	4.60	4.70			4.41
500	3.93	4.00	3.94	3.82 (518.5 kev)		3.75
600	3.42	3.40	3.40	3.82		3.28
700	3.04	3.00				2.92
800	2.75	2.75		2.73 (778.7 kev)		2.64
900	2.50	2.50				2.41
1037	2.24	2.35		2.14		2.16
1555	1.62	1.64		1.53		1.57
2047	1.30	1.21		1.22		1.24
2591	1.07	1.07		1.04		1.04

*Anderson and Ziegler [12] note that the data in reference [14] appear to be constantly high by amount ranging from 5 percent to 10 percent.

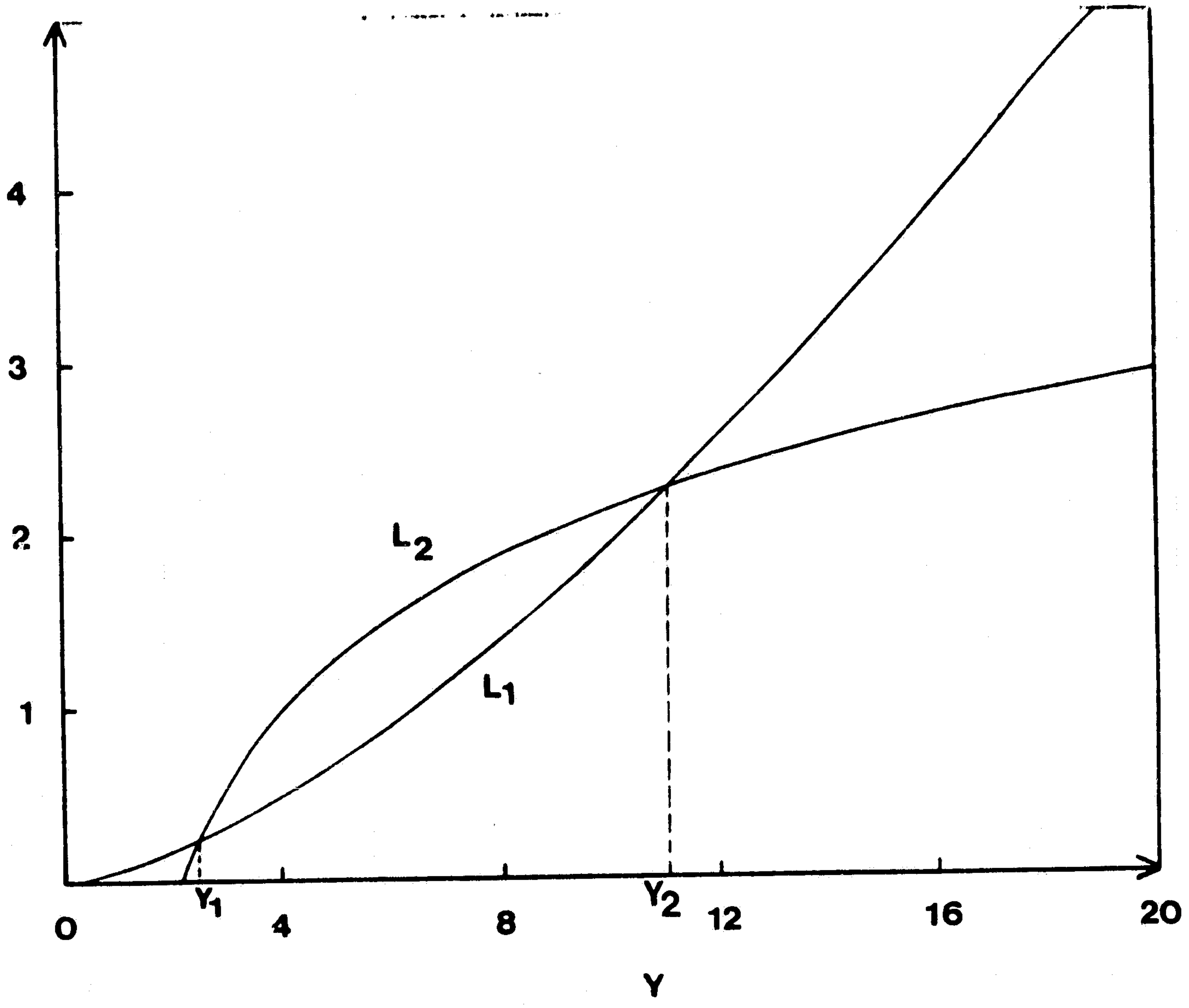
Summary of the stopping cross sections · (in units of ev x 10^{-15} cm^2/atom) for a Helium atom for various proton energies

E (Kev)	Theoretical Values of the Present Paper	Curve Fitted Values Anderson and Ziegler [12]	Best Available Experimental Results					Theoretical Values Calculated from Bonderup's work [6]
			Reynolds et al.* [14]	Park and Zimmerman [16]	Bonderup and Hrelpland [15]	Phillips [17]	Brolley and Ribe [5]	
80	6.83		7.37	7.15		6.6		
100	6.52	7.16	7.30	7.05	7.02			5.45
200	5.16	5.64	5.55	5.64	5.60			4.49
300	4.19	4.39	4.41					3.78
400	3.53	3.60	3.69					3.25
500	3.07	3.07	3.18					2.85
600	2.71	2.69	2.81					2.54
700	2.44	2.41						2.29
800	2.22	2.19						2.09
900	2.04	2.00						1.92
1000	1.89	1.92						1.79
2000	1.12	1.14						1.07
4400	0.595	0.600					0.585	0.576

*Anderson and Ziegler [12] note that the data in reference [14] appear to be constantly high by amount ranging from 5 percent to 10 percent.

FIGURE CAPTION

The low and high energy stopping number functions as functions of the variable Y. A typical value equal to 0.1 of the quantity χ^2 was chosen.


4
3
2
1
L2
L1
Y1
Y2
0
4
8
12
16
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Low-energy proton stopping power of N_2, O_2, and water vapor, and deviations from Bragg's rule

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ABSTRACT

A modified local plasma model, based on the works of Lindhard and Winther; Bethe, Brown, and Walske, is established. The Gordon-Kim model for molecular electron density is used to calculate stopping power of N_2, O_2, and water vapor for protons of energy ranging from 40 keV to 2.5 MeV, resulting in good agreement with experimental data. Deviations from Bragg's rule are evaluated and are discussed under the present theoretical model.

Recently, departures from Bragg's rule have been noticed in the theoretical calculations of the mean excitation energies of various molecular systems.[1,2] Analysis of the experimental data on energy loss of low energy α particles in gases also indicates deviations from Bragg's rule.[3-5] In this paper, the stopping power theory of Lindhard and Winther,[6] and the local plasma theory of Lindhard and Scharff,[7] are used to perform calculations in the low energy region. Modifications are introduced through a simplifying model which incorporates the effects of the shell corrections and of the screening of the projectile. The model is justified on the basis of fulfilling the more ambitious aim of obtaining the molecular stopping power. The Gordon-Kim[8] electron density model of molecular wave functions is utilized in the calculations. Such a model, as is known, allows a successful method of calculating chemical bond effects. Calculations done on N_2, O_2 and water vapor are found to be in fair agreement with experiments. Furthermore, departures from the Bragg's rule are noticed for all these systems.

The celebrated stopping power formula for an energetic charged particle of charge ze and velocity v, traversing matter of charge number Z is given by

$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4}{mv^2} NZL , \qquad (1)$$

where m is the mass of an electron, and N is the number of atoms per unit volume of the medium.

The stopping number L of Eq. (1) has been a topic of considerable study. For instance, Lindhard and Winther have investigated the function L for a free electron gas in the regions of low and high energy incident charged particles. These authors give for the high energy case, the expression for L to order $\frac{1}{v^2}$ as

$$L = \ln Y - \frac{\langle T \rangle}{\frac{1}{2} mv^2} , \tag{2}$$

where, $Y = \frac{2mv^2}{h\omega_p}$, the classical plasma frequency $\omega_p = \left(\frac{4\pi\rho e^2}{m}\right)^{1/2}$, ρ the electron density, and $\langle T \rangle$, the average kinetic energy is given by

$$\langle T \rangle = (\tfrac{3}{10})\, mv_F{}^2 ,$$

where v_F is the Fermi velocity.

For the low energy case, they give

$$L = (\tfrac{\chi^2}{3})^{3/4} \quad Y^{3/2} \quad C_1(\chi) , \tag{3}$$

where

$$C_1(\chi) = \frac{1}{2\,(1 - \frac{\chi^2}{3})^2} \left(\log_e \frac{1 + \frac{2}{3}\chi^2}{\chi^2} - \frac{1 - \frac{1}{3}\chi^2}{1 + \frac{2}{3}\chi^2} \right)$$

with

$$\chi^2 = \frac{e^2}{\pi \hbar v_F} , \quad \hbar = \frac{h}{2\pi} .$$

Equation (2) for the L function warrants some discussion. First, one notes that the L function of Eqs. (2) and (3) are derived by Lindhard and Winther for free electron system. Transition to an atomic system of the first term of Eq. (2), as studied widely, is accomplished under the so-called local plasma model in which density $\rho(\vec{r})$ is evaluated by using quantum mechanical wave functions. The local plasma model is equivalent to replacing the molecular dipole oscillator strengths by the corresponding classical plasma absorption spectrum. The adequacy of such a replacement was recently shown by Johnson and Inokuti[9] to be most accurate for evaluating atomic quantities associated with stopping power inspite of differences between the plasma spectrum and the actual oscillator strength distribution. A quantum mechanical analogue of the second term of Eq. (2) would be of interest. In this context, a result first derived by Brown would prove to be useful. Brown[10] studied the K-shell asymptotic stopping power of an hydrogenic system (with 2 K-electrons) for a fast projectile, taking the maximum momentum transfer equal to 2mv as if the electron was free. The asymptotic stopping power equation obtained by Brown can be expressed in a form similar to the Eq. (2). The first terms of both of these equations, since they involve the mean excitation energy, can be assumed essentially equivalent within the local plasma approximation. He obtained for the second term in Eq. (2) for an hydrogenic system, the quantity $1/n_s$ where, $n_s = \frac{1}{2} m\, v^2/Z_s^2 R$ where Z_s is the effective nuclear charge for s-shell (s=K,L,...) and R is the Rydberg Constant. Walske,[11] on the other hand, took the upper limit for momentum transfer to be infinity, thus overestimating the nuclear momentum recoiling and obtained instead $2/n_s$. In reality, however, due to the recoiling of the nucleus. the result should be expected to fall somewhere between $1/n_s$ and $2/n_s$. This fact will be incorporated later (see Eq. (6)) as a parameter which we later estimate. At the present, however, for the sake of simplicity, combining Brown's result for the K-shell with Walske's result for the L-shell,[12] but retaining the consistency with the free election model, we write the analogous second term (known as shell correction) for an hydrogenic system with Z electrons as

$$C = C_{K,\ total} + C_L = \frac{1}{n_K} + \frac{1}{n_L}\left(\frac{Z-2}{8}\right) , \tag{4}$$

which can be rewritten for a real atom as

$$C = \frac{1}{2}\ \frac{\langle T\rangle}{\frac{1}{2}mv^2}\ \phi(Z)\cdot , \tag{5}$$

$$\text{where } \phi(Z) = Z\cdot f(Z)g \tag{6}$$

$$\text{and } \langle T\rangle = \frac{1}{Z}\left[Z_K^2 R + (Z-2)\frac{1}{4} Z_L^2 R\right]. \tag{7}$$

In the above, a coefficient $f(Z)$ has been introduced to distinguish a real atom from an hydrogenic one. The coefficient $f(Z)$ is known to be less than unity for L-shells for low atomic number targets. The coefficient g is introduced to incorporate the effect due to the recoiling of the nucleus.

At this stage, it is appropriate to discuss various features associated with the low energy projectiles and the low atomic number targets. First, in the low energy region, the projectile's full charge z will not be operational in the stopping process due to electron capture that is influenced mainly by the outer shell electrons of the medium. Second, Walske has pointed out that the coefficients f(Z) are unreliable for the low atomic numbers $Z < 30$ due to use of the hydrogenic wave functions.

It is, evident from the above observations that some sort of crude estimate of the quantity C is in order. This is justified since the usual incorporation of these effects involves the fitting with the experimental data. The inclusion of the effect of projectile's effective charge should decrease the stopping number for all the elements; for Li the most and for Ne the least. In order to incorporate this effect and the other problem of the need for an accurate value of the coefficient f(Z) as stated above, it is reasonable as a first approximation to assume a semiempirical constant value of the quantity ϕ (Z) equal to half the total number of electrons in noble gas atoms. Such a division should over-estimate shell corrections for lithium and beryllium in decreasing fashion and under-estimate that for helium, neon, carbon, nitrogen, oxygen and fluorine also in a decreasing manner. Such a change in shell corrections is indeed what is needed as almost entirely compensating the effect of the effective charge of the projectile on the stopping power. Since, in this paper we are interested in the atoms with atomic number below 10 this assumption implies that

$$\begin{aligned} \phi(Z) &= 1 \qquad \text{for } Z < 2, \\ \phi(Z) &= 5 \qquad \text{for } 3 < Z < 10. \end{aligned} \tag{8}$$

Implicit in the above partition of ϕ is the fact that the quantity C no longer represents the so-called shell corrections only, but presumably also some other effects including that due to the projectile's effective charge as well as due to the neglect of the higher order terms in Eq. (2). One can now write Eq. (5) as:

$$\frac{C}{Z} = \frac{1}{2}\,\frac{\langle T\rangle}{\frac{1}{2}mv^2}\cdot\frac{1}{Z} \quad \text{for } Z < 2,$$

and

$$\frac{C}{Z} = \frac{1}{2}\,\frac{\langle T\rangle}{\frac{1}{2}mv^2}\cdot\frac{5}{Z} \quad \text{for } 3 < Z < 10, \tag{9}$$

where $\langle T\rangle$ by virial theorem is just the average kinetic energy of the electron and should be averaged over all the Z electrons in the atom.

In order to make a transition to an atomic system, we assume the above results and accordingly replace Eq. (2) with

$$L = \ln Y - \frac{3^{1.5}}{10\chi Z}\cdot\frac{1}{Y} \quad \text{for } Z < 2,$$

$$L = \ln Y - \frac{3^{1.5}}{2\chi Z}\cdot\frac{1}{Y} \quad \text{for } 3 < Z < 10, \tag{10}$$

The low and high energy L functions should now be combined to determine the appropriate dependence of the stopping power on energy. To do this, we used Eqs. (3) and (10) for our desired results after replacing ω_p

by $\gamma\omega_p$ in them, where nonconstant values of γ were obtained from reference 2. Bonderup,[13] had combined Eqs. (2) and (3) and assumed a constant value of γ equal to $\sqrt{2}$. Unlike Bonderup, we tried to preserve the continuity between the low energy stopping number function given by Eq. (3) and the high energy function given by Eq. (10). In this way, stopping number values for a system can be obtained given the velocity of the projectile and the density $\rho(\vec{r})$.

For a diatomic molecule, the Gordon-Kim model gives the density as:

$$\rho\ \text{molecule} = \rho_a(\vec{r}) + \rho_b(\vec{r} - \vec{R}_{ab}), \tag{11}$$

where $\rho_a(\vec{r})$ is the atomic groundstate density. R_{ab} is the distance between the two atoms, which is known to be 1.094Å for N_2 and 1.207Å for the O_2 molecule. Equation (11) was generalized for water vapor including its partial ionic bond nature and neglecting the overlap between the two H-atoms. The distance between the O and H nuclei was taken equal to 0.958Å.

The molecular stopping power for protons was obtained by averaging the stopping number over $\vec{r}$ for N_2, O_2 and water vapor molecules. Hartree-Fock wave functions were employed in these calculations.

Table I lists the results of this paper, together with Andersen-Ziegler curve fitted results,[14] and two sets of experimental data for the O_2 molecules. Table II lists these values for the N_2 molecule. In table III, the results of this paper for water vapor are compared with the available experimental data for energy ranging from 40 keV to 500 keV. Good agreement, within 10 percent, is found with the experimental data.

In order to discuss the departures from Bragg's rule, it would be relevant to cite a systematic study carried out in a series of experiments at Baylor University.[3-5] The study revealed that for low energy projectiles there may exist a deviation from Bragg's rule depending on the physical state, but most importantly, on the chemical structure of the compounds. The confusing status of the dependence on the chemical structure can best be described by citing these studies in chronological order. First in 1971, the Baylor group[3] summarized that the compounds with single bond and double bonds should obey Bragg's rule. The compounds containing triple-bond structure were found to deviate from Bragg's rule by as much as 12.8% (α particles of energy between 0.3 and 2.0 MeV often were the projectiles). In particular, these authors indicated that the molecular hydrogen (single bonded molecule) should obey Bragg's rule. Later in 1972, the Baylor group[4] critically looked again on their previous conclusions. They indicated that perhaps the hydrogen atomic stopping cross section may be considerably different than one-half of the molecular stopping cross section and thus should cause considerable deviations. However, the Baylor group in 1974,[5] recognizing the difficulty of obtaining atomic cross sections experimentally, based their analysis on the existence of some modified, but unique atomic stopping cross sections.

It is therefore imperative that in order to discuss the deviations from the Bragg's rule, one must have access to the atomic and molecular stopping cross sections. We calculated both the atomic and the molecular stopping cross sections as a function of projectile energy for the molecules O_2, N_2, and H_2. These results together with the deviations from Bragg's rule are exhibited in tables IV, V, and VI. One sees that the deviations from Bragg's rule become small as incident energy increases -- in agreement with observations made by many workers including those at Baylor University.[1] It is to be noted that N_2 is a triple-bonded, O_2 a double-bonded (from the bond energy point of view) and H_2 is a single-bonded molecule. The maximum deviations from Bragg's rule for energy 100 keV and above are 6.1%, 2.6%, and 10%, respectively, for these molecules. Thus, the deviation depends on the chemical structure. When the Gordon-Kim model is used, the overlap of electron density determines the deviation or molecular binding effects. For instance, for the hydrogen molecule, the distance between nucleons is very small, equal to 0.74Å. It is expected that the overlap of electron density is large, thus explaining the considerable deviation from the Bragg's rule. The stronger the bond energy, the shorter the distance will be. It is interesting to note that single-bonded, double-bonded and triple-bonded carbon molecules have internuclear distances equal to 2.94, 2.52 and 2.24 in Bohr units, respectively. We may thus expect that the triple-bonded carbon will have more deviation from Bragg's rule than the single-bonded carbon.

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TABLE I. Proton stopping cross section values (in units of 10^{-15}eV cm^2) per atom. These were obtained by dividing by two, the stopping cross section per molecule of the oxygen molecule.

E(keV)	Theoretical Values of the Present Paper	Curve Fitted Values Andersen and Ziegler[14]	EXPERIMENTAL RESULTS	
			Reynolds *et al.*[15]	Langley[16]
40	15.89	14.6	15.2 ±2.6	-
80	17.48	17.0	17.25±2.6	-
100	17.43	17.0	17.17±2.6	-
300	11.84	11.9	11.99±1.7	-
500	8.92	8.8	8.84±1.7	-
1037	5.64	-	-	5.25
2591	2.97	-	-	2.85

TABLE II. Proton stopping cross section values (in units of 10^{-15}eV cm^2) per atom. These were obtained by dividing by two, the stopping cross section per molecule of the nitrogen molecule.

E(keV)	Theoretical Values of the Present Paper	Curve Fitted Values Andersen and Ziegler[14]	EXPERIMENTAL RESULTS	
			Reynolds *et al.*[15]	Langley[16]
40	17.20	16	17.1 ±2.6	
80	18.41	17.9	18.5 ±2.6	
100	17.79	17.7	17.9 ±2.6	
300	10.85	11.2	11.2 ±1.7	
500	8.10	8.1	8.08±1.7	
1037	5.20			4.78
2591	2.71			2.56

TABLE III. Proton stopping cross section values (in units of 10^{-15}eV cm^2) per molecule for water vapor.

E(keV)	40	80	100	300	500
Theoretical Values of the Present Paper	28.81	27.8	26.8	17.1	12.6
Reynolds *et al.*[14]	25.0±2.6	27.6±2.6	27.3±2.6	17.9±1.7	13.0±1.7

TABLE IV. Deviations from Bragg's rule in the case of oxygen molecule. ε(atomic), the atomic stopping cross section (in units of eV x 10^{-15} cm^2/atom) was obtained from Eqs. (3) and (10). ε (molecule) is in units of $\frac{1}{2}$ eV x 10^{-15} cm^2/molecule.

E(keV)	40	100	200	300	500	1037	100000
ε(atomic)	17.44	17.48	14.65	12.15	9.1	5.72	0.1492
ε(molecule)	15.89	17.43	14.36	11.84	8.92	5.64	0.1476
percentage deviation	8.9	0.3	2	2.6	2	1.4	1.1

TABLE V. Deviations from Bragg's rule in the case of nitrogen molecule. ε(atomic), the atomic stopping cross section (in units of eV x 10^{-15} cm^2/atom) was obtained from Eqs. (3) and (10). ε (molecule) is in units of $\frac{1}{2}$ eV x 10^{-15} cm^2/molecule.

E(keV)	40	100	200	300	500	1037	100000
ε(atomic)	19.33	18.57	14.32	11.56	8.53	5.30	0.1340
ε(molecule)	17.20	17.79	13.75	10.85	8.10	5.20	0.1319
percentage deviation	11	4.2	4.00	6.1	5.0	1.9	1.3

TABLE VI. Deviations from Bragg's rule in the case of hydrogen molecule ε(2xatomic), the atomic stopping cross section (in units of eV x 10^{-15} cm^2/atom) was obtained from Eqs. (3) and (10). ε (molecule) is in units of eV x 10^{-15} cm^2/molecule.

E(keV)	100	200	300	500	800	1037	2591
ε(2 x atomic)	12.7	8.13	6.1	4.17	2.89	2.36	1.11
ε(molecule)	11.43	7.53	5.71	3.93	2.75	2.24	1.07
percentage deviation	10	7.4	6.4	5.8	4.8	5.1	3.6

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A THEORETICAL MODEL FOR CALCULATION OF MOLECULAR STOPPING POWER

by

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ABSTRACT

A modified local plasma model based on Linhard-Winther, Bethe, Brown, and Walske is established. The Gordon-Kim's molecular charged density model is employed to obtain a formula to evaluate the stopping power of many useful molecular systems. The stopping power of H_2 and He gas was calculated for incident proton energy ranging from 100 keV to 2.5 MeV. The stopping power of O_2, N_2 and water vapor was also calculated for incident proton energy ranging from 40 keV to 2.5 MeV. Good agreement with experimental data was obtained.

A discussion of molecular effects leading to departure from Bragg's rule are presented in this thesis. The equipartition rule and the effect of nuclear momentum recoiling in stopping power are also discussed in the appendix. The calculational procedure presented in this thesis hopefully can easily be extended to include the most useful organic systems such as the molecules compound of carbon, nitrogen, hydrogen and oxygen which are useful in radiation protection field.

TABLE OF CONTENTS

INTRODUCTION

The subject of energy loss of heavy ions such as protons, or α particles passing through matter, has been studied for more than sixty years. Research in this area began with the study of a mechanism under which charged particles lose their energy mainly to the atomic electrons. These studies have contributed to the basic understanding of the interaction of charged particles with matter-atoms-molecules and, more recently, to materials. The energy loss parameters have found their use in various applications. The list includes: radiation dose effects on solid state devices; shielding problem; space radiation research; design and calibration of spectrometers and dosimeters; proton doses in manned or unmanned space flights; energy transfer to living cells, and radiation effects in materials, etc.

The Bethe [1] theory of energy loss of fast charged particles rests on the knowledge of the so-called mean excitation energy of the medium. Once this parameter is known, the high energy stopping power of an atom can readily be calculated. The determination of this parameter, however, is very laborious, as is seen in the works of Dehmer, Inokuti, Saxon, and Baer [2], [3], [4], who calculated the mean excitation energy parameter for atoms of atomic number ranging from Z = 1 to Z = 38. The numerical evaluations involving the Hartree-Slater wave functions in these calculations are so involved that the estimating of the errors is difficult to ascertain.

The Bethe theory, although developed for the atoms, has also been extended to obtain the stopping power of molecules under the Bragg's rule [5]. One essentially ignores the chemical binding of molecules under this rule. Recently, however, several experiments [6], [7], [8], have revealed that for low energy regions there may exist deviations from the Bragg's rule. Furthermore, there are some indications (see, for instance, a series of papers by Wilson and his co-workers) that the Bragg's rule may not be obeyed in the determination of the mean excitation energy parameter for molecules, although this departure does not have much effect on stopping power because of the dominance of the velocity of the projectile on the stopping power.

It is evident from the above discussion that the traditional approach of obtaining the molecular stopping power from the atomic stopping power via the Bragg's rule should be abandoned, at least for the low energy projectile. The local plasma model which has been successful in predicting the mean excitation energy could serve as the appropriate candidate for an alternative approach.

This report discusses the establishment of a modified local plasma model by employing the Gordon-Kim molecular [9] density model, which provides a method of calculating molecular stopping power even at quite low proton energies. In spite of the fact that it is a somewhat average model, calculation is relatively simple, and the calculation of stopping powers of H_2, He, O_2, N_2 and water vapor are in fair agreement with experimental data. Modifications to the local plasma model are mainly due to the complexity of real atomic and molecular situations. Besides the effects of shell corrections, and the screening of projectiles, other effects such as nuclear recoiling are also involved. Interesting discussions on deviation from the Bragg's rule and on the modified local plasma model and the conclusions deduced from experimental data are presented in the last section of this report, "Molecular Effect of Stopping Power."

From the theoretical model established in this report, the departure of stopping power from Bragg's rule only occurs for low velocity projectile cases. Deviation from the Bragg's rule also is found to depend on the chemical structure of molecules. More overlap of electron clouds is found to cause more deviation from the Bragg's rule when the Gordon-Kim model is employed. The geometric structure gives the most important information on molecular effects.

The basic stopping power theories assume the interaction between the projectile and the atomic electron, which is assumed initially to be at rest. While it is true that the overall energy loss must, indeed, take place in this manner, in some collisions the recoiling of the nucleus cannot be neglected. This is especially true for relatively low incident energies of the heavy ion. Although the recoil energy may be small due to the heavy mass of the target nucleus, the recoiling momentum may be very large. Thus, the conservation of momentum will lead to a different value of the momentum of electrons than has previously been assumed in these theories.

This observation lends itself to solving a three body problem. Thus, in this report, a semi-classical three body model is established to calculate relevant quantities. Specifically, exact semi-classical three body calculations are made for a proton incident on a hydrogen atom with the electron in its first Bohr orbit. The model and the resulting conclusions especially in regards to the equipartition theorem for shell corrections are presented in the appendix.

Historical Review

The three prominent theories of penetration of charged particles in matter are: Bohr's semi-classical theory, Bethe's quantum theory, and Lindhard's local plasma theory based on the treatment of free electron gas. Since this paper touches upon all three theories, it is helpful to outline their main features and assumptions of interest. When appropriate, the detailed structure of these theories will also be given, in later sections.

Semi-Classical Theory

Bohr's semi-classical treatment of the slowing down charged particles, done as early as 1913 [10], [11], was the first to give the overall characteristic structure and the features of the penetration theory. The classical parameters appearing in this theory, surprisingly, could later be calculated or related to the quantum treatment. The main underlying assumptions and the characteristics of the theory are:

1. The coulomb interaction between the incident-charged particle of velocity v and the atomic electrons is assumed to be responsible for energy loss.
2. The momentum transfer is sufficiently small so that the projectile's path is a straight line.
3. The atomic electron is assumed to be at rest.
4. The minimum impact parameter is determined from the knowledge of the maximum momentum transfer of the projectile to a free electron. The maximum impact parameter is determined under the assumption that the interaction time must be larger than the orbital period of the atomic electron.

Based on the above assumptions, Bohr obtained the stopping power formula as:

$$- \frac{dE}{dx} = 4\pi NZ \frac{z^2 e^4}{mv^2} \ln \frac{mv^3}{e^2\omega} \qquad (1)$$

where, ze is the charge of the projectile and N is the number of atoms per unit volume, with Z electrons per atom, and ω is the characteristic atomic frequency.

Equation (1), even though the derivation was based on classical considerations, embodies the main features of the quantum mechanical description given in the later section. As is known, in both theories, the properties of the incident ion such as its charge ze, and its velocity v occur in this equation, m being the mass of the electron. The properties of the medium are contained in the quantities N, Z, and ω.

Quantal Theory

Bethe's non-relativistic calculation of stopping power was performed in 1933 in the first Born approximation [1] and rests mainly on the following assumptions.

1. The interaction responsible for energy loss is the coulomb interaction between the incident ion and the atomic electron.
2. The speed of the ion is much greater than that of the atomic electrons.
3. The calculation of the maximum momentum transfer entails the collision with the electron initially at rest.
4. Within the plane wave Born approximation, the assumption that the electronic positions are correlated only over relatively small distances implies the use of the dipole oscillator strengths.

Based on the above assumptions, Bethe arrived at the following energy-loss formula:

$$-\frac{dE}{dx} = \frac{4\pi N Z z^2 e^4}{mv^2} \ln \frac{2mv^2}{I} \qquad (2)$$

where I, the mean excitation energy of the medium, is defined through the electric dipole strength f_n by:

$$Z \ln I = \sum_n f_n \ln E_n$$

with E_n being the eigenenergy of the electron.

Notice the similarity between equations (1) and (2) obtained under classical and quantal considerations, respectively. Notice also the occurance of the factor $2mv^2$ (which represents the maximum energy transfer of the assumption (3)) in the argument of log in equation (2).

Theories Based on the Thomas-Fermi Model

Bloch [13], in 1933, calculated the stopping power by using the Thomas-Fermi model for the many electrons of the atoms of the medium. Useful results were later obtained by Lindhard [14], [15], [16], and his co-workers. Lindhard showed that for a swift heavy particle of low charge the stopping power of a free electron gas is given by

$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4}{mv^2} \rho \ln \left(\frac{2mv^2}{\gamma h\omega_p}\right) \tag{3}$$

where, ρ is the electron density, and ω_p is the classical plasma frequency given by $\omega_p^2 = \frac{4\pi e^2}{m} \rho$, and γ is a parameter calculated by Lindhard to be equal to $\sqrt{2}$. Lindhard made the bold assumption that the theory can be extended to the atoms if one writes the above equation as:

$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4 N}{mv^2} \int \ln \left[\frac{2mv^2}{\gamma h\omega_p(\vec{r})}\right] \rho(\vec{r})\, d^3r \tag{3a}$$

where, now $\rho(\vec{r})$ is to be evaluated by employing the quantal wave functions of the electrons. This model is often called a local plasma model, in literature.

Further Discussion of the Bethe and Lindhard Theories.

The simplicity in Bethe's theory results from several factors. The first factor allows all the atomic electrons to participate in the stopping process. Indeed, this is not valid for the inner shell electrons which are tightly bound and may not always participate in the stopping process. The second factor is the inclusion only of the dipole transitions in the theory, although other transitions (though less probable) may possibly take place. This, as indicated earlier, is tantamount to assuming that the electronic positions are correlated only over relatively small distances. These corrections to the Bethe theory have been extensively investigated.

Lindhard's local plasma theory, as mentioned earlier, makes the bold assumption through equation (3) for its application to atomic systems. This approach, surprisingly, works well for atoms as is shown recently in the evaluation of the mean excitation energy parameter [17]. The approach rests with the comparison of equation (3) of Lindhard with the Bethe formula equation (2):

$$Z \ln I = \int \rho(\vec{r}) \ln (\gamma h\omega_p) \cdot d^3r \qquad (4)$$

The local plasma model is also relatively easy to extend to molecules for ionic bonded gases, covalent bond gases and metals. Such progress has recently been made by various authors. (See, for instance, a series of papers by Wilson and his co-workers).

STOPPING NUMBER FUNCTION

The energy loss of fast charged particles caused by their inelastic collision with atoms, is given with good approximation by Bethe's formula, which is based on the quantum perturbation theory. However, the mean excitation energy in his formula is too complicated to evaluate theoretically for many practical problems especially for molecules. It appears the local plasma model affords a simple method to calculate the mean excitation energy of elements as well as compounds. There still remain three problems: 1) people have more interest in stopping power than in mean excitation energy; 2) how to extend this method to evaluate molecular stopping power; 3) how to extend this method to slow charged particle cases as well as to fast charged particles cases. Now let us recall the basic formula of local plasma model for fast charged particles.

$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4 N}{mv^2} \int \ln\left(\frac{2mv^2}{\gamma \hbar\omega_p(\bar{r})}\right)\rho(\bar{r})\, d^3r \qquad (5)$$

where $\omega_p^2(\bar{r}) = \frac{4\pi e^2 \rho(\bar{r})}{m}$ is the plasma frequency. We can see in the above formula that once the parameter γ and the electron density $\rho(\bar{r})$ are known, the stopping power can be determined immediately. We will discuss the problem of parameter γ in the section "Local Plasma Model for High Projectile's Energy Cases."

The atomic electron density is just the square of the wave function of the ground state of the atom. It is not easy to find the molecular wave function. Fortunately, we have a very simple molecular electron density model, namely the Gordon-Kim model [9]. It is a rough model, but as a first order approximation this model gives the main features of molecular effects. Detailed discussion will be presented in the next chapter. To extend this model to low energy regions is of considerable interest from both a practical and theoretical point of view. Unfortunately, many effects arise at low energies including projectile charge screening, nuclear momentum recoiling, forbidden transition, etc. On one hand we have to consider the above complexity in realistic atomic and molecular world. On the other hand we still need to keep the simplicity of the local plasma model, otherwise no results can be obtained in practice. This section is devoted to establish a modified local plasma model. We will concentrate on finding a stopping number function L. It should be valid for low energy as well as high energy cases, and should still retain the simplicity of the local plasma model. It will also approach the realistic cases as closely as possible. However, it is only an average model and some estimating is involved.

Local Plasma Model for High Projectiles Energy Case

When the projectiles move rather fast the stopping power can be determined by Bethe's formula with good accuracy,

$$- \frac{dE}{dx} = \frac{4\pi z^2 e^4 N}{mv^2} Z \ln\left(\frac{2mv^2}{I}\right) \tag{6}$$

where I, the mean excitation energy has been of considerable study. This is because once the parameter is known, the energy loss can be obtained immediately. However, the evaluation of this parameter is considerably laborious. In principle, the parameter can be calculated exactly only for the H-atom for which accurate wave functions are known. More recently, Dehmer, Inokuti and Saxon [2] used the tabulation of Hartree-Slater potential given by Herman and Skillman. They solved the Schroedinger equation to obtain the radial matrix element R (nl, n'l') where (n, l), (n', l') are initial and final states of atom. Knowing these values they calculated the mean excitation energy parameter I for atoms ranging from Z=1 to Z=38. However, there are difficulties with the above approach. In practice, the extreme complexity of numerical calculations renders it impossible to extend the approach to evaluate the mean excitation energy of molecules.

An alternative approach is the possibility of using the local plasma model, formula (5). There are, however, two central quantities which should be known. These are function γ and $\rho(\bar{r})$. The evaluation of $\rho(\bar{r})$ rests on the determination of the wave functions of electron only in ground states, such Hartree wave function for various atoms have recently been available in the work of Clementi and Roetti. The problem is then the determination of parameter γ.

Calculation of Parameter γ

In his original theory of stopping power of electron gas Lindhard gave a quantitative discussion for the values of parameter γ. The first term in high energy expansion of stopping number L is given by $\ln\left(\frac{2mv^2}{\hbar\omega p} C(x)\right)$ where $C(x) = \frac{1}{\gamma}$. Linhard discussed the function C(x) as a function of electron density. He surmised that the function C(x) depends on the density slightly only. It should be a little bit less than one for moderate density and should approach unity for both extremely low and extremely high densities. Furthermore, Lindhard suggested that the values of γ can be taken to be unity for light atoms without large error. Later, Lindhard and Scharff [14] suggested on the basis of a simple model that $\gamma = \sqrt{2}$ can be chosen for heavier elements.

Chu and Power using constant value of $\gamma = \sqrt{2}$ obtained the parameter I for various atoms. [17] Their calculated values however were found to exceed the values calculated by Delmer et al. (based on oscillator strength method) by 20% to 30%. The most satisfying thing, however, was the similar trend in the variation of I values in both cases as a function of atomic numbers. This points towards a greater confidence in the local plasma theory. Some authors encouraged by this, and also not satisfied with Chu and Power's results treated the parameter γ as an empirical parameter to fit the data. Unsatisfied with this type of empirical treatment, we adopt the following approach. Bohm and Pine [18], [19] have treated the problem of collective long range interaction in a quantum electron gas. They introduced normal coordinates of collective motion of electron beyond some screening radius r_c and the individual particle motion was considered to be more important for radius smaller than r_c.

Bohm and Pine showed that the average plasma frequency $\langle\omega\rangle$ (which is the average over the frequency of the collective oscillations, say ω) is a linear function of the classical plasma frequency ω_p and is given by

$$\langle\omega\rangle = [1 + \frac{3}{2}\frac{\beta}{\lambda_s}(1 + \frac{3}{10}\beta^2)]\,\omega_p \tag{7}$$

where $\lambda_s = r_s/a_0$ is a dimensionless parameter and is the average distance between electrons, and where a_0 is the Bohr radius.

The parameter β can be determined by minimizing the electron long range correlation energy (the long range part of correlation energy is obtained by subtracting short range exchange energy from the cohesive energy)

$$E_{corr}^{lr} = \frac{0.866\ \beta^3}{\lambda_s^{3/2}} - \frac{0.458\ \beta^2}{\lambda_s} + \frac{0.019\ \beta^4}{\lambda_s} \qquad (8)$$

The minimization of the above equation leads to the following equation for β

$$0.076\ \beta^2 + \frac{2.598\ \beta}{\sqrt{\lambda_s}} - 0.916 = 0 \qquad (9)$$

At this stage let us recall that Bohr's semi-classical theory and Bethe's quantum theory have the similar first term in the high velocity expansion of

$$L = \ln\left(\frac{2mv^2}{E}\right)$$

One must note that E is some average energy which in the case of the Bethe theory is the mean excitation energy I. Thus, some sort of average quantity must occur in the argument of log term, therefore, recalling equation (4) of Lindhard's theory

$$L = \ln\left(\frac{2mv^2}{\gamma\hbar\omega_p}\right)$$

It was shown by Bohm and Pines that $\gamma\hbar\omega_p$ may be replaced by $\hbar\langle\omega\rangle$ where $\langle\omega\rangle$ is given by equation (7). Thus $\gamma = 1 + 3/2\,\frac{\beta^2}{\lambda_s}\,(1 + 3/10\,\beta^2)$. Once we know λ_s then β can be determined by equation (9), hence γ can be determined by equation (7). Now let us use this average model to evaluate γ as function of Z for various atoms. We took average distance between electrons in an atom as $r_s^3 = \frac{4}{3}\pi\, r_0^3/Z$ where r_0 is atom's radius. Then $\lambda_s = r_s/a_0$ where a_0 is Bohr radius. Table 1 shows r_s, β, λ_s as functions of Z for some selected values of Z ranging from $Z=2$ to $Z=54$.

Table 1. r_s, β as functions of Z

Z	r_s	λ_s	β
2	1	2.42	0.54
3	1.55	3.27	0.62
4	1.12	2.15	0.51
5	0.98	1.75	0.46
6	0.91	1.53	0.43
7	0.9	1.43	0.42
10	1.17	1.65	0.45
11	1.9	2.60	0.55
12	1.6	2.13	0.50
13	1.43	1.85	0.47
14	1.32	1.67	0.45
15	1.28	1.58	0.44
16	1.27	1.54	0.43
18	1.43	1.66	0.45
36	1.59	1.47	0.42
54	1.75	1.41	0.41

Table 2 shows γ as a function of Z. From table 2 we can see γ is nearly a constant equal to 1.19. This is reasonable, since other workers have chosen values of γ ranging from $\gamma = 1.1$ to $\gamma = 1.5$. Actually in

Lindhard's description of γ it is a function that slightly depends on density or λ_s, and is not a constant. We obtained $\gamma = 1.19$ partly because we took an average model. Table 3 lists γ as a function of λ_s, (ranging from 10^{-18} to 10^7). Since $\rho(r) = \frac{1}{\lambda_s^3}$ from the table we can see that γ is very slightly dependent on density; a little bit greater than one for moderate density and approaches unity for both extreme cases - very low and very high density. Compared with Lindhard's qualitative description of $C(X) = \frac{1}{\gamma}$ in his theory, as mentioned earlier in this section, we reach agreement with Lindhard for these two different cases. In the exact calculations of mean excitation energy using local plasma model, we took γ as function of distance r (distance from electron to nuclei), instead of a constant.

Recent development confirmed the concept of γ obtained here in improving the work of Chu and Powers. Furthermore, the above consideration will be used in the following section for low energy stopping power.

Low Energy Stopping Number Function

Lindhard-Winther expanded the stopping number function of free electron gas in high energy case and in low energy case as follows:

$$L_2 = \ln\left(\frac{2mv^2}{h\omega_p}\right) - \langle T\rangle \Big/ \frac{mv^2}{2} \quad \text{(high energy case)} \qquad (10)$$

Table 2. γ as functions of Z

Z	2	3	4	5	6	7	10	11	12	13	14	15	16	18	36	54
γ	1.193	1.191	1.192	1.191	1.191	1.191	1.191	1.193	1.192	1.192	1.191	1.191	1.191	1.191	1.191	1.191

Table 3. γ as functions of λ_s

λ_s(a0)	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1	10	100	1000	10^4	10^5	10^6	10^7
γ	1	1	1.06	1.10	1.19	1.19	1.19	1.19	1.19	1.20	1.17	1.05	1.007	1.001	1	1

$$L_1 = \left(\frac{X^2}{3}\right)^{\frac{3}{4}} C_1(X) \left(\frac{2mv^2}{h\omega_p}\right)^{\frac{3}{2}} \quad \text{(low energy case)} \qquad (11)$$

$$\text{where } C_1(X) = \frac{1}{2\left(1-\frac{X^2}{3}\right)^2}\left[\ln\left(\frac{1+\frac{2}{3}X^2}{X^2}\right) - \frac{1-\frac{X^2}{3}}{1+\frac{X^2}{3}}\right] \qquad (12)$$

$X^2 = \frac{e^2}{\pi h V_F}$, $\omega_p^2 = \frac{4\pi\rho e^2}{m}$ is the plasma frequency, ρ is the electron density V_F is the Fermi velocity.

Bonderup [20] directly combined low energy L function L_1 and high energy L function L_2 and used $\sqrt{2}$ instead $C(X)$ in the first term in L_2. (In [15] Lindhard and Winther assumed $C(X) = 1$ see last few lines of page 10). He then performed calculations for the stopping power of some elements using the above L function and local plasma model. Good agreement was found with experimental data for proton energy over 500 kev. Unfortunately, for low energy regions, his simple approach is not valid.

We establish our modified L function based on the following principles:

1. smoothly join Linhard-Winther's high energy L function L_2 and low energy function L_1;
2. involve Pine correction using $\gamma h\omega_p$ instead of $h\omega_p$ in all the terms in L function;
3. apply correction on the second term of L_2.

The correction on the second term warrants some discussion.

Many complicated physical effects are involved in the low energy region We will discuss them in detail to approach the realistic atomic and molecular world. Bethe, Walske, and Brown [21], [22], [23], developed quantum mechanical theory of stopping power of innershells of atoms. Calculations are done under plane wave Born approximation using hydrogenic wave functions. Brown [21] and Walske [22] had calculated the stopping power of K shell electron. Walske [23] also calculated the stopping power of L shell electrons. Khandelwal and Merzbacher [24] calculated the stopping power of M-shell electrons. Khandelwal more recently evaluated K and L shell corrections [25].

They defined a stopping number function B as follows.

$$-\frac{dE}{dx} = \frac{4\pi e^4 z^2}{mv^2} N \sum_{i=K,L,M} B_i \tag{13}$$

where $$B_i = \int_{w_{min}}^{w_{max}} w dw \int_{q_{min}}^{q_{max}} |Fw_i (q)|^2 \frac{2dq}{q^3} \tag{14}$$

where $|Fw_i(q)|^2$ is the form factor, q is the change in incident particles momentum divided by $(2m Z^2_{ieff} Ry)^{\frac{1}{2}}$. For high energy projectiles, they also give an asymptotic stopping number formula of the form $B_s(\theta_s, \eta_s) = S_s(\theta_s) \ln \eta_s + T_s(\theta_s) - C_s(\theta_s, \eta_s)$ where $s = K,L,M$ and where C_s are the so called shell correction terms. Equation (13) can also be written in terms of

$$B = Z \ln\left(\frac{2mv^2}{I}\right) - \sum_s C_s (\theta_s, \eta_s) \tag{13a}$$

where I is the mean excitation energy, θ_s is dimensionless screening parameter denoting the observed ionization potential in units of ideal ionization potential $Z^2 sRy/s^2$. η_s is also a dimensionless quantity and is given by $\frac{1}{2}mv^2$ divided by Z_{effs}^2 Ry.

The calculations of the shell corrections are extremely complex. Bethe, Brown, and Walske expanded them in power series of $\frac{1}{\eta_s}$. The first term of shell correction given by Brown [21] is C_k total $\sim \frac{1}{\eta_k}$ for K shell electron meanwhile Walske's [23] results are C_k total $\sim \frac{2}{\eta_L}$. The difference between Brown and Walske is mainly due to the fact that they took different upper limits to estimate maximum momentum and energy transfer. As is well known when a heavy particle collides with a free electron, the maximum momentum transferred to the electron is 2mv and maximum energy transfer is $2mv^2$ these values are the ones taken in by Brown in doing his calculations. But if one considers the nuclear recoiling and the binding effects, then the upper limit of momentum transfer is no longer 2mv. Walske took the upper limit of both momentum transfer and energy transfer as infinity. Indeed, both Brown and Walske simplified the problem in this manner. Later, we'll use an exact three body semi-classical model to estimate the upper limit of momentum transfer. Right now, at this stage, we'll use Brown's assumption for consistency with the free electron gas of plasma model, but keep in mind that there are some errors due to Brown's assumption. The accurate result should be expected to be between Brown's and Walske's results. Now we try to establish some relationship between plasma model and quantum mechanical calculation based on Bethe, Brown, and Walske's theory. Following Brown

$$C_k \text{ total} \sim \frac{1}{n_k} = \frac{1}{\langle n\rangle}\frac{\langle n\rangle}{n_k}$$

where we define $\langle n\rangle = \frac{1}{2} mv^2/\langle T\rangle$, $\langle T\rangle$ is the average kinetic energy of electron of atoms then

$$\frac{\langle n\rangle}{n_k} = \frac{\frac{1}{2}mv^2}{\langle T\rangle}\;\frac{Z_{keff}^{2}\,Ry}{\frac{1}{2}mv^2}$$

by virial theorem $\langle T\rangle = |\langle E\rangle|$ we have

$$\frac{\langle n\rangle}{n_k} = \frac{Z_{keff}^{2}\,Ry}{|\langle E\rangle|}$$

For $Z = 1$ we get

$$C_k|_{z=1} = \frac{1}{2} C_k \text{ total}$$

hence, we have

$$\frac{C_k|_{Z=1}}{Z|_{Z=1}} = \frac{1}{2}\,\frac{1}{\langle n\rangle} = \frac{\langle T\rangle}{mv^2} = \frac{1}{2}$$ (Linhard-Winther's second term of L_2 function)

For $Z = 2$ we get

$$C_k|_{z=2} = C_k \text{ total}$$

so that

$$\frac{C_k|_{z=2}}{Z|_{z=2}} = \frac{1}{2}\;\frac{1}{\langle n\rangle} = \frac{1}{2} \quad \text{(Linhard - Winther's second term of } L_2 \text{ function)}$$

Now, let us consider atoms which contain L shell electrons.

Walske also showed that the total shell correction of L electron C_L total $\sim \frac{2}{n_L}$, which is still due to the value infinity for the upper limit of momentum transfer and energy transfer. If we keep Brown's model, i.e. assume that the incident particle collides with free electron, we have C_L total $\sim \frac{1}{n_L}$ where $n_L = \frac{\frac{1}{2}mv^2}{Z_{Leff}{}^2 Ry}$. Now consider L shell closed. The total K and L shell corrections is

$$C_K \text{ total} + C_L \text{ total} = \frac{1}{n_K} + \frac{1}{n_L} = \frac{1}{n_K}\left[1 + \frac{n_K}{n_L}\right]$$

$$= \frac{1}{n_K}\left[1 + \frac{Z_{Leff^2}}{Z_{Keff^2}}\right] = \frac{1}{\langle n\rangle}\left[1 + \frac{Z_{Leff^2}}{Z_{Keff^2}}\right]\frac{\langle n\rangle}{n_K}$$

$$= \frac{1}{\langle n\rangle}\left[1 + \frac{Z_{Leff^2}}{Z_{Keff^2}}\right]\frac{\frac{1}{2}mv^2/\langle T\rangle}{\frac{1}{2}mv^2/Z_{Keff^2}\,Ry}$$

$$= \frac{1}{\langle n\rangle}\left[1 + \frac{Z_{Leff^2}}{Z_{Keff^2}}\right]\frac{Z_{Keff^2}\;Ry}{|\langle E\rangle|}$$

for hydrogenic atom

$$|\langle E\rangle| = \frac{2Z_{Keff^2}\,Ry + \frac{1}{4}Z_{Leff^2}\,Ry \cdot 8}{Z} = 2Z_{Keff^2}Ry \cdot \left(1+\frac{Z_{Leff^2}}{Z_{Keff^2}}\right)\frac{1}{Z}$$

hence, $$\frac{C_K\ \text{total} + C_L\ \text{total}}{Z} = \frac{1}{2}\ \frac{1}{\langle n\rangle}$$

Now consider L shell open:

$$C_K\ \text{total} + C_L = \frac{1}{n_K} + \frac{1}{n_L}\ \frac{(Z-2)}{8} = \frac{1}{n_K}\left[1 + \frac{(Z-2)}{8}\ \frac{n_K}{n_L}\right]$$

$$= \frac{1}{\langle n\rangle}\left[1 + \frac{(Z-2)}{8}\ \frac{Z_{Leff^2}}{Z_{Keff^2}}\right]\frac{Z_{Keff^2}Ry}{|\langle E\rangle|}$$

where, $$\frac{Z_{Keff^2}Ry}{|\langle E\rangle|} = \frac{\langle n\rangle}{n_k}$$

Now $$|\langle E\rangle| = \frac{1}{Z}\left[2\ Z_{Keff^2}Ry + \frac{1}{2^2}\ Z_{Leff^2}Ry\ (Z-2)\right]$$

$$= \frac{2}{Z}\ Z_{keff^2}Ry\left[1 + \frac{(Z-2)}{8}\ \frac{Z_{Leff^2}}{Z_{Keff^2}}\right]$$

hence,

$$C_{k\ \mathrm{total}} + C_L = \frac{1}{\langle n\rangle}\left[1 + \frac{(Z-2)}{8}\,\frac{Z_{Leff^2}}{Z_{keff^2}}\right]\frac{Z}{2} \Big/ \left(1 + \frac{(Z-2)}{8}\,\frac{Z_{Leff^2}}{Z_{Keff^2}}\right)$$

or $$\frac{C_K + C_L}{Z} = \frac{1}{2}\,\frac{1}{\langle n\rangle}$$

In both cases either closed shell or open shell we obtained the same results

$$\frac{C}{Z} = \frac{1}{2}\,\frac{1}{\langle n\rangle} = \frac{1}{2}\,\frac{\langle T\rangle}{\frac{1}{2}mv^2} = \frac{\langle T\rangle}{mv^2} = \frac{1}{2} \quad \text{(Lindhard-Winther's second term of } L_2 \text{ function)} \tag{15}$$

It appears that from quantum perturbation theory we obtained the similar result as of plasma theory except a factor of $\frac{1}{2}$. Actually if we use Walske's result exactly the same results are obtained from both quite different approaches. What is implied in this surprising similarity? We believe this similarity is the real background of local plasma model. In plasma model average kinetic energy $\langle T\rangle$ is related to the plasma density. On another side in Bethe-Brown-Walske's theory as we have shown the average kinetic energy $\langle T\rangle$ is related to atomic wave function by using virial theorem or averge kinetic energy is related to atomic electron density. Since these two approaches give the same stopping power expressions, we may say that plasma model can be localized by the equivalence of these two approaches. But for low energy projectile, especially for light elements which contain L shell electrons, this formula is too simple to describe the stopping power due to various physical effects. First, one should take into account the transitions that are forbidden by Pauli's principle (for the importance of this in the case of asymptotic stopping numbers see Khandelwal [26]). There is a modification factor on $\frac{1}{\eta_K}$ or $\frac{1}{\eta_L}$ or $\frac{1}{\eta_M}$ which depends on Z and also depends on the shell. The following tables 4 and 5 list the coefficients of η_L for different θ_L (where θ_L is the energy difference between ground state and lowest occupied state in units of $Z_{Leff^2}Ry/n^2$ for L shell n = 2) according to Walske for $\theta_L = 1$ the coefficient of η_L^{-1} is 2.

Table 4. Coefficent of η_L^{-1}

θ_L	0.35	0.45	0.55	0.65	1
Coefficients of η_L^{-1}	1.5032	1.0756	1.9890	2.0000	2

Table 5. Coefficent of η_K^{-1}

θ_L	0.7	0.75	0.8	0.85	0.9
Coefficients of η_K^{-1}	2.0662	2.0999	2.1196	2.1290	2.1309

Second, at low energy we also need to consider high order expansion terms which are not completely known. Walske's expansion for the L shell for the η_L^{-3}, η_L^{-4} forms involves fitting.

Third, Brown and Walske's calculations are based on hydrogenic wave functions, as Walske has pointed out, for $Z<30$ the results are not accurate.

Fourth, as mentioned, Brown's model of upper limit of momentum transfer was used and this involves an uncertain factor between 1 and 2. This is because due to the nuclear recoiling, the real value should be between that of Brown and Walske, and should depend on projectiles energy.

Furthermore, there exists a screening effect on low energy projectiles charge. It is easy for the element like Li to loose its valence electron, when positive heavy ion projectile moves rather slow. There is some chance that the projectile can capture the eletron. This will cause screening effect on projectile which in turn will decrease the stopping power. All these complicated effects should be taken into account.

In formula (15)

$$\frac{C_K + C_L}{Z} = \frac{1}{Z} \left\{ \frac{1}{\langle \eta \rangle} \quad \frac{Z}{2} \right\}$$

$$= \frac{1}{Z} \left\{ \frac{1}{2} \text{ Linhard-Winther's Second term of } L_2 \text{ function times } Z \right\}$$

the factor $\frac{1}{Z}$ is due to the definition of $\frac{C}{Z}$ as another Z in the bracket is mainly due to each electron's contribution to total shell correction, $\frac{1}{\eta_K}$ or $\frac{1}{\eta_L}$ is full shell's shell correction, it looks like these two Z factor cancel each other but taking into account all the above effects the situation is not so simple.

As we know the quantity Z in the bracket of formula (15) is mainly due to each electrons contribution to total shell correction but at least the screening effect has a negative influence. As is well known, Li's first ionization potential is about 5 ev. It means only 5 ev additional energy can cause Li to loose its valence electron. Meanwhile, neon's first ionization potential is about 20 ev. The ionization potential rises linearly in Z between lithium and neon. It appears for Li screening effect is much more important than for Neon. At least for $2 < Z < 10$ elements of small Z have more influence on reducing the stopping power through screening than large Z.

Formally, we absorb this effect into the bracket. Now, in the bracket we have two contradictory effects. The shell correction proportional to Z, the screening effect is in the inverse direction. In addition, there are many other unclear effects which we have mentioned above. Roughly now, we have the following assumption, suppose these two contradictory effects roughly cancel each other also with other effects. We may use a half full shell number as an average instead of Z in the bracket.

Thus, we obtain the expression for L_2:

$$L_2 = \ln \left(\frac{2mv^2}{h\omega_p}\right) - \frac{1}{Z} \frac{\langle T \rangle}{mv^2} \quad \text{for } Z < 2$$

$$L_2 = \ln \left(\frac{2mv^2}{h\omega_p}\right) - \frac{5}{Z} \frac{\langle T \rangle}{mv^2} \quad \text{for } 2 < Z < 10 \tag{16}$$

where $\frac{\langle T\rangle}{mv^2} = \frac{1}{2}$ (Lindhard-Winther's second term in L_2 function) .

As mentioned earlier the equivalance of the shell correction term from Lindhard-Winther's theory and Bethe-Walske's theory actually gives somewhat the explanation of the local plasma model. Furthermore, for real atoms we also give the correction on Lindhard's theory. Also we can tell how far the local plasma model can be applied to real situations. Lindhard and Winther also used a parameter γ in both the first term and terms of L_2 to simplify the calculations we will show in the note at the end of this section in detail.

Now (16) becomes

$$L_2 = \ln Y - \frac{1}{Z}\,\frac{3^{1.5}}{10X}\,\frac{1}{Y} \qquad \text{for } Z < 2$$

$$L_2 = \ln Y - \frac{5}{Z}\,\frac{3^{1.5}}{10X}\,\frac{1}{Y} \qquad \text{for } 2 < Z < 10$$

where $X^2 = \frac{e^2}{\pi h V_F}$ V_F is the Fermi velocity and $Y = \frac{2mv^2}{\hbar\omega_p}$

Now we apply the Pine correction on L, i.e. use $\gamma\hbar\omega_p$ instead of $\hbar\omega_p$ in L_2 as well as in L_1 or using $Y = \frac{2mv^2}{\gamma\hbar\omega_p}$ instead of $Y = \frac{2mv^2}{\hbar\omega_p}$ in L function.

Finally, we smoothly join L_1 and L_2 thus obtaining L function by the following manner. Extensive numerical evaluations using a computer program of the function L_1 and L_2 for various values of the variable Y revealed that in most useful cases there were found two roots Y_1 and Y_2 of the equation $L_1 = L_2$ where $Y_1 < Y_2$. Furthermore, the slope M of the function L_2 for values of Y greater than Y_2 was always small. On the other hand, the slope of L_2 for Y values less than Y_1 was very steep. These observations, including the behavior of these functions (see figure 1), led us to the following recipe to preserve the continuity consistent with the physics of the situation

$$\begin{aligned} L &= L_2 && \text{when } MY < L_2 \\ L_2 &= \text{Max}\,[L_1, L_2] && \text{when } MY > L_2 \end{aligned}$$

actually we have

$$L = \begin{cases} L_1 & Y < Y_1 \\ L_2 & Y > Y_1 \end{cases}$$

which was found to be convenient for the computer programming. The functions L_1 and L_2 are defined as follows

$$L_1 = \left(\frac{X^2}{3}\right)^{\frac{3}{4}} Y^{\frac{3}{2}} \; C_1(X)$$

$$\text{where} \quad C_1(X) = \frac{1}{2\left(1 - \frac{X^2}{3}\right)^2} \left(\ln\left(\frac{1 + \frac{2}{3} X^2}{X^2} \right) - \frac{1 - \frac{1}{3} X^2}{1 + \frac{2}{3} X^2} \right)$$

$$L_2 = \ln Y - \frac{N}{Z} \frac{3^{1.5}}{10X} \frac{1}{X}$$

where N is the half full shell number

$$N = \begin{cases} 1 & \text{for } Z < 2 \\ 5 & \text{for } 2 < Z < 10 \end{cases}$$

NOTE: Lindhard and Winther used a parameter Y in both first and second terms of the L_2 function, i.e.

$$L_2 = \ln Y - \frac{3^{1.5}}{5x} \frac{1}{Y}$$

instead of

$$L_2 = \ln \frac{2mv^2}{h\omega_p} - \frac{\langle T \rangle}{\frac{1}{2} mv^2}$$

where $Y = \frac{2mv^2}{h\omega_p}$ and $X^2 = \frac{e^2}{\pi h V_F}$

where V_F is the Fermi velocity $V_F = \frac{h}{m} (3\pi^2 n)^{\frac{1}{3}}$ and $\omega_p{}^2 = \frac{4\pi e^2 n}{m}$

n is the density of plasma.

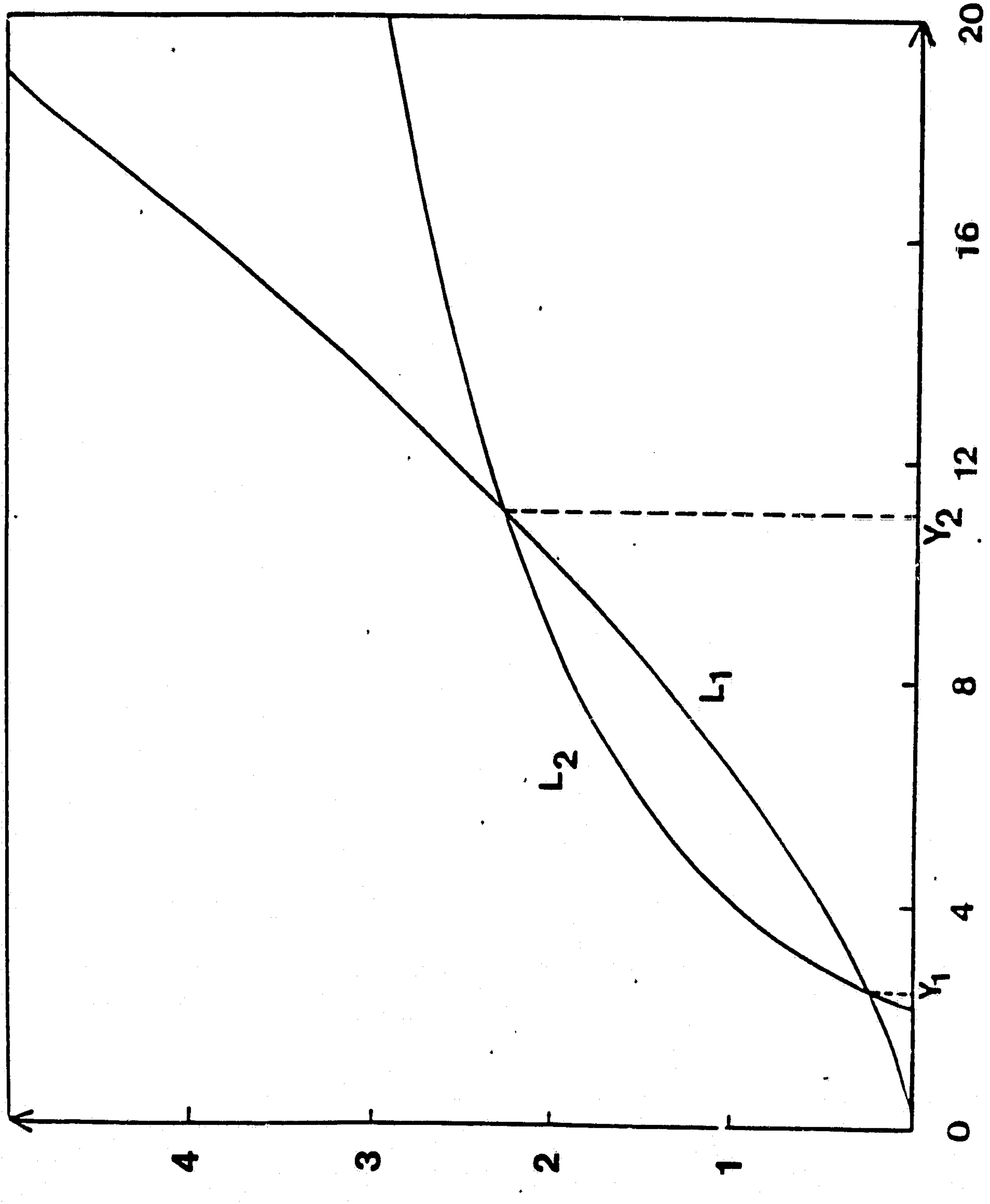


Figure 1.

Applying this formula in the atomic or molecular scale, i.e. in the local plasma model n is the electronic wave function square of ground state. Thus Y and X are the function of density since we know the wave function, L_2 can be easily obtained. Now we will show that the second term of L_2

$$\frac{\langle T\rangle}{\frac{1}{2} mv^2} \text{ is equal to } \frac{3^{1.5}}{5X} \frac{1}{Y}$$

the following formulae are used

$$X^2 = \frac{e^2}{\pi h v_F} \quad \text{definition of } X \tag{17.1}$$

$$\omega_p{}^2 = \frac{4\pi e^2 n}{m} \tag{17.2}$$

$$\varepsilon_F = \frac{1}{2} m \, V_F{}^2 = \frac{h^2}{2m} (3\pi^2 n)^{\frac{2}{3}} \tag{17.3}$$

$$\langle T\rangle = \frac{3}{10} m \, V_F{}^2 \tag{17.4}$$

From (17.3) we have $\sqrt{n} = \frac{m}{\pi h} \cdot \sqrt{\frac{m}{3h}} \, V_F \cdot \sqrt{V_F}$

from (17.2) we have $\omega_p^2 = \frac{4\pi e^2}{m} \cdot n$

thus

$$h\omega_p = \sqrt{\frac{4n}{m}}\ eh\ \frac{m}{\pi h}\ \sqrt{\frac{m}{3h}}\quad V_F\sqrt{V_F} = A\ V_F\ \sqrt{V_F}$$

where $A = 2\ me\sqrt{\frac{1}{3\pi h}}$

$$Y = \frac{2mv^2}{h\omega_p} = \frac{2mv^2}{A\ V_F{}^2}\ \sqrt{V_F} = \frac{2m\sqrt{V_F}}{A}\ \left(\frac{V}{V_F}\right)^2$$

from (17.1) we have $\sqrt{V_F} = \frac{1}{X}\sqrt{\frac{e^2}{\pi h}}$

thus

$$Y = \frac{\sqrt{3}}{X}\ \left(\frac{V}{V_F}\right)^2$$

since from (17.4) we know $\langle T\rangle = \frac{3}{10}\ m\ V_F^2$, finally we have

$$L_2 = \ln\ Y - \frac{3^{1.5}}{5x}\ \frac{1}{Y}$$

CALCULATION OF MOLECULAR STOPPING POWER

In this section, we perform calculations on the molecular stopping power of H_2, He, N_2, O_2 and water vapor for wide proton projectile energy regions (for H_2, He, 100 Kev - 2.5 Mev, 40 Kev - 2.5 Mev else). Comparisons of the experimental data are indicated in tables 6 to 11, (see reference [27] and [28]).

The basic formula for the stopping power of local plasma is as follows:

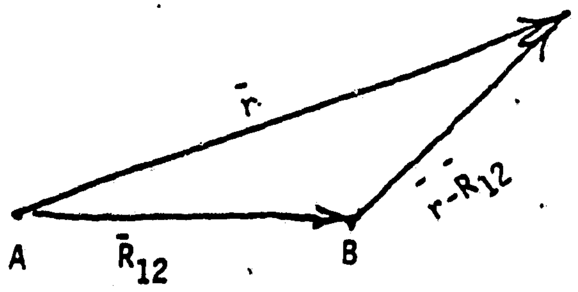
$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4 N}{m v_p^2} \int \rho(r) \ln\left(\frac{2mv_p^2}{\gamma h\omega_p(r)}\right) d^3r$$

To extend the formula to low energy regions, it is only necessary to replace $\ln\left(\frac{2mv_p^2}{\gamma h\omega_p(r)}\right)$ by L function, which we have established in the section entitled "Stopping Number Function."

Now we are interested in molecular stopping power. The charge density in the integral should be the electron density of molecules. As we mentioned in the section titled "Stopping Number Function," the Gordon-Kim model is a rough model of molecular electron density. They assumed that no arrangement or distortion of the separate atomic density takes place when the atoms are brought together. The total electron density of two interacting atoms is, therefore, taken simply as the sum of the two atomic densities.

$$\rho_{\text{molecule}}(\bar{r}) = \rho_A(\bar{r}) + \rho_B(\bar{r} - \bar{R}_{12}) \qquad (18)$$

where $\bar{R}_{12}$ is the internuclear distance.



Let us use H_2 as an example to explain how to apply formula (18). The ground state wave function of the hydrogen atom is $\frac{1}{\pi} e^{-r}$. The electron density of hydrogen atom is $\frac{1}{\pi} e^{-2r}$. According to (18)

$$\rho_{H_2} = \frac{1}{\pi} e^{-2r} + \frac{1}{\pi} e^{-(2\sqrt{r^2 + R_{12}^2 - 2rR_{12}\cos\theta})}$$

For other atoms the atomic wave functions are obtained by Clementi, Roetti [29] (published in atomic data and nuclear data). They used Roothan-Hartree-Fock method to calculate basic function and their coefficients for ground and certain excited states of neutral and ionic atoms for $Z<54$. For molecules which contain more than two atoms the model can be extended as follows

$$\rho_{\text{molecule}} = \rho_A(\bar{r}) + \rho_B(\bar{r} - \bar{R}_{BA}) + \rho_C(\bar{r} - \bar{R}_{AC}) \qquad (19)$$

Here we present the calculation of water vapor which contains three atoms.

The angle between two OH bounds is about 105°. It should be calculated by formula (19), but for simplicity in this section we neglected the H-H overlap simply as follows

$$\rho_{H_2O} = \rho_O(\bar{r}) + 2\,\rho_H(\bar{r} - \bar{OH})$$

Also we need to consider partial ionic bond effect. Many compounds exhibit partial ionic bond rather than pure covalent bond. Pauling defined partial ionic fraction [30] as the measured dipole moment divided by ideal dipole moment. Consider, for example, the compound, HCl. The distance between two nuclei is 1.275A°, the partial ionic fraction is $p = \frac{\mu}{\mu^{\circ}} \times 100\%$, $\mu^{\circ} = e \times R_0 = 4.80 \times 1.275 = 6.12$ D, but the actual measured dipole moment $\mu^{\circ} = 1.03$ D. Hence, $p = \frac{1.03}{6.12} \times 100\% = 17\%$. H_2O is also partial ionic bonded compound. The actual measured dipoment is $\mu = 1.94$D the ideal dipoment $\mu^{\circ} = e\,R_0 = 4.8 \times 0.958$ D $=$ 4.598D the partial ionic fraction $p = \frac{\mu}{\mu^{\circ}} = 0.42$. The mole-cule's electron density of partial ionic bonded compounds can be expressed as follows

$$\rho_{molecule} = \rho_A^{+}(\bar{r}) + \rho_B^{-}(\bar{r} - \bar{R}_{AB})$$

with $\rho^{\pm} = (1 - p)\,\rho(\bar{r}) + p\,\rho^{\pm}(\bar{r})$

The case $p = 1$ (pure ionic bond) physically corresponds to moving one electron from one atom to another atom. Now for one atom we use wave function of positive ion, for another atom we use wave function of negative ion. For the case p=0, that is the pure covalent bond, we still use the neutral atom's wave function. H_2, O_2, N_2, are all pure covalent bond molecules.

Water vapor is a partial ionic bonded compound. The distances between nuclei are listed in table 6.

Table 6.

	H-H	H-O	N-N	O-O
R(A)	0.74	0.958	1.094	1.207

Table 7 lists the results of this paper together with Andersen and Ziegler [31], curve fitted results and three sets of experimental data for H_2 molecules. Good agreement within 20 percent is found with experimental data from proton energy 100 Kev. - 2.5 Mev. Calculations from the equations established by Bonderup [20] were also undertaken by extending them to molecular system. Table 7 lists these values for H_2 molecules in the last column. These differ from our results in the low energy regions. Table 8 lists the same physical quantities for helium gas. The same trend is observed as in the case of the H_2 molecule.

Table 9 lists the results of this model together with Andersen-Zeigler and three sets of experimental data from proton energy 40 Kev - 2.5 Mev for

N_2 molecule. Table 10 lists the same physical quantities for O_2. Table 11 lists the results of this model together with Reynolds et al. experimental data for water vapor all these tables show theoretical results of this model are in good agreement with experimental data.

for the hydrogen molecule for various proton energies.

E (keV)	Theoretical Values of the Present Paper	Curve Fitted Values Andersen and Ziegler [31]	Reynolds et al.* [32]	Langley [33]	Bonderup and Hrelpland [34]	Theoretical Values Calculated from Bonderup's Work [20]
100	11.41	11.6	11.66		11.2	10.23
200	7.52	8.0	7.80		7.64	7.02
300	5.70	5.95	5.82	4.54 (311 kev)		5.39
400	4.63	4.60	4.70			4.41
500	3.93	4.00	3.94			3.75
600	3.42	3.40	3.40	3.82 (581.5 kev)		3.28
700	3.04	3.00				2.92
800	2.75	2.75		2.73 (778.7 kev)		2.64
900	2.50	2.50				2.41
1037	2.24	2.35		2.14		2.16
1555	1.62	1.64		1.53		1.57
2047	1.30	1.21		1.22		1.24
2591	1.07	1.07		1.04		1.04

*Andersen and Ziegler [31] note that the data in reference [32] appear to be constantly high by amount ranging from 5 percent to 10 percent.

Best Available Experimental Results								
E(keV)	Theoretical Values of the Present Paper	Curve Fitted Values Andersen and Ziegler [31]	Reynolds et al. [32]	Park and Zimmerman [35]	Bonderup and Hrelpland [34]	Philips [36]	Brolley and Ribe [37]	Theoretical Values Calculated from Bonderup's Work [20]
80	7.46		7.37	7.15		6.6		
100	7.07	7.16	7.30	7.05	7.02			5.45
200	5.38	5.64	5.55	5.64	5.60			4.49
300	4.26	4.39	4.41					3.78
400	3.59	3.60	3.69					3.25
500	3.10	3.07	3.18					2.85
600	2.73	2.69	2.81					2.54
700	2.45	2.41						2.29
800	2.23	2.19						2.09
900	2.15	2.00						1.92
1000	1.89	1.92						1.79
2000	1.12	1.14						1.07
4400	05.95	0.600					0.585	0.576

Table 9. Proton stopping cross section values (in units of 10^{-15}eV cm^2) or more exactly $\frac{1}{2}$ stopping cross section per molecule (10^{-15}eV-cm^2) of N_2 gas

E(keV)	Theoretical Value of the Present Paper	Curve Fitted Values Andersen and Ziegler[31]	Best Available EXPERIMENTAL RESULTS		
			Reynolds et al. [32]	Philips [36]	Langley [33]
40	17.20	16	17.1 ±2.6	14.1	
50	17.81	16.9	17.8 ±2.6	14.8	
60	18.24	17.3	18.2 ±2.6	15	
70	18.48	17.8	18.5 ±2.6	14.9	
80	18.41	17.9	18.5 ±2.6		
90			18.25±2.6		
100	17.79	17.7	17.9 ±2.6		
200	13.26	14.1	14.7 ±2.6		
300	10.85	11.2	11.2 ±1.7		
400	9.24	9.3	9.34±1.7		
500	8.10	8.1	8.08±1.7		
600	7.25	7.2	7.21±1.7		
700		6.7			
800		6.0			
900		5.65			
1037	5.20				4.78
2074					
2591	2.71	2.72			

Table 10. Proton stopping cross section per atom (in units of 10^{-15}eV cm^2) or more exactly $\frac{1}{2}$ stopping cross section per molecule (10^{-15} eV-cm^2) of O_2 gas

E(keV)	Theoretical Value of the Present Paper	Curve Fitted Values Andersen and Ziegler [31]	Best Available EXPERIMENTAL RESULTS		
			Reynolds et al [32]	Philips [36]	Langley [33]
40	15.89	14.6	15.2 ±2.6	12.5	
50	16.52	15.5	16.4 ±2.6		
60	16.99	16.2	16.9 ±2.6	14.2	
70	17.29	16.7	17.15±2.6	13.8	
80	17.48	17	17.25±2.6	13.8	
90		17.1	17.25±2.6		
100	17.43	17.0	17.17±2.6		
200	14.36	14.6	14.7 ±2.6		
300	11.84	11.9	11.99±1.7		
400	10.14	10	9.76±1.7		
500	8.92	8.8	8.84±1.7		
600	7.99	7.9	7.91±1.7		
700		7.0			
800		6.5			
900		6			
1037	5.64				5.25
2074					
2591	2.97				2.85

Table. 11. Proton stopping cross section per molecule (10^{-15} eV-cm^2) of H_2O vapor

E (keV)	Theoretical Values of Present Report	Reynolds et al. [32]
40	28.81	25.0 ± 2.6
50	28.81	26.1 ± 2.6
60	28.59	26.9 ± 2.6
70	28.22	27.5 ± 2.6
80	27.77	27.6 ± 2.6
90	28.28	27.5 ± 2.6
100	26.77	27.3 ± 2.6
200	21.04	22.0 ± 1.7
300	17.06	17.9 ± 1.7
400	14.43	15.0 ± 1.7
500	12.59	13.0 ± 1.7
600	11.20	
700	10.13	
800	9.28	
900	8.56	
1000	7.97	

MOLECULAR EFFECT OF STOPPING POWER

Deviations from Bragg's rule due to chemical structure have been recently systematically studied by several experimenters. Some interesting conclusions were summarized from these experiments. Now, we have already obtained stopping cross section of molecules by using method established in the sections titled "Stopping Number Function" and "Calculation of Molecular Stopping Power." We can also easily obtain the atomic stopping cross section by calculating the difference of these two quantities. In this way we can obtain the deviation from Bragg's rule theoretically. A discussion, based on this evaluation and on conclusion from the experimental side, will be presented in this section.

Discussion on deviation from Bragg's rule due to chemical structure of stopping power of molecules is of great interest. In 1905, Bragg and Kleemman first proposed the Bragg's rule [5]. It states that the stopping power (or stopping cross section) of a molecular substance is the additive sum of the atomic stopping powers multiplied by the number of times each atom occurs in the molecule. Bragg's rule has been shown by Thompson [38], for very high velocity proton to be valid within about 1%. Wilson and his co-workers [39], [40], [41], [42] systematically studied the molecular effect on mean excitation energy. Considerable deviations from Bragg's rule on mean excitation energy were found. This is not contradictory to Thompson because due to Bethe's formula

$$-\frac{dE}{dx} = \frac{4\pi e^4 Z}{mv^2} N \ln \frac{2mv^2}{I}$$

even though there may be considerable difference in mean excitation energy I, for very high velocity case the percentage deviation on stopping power can still be very small.

For low energy projectile the situation is more complex. Many authors found no molecular effect on stopping power. Reynolds et al. [32], and Park and Zimmerman [35], found there existed deviation from Bragg's rule. Since 1971, Baylor group did several experiments and thus systematically studied deviation from Bragg's rule due to chemical structure, [6], [7], and [8]. They used α particle as the projectile from 300 keV to 2 MeV and many gaseous compounds as targets in their experiments. The following conclusion have been given:

1. Physical effects appear to have caused deviation from Bragg's rule. The stopping power of H_2O vapor obtained by Reynolds, et al. [32], was found to be an average 11% higher than that of D_2O ice obtained by Wenzel and Waling for proton of 30-600 keV [43].
2. Chemical binding effects are more likely to cause departure from Bragg's rule for low velocity projectile.
3. Bourland and Power [7] said Bragg's rule applies to the gaseous compounds which contain single and double bonded molecules. Bragg rule does not apply to compounds containing triple bonds. For α particles of energy 0.3 - 2 Mev, the deviation of Bragg's rule are found as much as 12.8%. Especially they indicated that molecular hydrogen obeys Bragg's rule. One year later, Power et al. [6] wondered about their previous conclusion. They said "this observation greatly weakens the assumption that a physical state effect is possibly the cause of deviation from Bragg's rule and may even imply that the problem is not due to a difference in $\varepsilon(C)$ (stopping cross section) under certain circumstances but rather than the atomic stopping cross section $\varepsilon(H)$ may be considerably different than one-half the molecular stopping cross section $\varepsilon(H_2)$ as has usually been assumed in the past. In 1974 Lodhi and Power [8] gave a more careful conclusion. They said that single bonded compounds involving C, H, F and Br have been shown to have molecular stopping cross sections that are predictable with errors of a very few percent by using vapor deposited solid carbon $\varepsilon(C)$ along with an $\varepsilon(H)$ that is common to eleven compounds. It appears that there exists no unique atomic stopping power for carbon and hydrogen which satisfies Bragg's rule for double bond compounds and that due consideration must be given to molecular structure when pre-

> dicting molecular stopping power from atomic stopping power for those compounds.

It appears they corrected their previous conclusion that the double bonded compounds have no deviation from Bragg's rule. However, their main difficulties lie in the fact that it is very hard to determine the atomic stopping power from experimental data.

Discussion on Deviation from Bragg's Rule, Due to Chemical Structure from Theoretical Model.

In the above section, we found the Baylor group met difficulties with determining the atomic stopping cross section from experiments. Actually, it is very hard to obtain atomic state hydrogen. However, from the local plasma model it is quite easy to calculate the atomic cross section, since atomic electron ground wave functions are employed in obtaining the density in local plasma model.

Table 11, 12, 13 show the calculated atomic and molecular stopping cross section of O_2, N_2, H_2, respectively. The percentage deviation from Bragg's rule are also listed.

Table 11. Atomic and molecular stopping cross section and deviation from Bragg's rule of O_2

E(keV)	40	100	200	300	500	1037	100000
S(atomic) $\frac{eV + 15^{-15}\ cm^2}{atom}$	17.44	17.48	14.65	12.15	9.1	5.72	0.1429
S(molecular) $\frac{1}{2}\frac{eV \times 10^{-15}\ cm^2}{molecule}$	15.89	17.43	14.36	11.84	8.92	5.64	0.1476
deviation	8.9%	0.3%	2%	2.6%	2%	2.4%	1.1%

Table 12. Atomic and molecule stopping cross section and deviation from Bragg's rule of N_2

E(keV)	40	100	200	300	500	1037	100000
S(atomic) $\frac{eV \times 10^{-15}\ cm^2}{atom}$	19.33	18.57	14.52	11.56	8.53	5.30	0.1340
S(molecular) $\frac{1}{2}\frac{eV \times 10^{-15}\ cm^2}{molecule}$	17.70	17.79	13.26	10.55	8.10	5.20	0.1319
deviation	4%	4.2%	7.4%	6.1%	5%	1.9%	1.3%

Table 13. Atomic and molecular stopping cross section and deviation from Bragg's rule of H_2

E(keV)	100	200	300	500	800	1037	2591
S(2xatomic) $\frac{2\text{xeVx}10^{-15}\text{cm}^2}{\text{atom}}$	12.7	8.13	6.1	4.17	2.89	2.36	1.11
S(molecule) $\frac{\text{eVx}10^{-15}\text{cm}^2}{\text{molecule}}$	11.43	7.53	5.71	3.93	2.75	2.24	1.%
deviation	10%	7.4%	6.4%	5.8%	4.8%	5.1%	3.6%

From Table 11, 12, 13 the following facts are found:

1. When the projectile's velocity becomes extremely large, the deviation from Bragg's rule almost vanishes for N_2, O_2 gases. When the protons energy increased to 100 Mev, the deviation from Bragg's rule decreased to almost 1%. This result agrees with Thomson's predictions.

2. When the protons velocity becomes comparable to the atomic electron velocity (corresponding to proton energy 40-100 keV) there may exist considerable deviations from Bragg's rule.

3. Deviations from Bragg's rule are also found to depend on chemical structure of molecule. As is well known in chemistry O_2's structure is a little bit fuzzy. From bond energy point of view, O_2 is still a double bonded molecule. Meanwhile N_2 is 100% triple bonded molecule, H_2 is a single bonded molecule. It is also noticed that the maximum deviation for O_2, N_2 and H_2 above 100 Kev proton energy are about 2.6%, 7.4% and 10%, respectively. Meanwhile the internuclear distance for O_2, N_2, and H_2 are 1.20A°, 1.094A° and 0.74A°, respectively.

It appears, the smaller the internuclear distance the more the deviation will be. When Gordon-Kim model is employed, the smaller the internuclear distance always means that there is more overlap of electron clouds. Thus more overlap causes more deviation from Bragg's rule. In this model, the molecular binding effects are also determined by these overlap of electron clouds. However, Gordon-Kim model is a very simple model for diatomic molecules. The internuclear distance is the only relevant parameter but the most important information about the molecular effect is contained in this parameter. There is a very strong relationship between the bond energy and the distance between the nuclei. The stronger the bond energy, the shorter the distance will be. It is interesting to note that the single bonded, double bonded and triple bonded carbon molecules have inter-nuclear distances equal to 2.94, 2.52, and 2.24 in Bohr units respectively. It means that the triple bonded carbon has more overlap than the single bonded carbon. We may thus expect that the triple bond carbon will have more deviation from Bragg's rule than the single bonded carbon. It is expected from the above statement that for the same compounds the triple bonded molecules most likely have more deviation from Bragg's rule than single bonded molecules but it does not mean that we agree with the statement that the single bonded molecules have no deviation from Bragg's rule.

Actually from our calculation, it was found that H_2 had considerable deviation from Bragg's rule at low projectiles energy. (10% for 100 Kev proton energy) due to its small internuclear distance 1.074A° and relatively large overlap of electron cloud. It was also noticed that all these deviations due to molecular effect always decreased the stopping power.

One of the reasons to understand the above fact is that the binding effects always weaken momentum transfer and cause the upper limit of momentum transfer to be less than $2mv$ and thus reduce the stopping power. Another reason is due to the shell correction term. As we know the first shell correction term is proportion to $\langle T\rangle/mv^2$ for bond states $\langle T\rangle \sim |\langle E\rangle|$. Thus, more binding effect increased the kinetic energies thus decreasing of stopping power.

CONCLUSION

We have established a modified local plasma model which in conjunction with the Gordon-Kim model affords a method to calculate molecular stopping power even at low projectile energy. By using this model the main conclusion on deviation from Bragg's rule, summarized by Baylor group's experiments, can be understood. Some ambiguity on deviation from Bragg's rule of H_2 is now understood under the present model. The assumption that $\varepsilon(H) = \frac{1}{2}\ \varepsilon(H_2)$, is not correct from overlap point of view (where ε is the stopping cross section). The only conclusion by using simple Gordon-Kim model is that the more percentage overlap caused more deviations. In other words, the stronger the binding effect the more deviation from the Bragg's rule will be. It appears that for the same compounds, triple bonded molecules most likely caused more deviation than the single bonded molecules.

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APPENDIX

THE EQUIPARTITION RULE AND NUCLEAR MOMENTUM RECOILING

A semi-classical three body collision model has been established to estimate the upper limit of total momentum transfer of proton incident on hydrogen atoms. Numerical results revealed that the equipartition rule in shell correction deserves more careful study.

We have mentioned in the section titled "Stopping Number Function" that to apply a correction on the first term of shell correction we used Brown's results. Specifically the term $\langle T\rangle/mv^2$ was used instead of the term $\langle T\rangle/\frac{1}{2}mv^2$ of plasma model.

In their paper "Stopping Power of Electron Gas and Equipartition Rule" Lindhard and Winther [15] mentioned that their result of first term of shell correction was in agreement with Walske's result [22]. As is known, Walske's shell correction term is just twice that of Brown [21]. This result leads one to believe the existence of an equipartition rule in case of shell corrections. Lindhard and Winther noticed this, and surmised that there was a correspond-ing equipartition rule in the plasma model. This implies that the plasma resonance excitation and the close collision each had equal contribution to stopping power. It appears that plasma model gives exactly the same results as quantum perturbation theory. Lindhard and Winther emphasized this fact as a success of local plasma model. Fano also mentioned this fact in his paper "Penetration of Proton α Particles and Mesons" [44]. He used the results of plasma model to support the existence of the equipartition rule in shell corrections.

The so called equipartition rule has its origin in Bethe's stopping power formalism. Bethe divided the stopping power of fast charged particles into two parts, that due to the distant collision and the close collision. There was also found to have considerable contribution to stopping power for those particles which move not so fast. Thus besides the logarithm term, the so called shell correction terms should also be included in calculating the contributions to stopping power.

Brown had calculated the stopping number function and shell correction of K shell electron by using the hydrogenic wave functions. The expression for stopping number is as follows

$$B_K = \int_{Emin}^{Emax} EdE \int_{Qmin}^{Qmax} \frac{dQ}{Q^2} |F_n(Q)|^2$$

where $Q = (\bar{P} - \bar{P}')^2/2m$ $\bar{P}$ and $\bar{P}'$ being the momenta of incident particle before and after collision $|F_n(Q)|^2$ is the form factor. Brown took the simple two body collision model, namely particles colliding with a free electron to estimate the upper limit of momentum and energy transfer. Thus he obtained the maximum momentum transfer $\Delta P_{max} = 2mv$. Brown obtained an asymptotic expression for stopping power of K electron as $B_K = 2 \ln \eta_K + 2.57861 - \frac{1}{\eta_K}$ where $\eta_K = \frac{1}{2} mv^2$ in units of $Z^2_{eff_K}$ Ry is the first term of shell correction. Meanwhile Walske, took both the upper limit of momentum transfer and energy transfer as infinity and obtained the stopping number functions

$$B_i\ (\theta_n, \eta_0) = \int_{W_{in} = \theta_i/\eta_i^2}^{\infty} EdE \int_{w^2/4\eta_i}^{\infty} \frac{dQ}{Q^2} |F_{W_i}\ (Q)|^2$$

where $i = K, L, M$ denotes the different shell, $\eta_i = mv^2/2$ in units of $Z^2{}_{eff}$ Ry, θ_i is the observed ionization potential of ith shell divided by "ideal ionization potential."

Walske also defined the shell correction term $C_i(\theta_i, \eta_i)$ as follows $B_i\,(\theta_i, \eta_i) = S_i\,(\theta_i) \ln \eta_i + T_i\,(\theta_i) - C_i(\theta_i, \eta_i)$ and he thus obtained asymptotic formula B_K and B_L both for K and L shell. The correct coefficient of $1/\eta_{K2}$ is taken from Khandelwal's paper [25].

$$B_K = 2 \ln \eta_K + 2.57861 - 2\eta_K^{-1} - (\frac{25}{3})\, \eta_K{}^{-2}$$

$$B_L = 8 \ln \eta_L + 25.5766 - 2\eta_L^{-1} \text{ (to order } \eta_L^{-1})$$

Notice that the first shell correction terms are $2\eta_K^{-1}$ or $2\eta_L^{-1}$. The K-shell term $2\,\eta_K^{-1}$ thus is twice that of Brown's term η_K^{-1}.

In other words, shell correction can also be divided into two high and low momentum transfer parts. Such parts each contributes equally to stopping power. Indeed, Walske explicitly divided shell correction into two parts.

$$C\,(\theta, \eta) = C_1\,(\theta, \eta) + C_2(\theta, \eta)$$

where C_1 and C_2 are low and high momentum transfer parts respectively. Furthermore, he also showed that C_1 and C_2 are equal to the order of η_i^{-1} both for K and L shells and to order $1/\eta_{K2}$ for K-shell. Walske's results are only limited to K and L shell electrons of hydrogenic atoms. But Fano made an assumption that the conclusion $C_1 = C_2$ can be generalized to any shell of any atom. This is so called the equipartition rule of shell correction. All these conclusions are based on Walske's assumption that the upper limits of the momentum transfer and the energy transfer are infinity. The question is whether the assumption is true or not.

Brown took the upper limit of momentum transfer as 2mv and this is based on the assumption that the electron initially is free. Two factors are neglected in this assumption. First Brown neglected the binding effect of the electron. Second, he also neglected the nuclear momentum recoiling. It is obvious that if the nuclear motion is involved then due to its huge mass, the total momentum transfer may be greatly increased. But by how much? Is taking infinity a good approximation for the upper limit of momentum transfer? It appears the answer should be dependent on the velocity of projectile. For instance, if the projectile moves extremely slow then the nucleus may obtain sufficiently large momentum transfer. Otherwise due to the short interaction time, nuclear momentum could be small and the upper limit of total momentum transfer will not differ too much from 2mv.

In this appendix, we estimate the upper limit of momentum transfer by the projectile to a hydrogen atom by establishing a semi-classical three body collision model. For protons energy over 50 Kev a fitting formula from numerical results was obtained: (See for the general results later in this appendix)

$$\Delta P_{max} = 2\, m_e V_p \xi$$

where $\xi = \frac{1}{2} \left(1 + 8.9 \left(\frac{V_o}{V_p}\right)^5\right) \left(1 + \sqrt{1 - \left(\frac{V_o}{V_p}\right)^2}\right)$

where V_p is the velocity of proton and V_o is the Bohr velocity. Numerical results of ξ of various proton energies are listed in table 14.

Table 14.

E(keV)	50	75	100	200	400	1600
ξ	2.20	1.43	1.19	1.01	0.991	0.996

From the above formula and the table we see that for high energy projectiles Brown's assumption is correct. The values of ξ slightly less than unity is due to binding effect but for low energy proton the factor of nuclear momentum play a more important rule. There is a considerable correction to Brown's results. But even at 50 Kev protons energy the numerical result of ξ is only 2.2, still quite different from Walske's assumption of infinity. It is true that when protons energy becomes smaller, then the correction factor ξ is expected to increase rapidly, but then the expansion of stopping number function B_i should involve more terms than just the term η_i^{-1}. However Fano's assumption that $C_1 = C_2$ or equipartition rule of shell correction, deserves a careful study.

Nuclear Momentum Recoiling

In this section first we shall review the conservation laws and the resulting physical quantities when the collision is assumed to be taking place between two bodies only. Later, three body collision problems are handled numerically in a semi-classical manner. Nuclear momentum recoiling effect is estimated in the relatively low energy region of Bethe stopping power.

Semi-Classical Formulation of Three Body Problem for Relatively Low Energy Stopping Power

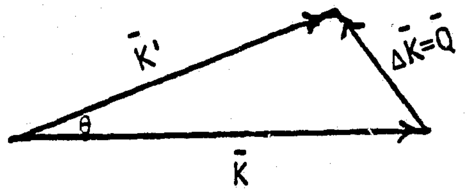
Estimating of the Quantities Q(min) and Q(max) Two Body Collision.

Let us first consider the energy regions such that we can always neglect the nuclear recoiling energy, i.e. we can express energy conservation law as

$$(E_n - E_o) = h^2 \ (K^2 - K'^2)/2M_p$$

where E_n and E_o are the eigen energy values of final state of electron and initial state of electron, $h\bar{K}$ and $h\bar{K}'$ are the initial and final momentum of projectile.

We know that in lab. coordinates the momentum changes of projectile are much smaller than the momentum of projectile itself, i.e. $\Delta K << K$ or $\theta << 1$ so, we have $(E_n - E_o) = h^2(K^2 - K^{2}{}')/2M_p \cong h^2 K(K-K')/M_p = hV_p(K-K')$



since θ is small

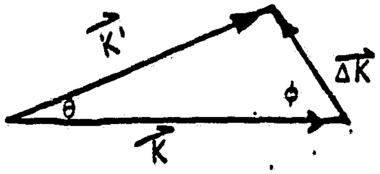
$$Q^2 = K^2 + K'^2 - 2KK' \cos(\theta) = (K-K')^2 + (K_\theta)^2$$

$$Q \cong \sqrt{(E_n - E_o/hV_p)^2 + (K_\theta)^2}$$

Thus $Q(min) = (E_n - E_o)/hV_p$

This Q(min) estimation is justified unless one deals with the extremely low energy case for hydrogen atom targets when proton's energy is lower than 10 kev (Andersen and Ziegler) for which we need to consider nuclear recoiling energy term. Now let us estimate Q(max) term very carefully. This upper limit estimation will involve a correction to Bethe's theory.

We use Landau's treatment of Bethe's theory for estimating the upper limit of momentum transfer. Essentially it neglects the nuclear recoiling displacement and momentum. Hence it becomes simply a two body collision. In this model, the projectile collides with a free electron.



The projectile's initial momentum is hK and the final momentum is hK'. All the momentum changes of projectile are transferred to the electron which is free in its initial state hence we write down the momentum and energy conservation laws as,

$$K'^2 = K^2 + \Delta K^2 - 2K\Delta K\cos\phi$$

$$\Delta E = \frac{K^2 - K'^2}{2M_p} = \frac{Q^2}{2m}$$

$$\Delta K = Q$$

where Q is the momentum of electron (in our case projectile momentum loss is entirely transferred to the electron) m is the mass of electron. From above conservation laws, we have

$$\frac{2K\Delta K\cos\phi \;-\Delta K^2}{2M_p} = \frac{Q^2}{2m}$$

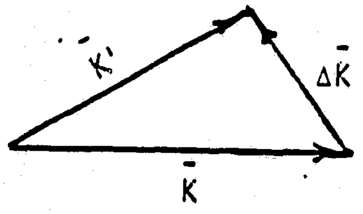
$$\frac{2KQ\cos\phi}{M_p} = \left(\frac{1}{m} + \frac{1}{M_p}\right) Q^2 \cong \frac{Q^2}{m}$$

or $Q(\max) = 2\ mV_p$

It is a very simple model, but it works at high energy. The main physical reason is that the projectile moves too fast to cause any significant displacement of the nucleus. At relatively low energy due to long interaction time, we need consider the nuclear recoiling momentum to correct the upper limit i.e. Q(max)

Semi-Classical Three Body Formulation

A model essentially based on classical three body problem was established. Consider a proton which collides with a hydrogen atom. The electron of the atom was initially assumed to be in its ground state. Somewhat semi-quantum conditions are involved in our model, besides usual classical columb interaction. Now let us see how the nuclear recoiling momentum influences the upper limit.



$$\Delta\bar{K}=\bar{K}'-\bar{K} = \Delta\bar{P}_e+\Delta\bar{P}_n$$

where $\Delta\bar{P}_e$ and $\Delta\bar{P}_n$ are the difference of the electron momentum and the nuclear momentum before and after collision. Now the projectiles momentum

C-2

not only can be transferred to the electron but also can be transferred to the nucleus. Furthermore as stated before we assume that the electron is in the ground state initially. Now let us set the initial momentum of nucleus to be zero i.e., $\Delta P_n = p_n$. Thus we have $\Delta\bar{K} = \Delta\bar{P}_e + \bar{P}_n$

$$\Delta K = |P_e| \sqrt{\frac{(\Delta P_e)^2 + 2\Delta\bar{P}_e \cdot \bar{P}_n + (P_n)^2}{P_e^2}} = |P_e|(1 + \eta)$$

where

$$1 + \eta = \sqrt{\frac{(\Delta P_e)^2 + 2\Delta\bar{P}_e \cdot \bar{P}_n + (P_n)^2}{P_e^2}} \tag{20}$$

We again write down the conservation laws;

$$\left\{ \begin{aligned} & K'^2 = K^2 + \Delta K^2 - 2K\Delta K \cos\phi && (21a) \\ & \frac{K^2}{2M_p} + E_0 = \frac{K'^2}{2M_p} + \frac{Pe^2}{2m} + \frac{Pn^2}{2M_n} + V_n && (21b) \\ & \Delta K = |P_e| \; (1 + \eta) && (21c) \end{aligned} \right.$$

For maximum momentum transfer $\cos(\phi) = 1$, as before. From (21a) we have $K^2 - K^{2\prime}/2M_p = (2K\Delta K - \Delta K^2)/2M_p$

from (21a), (21b), (21c)

we have

$$V_p |P_e| \; (1 + \eta) - \frac{P_e^{\,2}}{2M_p} (1 + \eta)^2 = \frac{P_e^{\,2}}{2m} + \frac{P_n^{\,2}}{2M_n} - (E_0 - V_n)$$

hence, $V_p|P_e|\,(1 + n) + (E_o - V_n) = \frac{1}{2}\, P_e^2 \, \{\frac{(1+n)^2}{M_p} + \frac{1}{m} + \frac{1}{M_n}\,\frac{Pn^2}{P_e^2}\}$

$$= \frac{1}{2}\, P_e^2 \alpha$$

where $\alpha = \frac{(1+n)^2}{M_p} + \frac{1}{m} + \frac{1}{M_n}\,\frac{P_n^2}{P_e^2}$

or $P_e{}^2 - \frac{2\, V_p P_e (1+n)}{\alpha} + \frac{2(V_n - E_o)}{\alpha} = 0$

$$P_e = \frac{V_p(1+n)}{\alpha}\Big[1 + \sqrt{1 - \frac{(V_n - E_o)\alpha}{\frac{1}{2}\, V_p^2 (1+n)}} \qquad (22)$$

$$\therefore \Delta K_{max} = P_e(1+n) = \frac{V_p(1+n)^2}{\alpha}\Big(1 + \sqrt{1 - \frac{(V_n - E_o)\alpha}{\frac{1}{2}\, V_p^2 (1+n)^2}}\Big) \qquad (23)$$

For high energy case $V_p >> V_0$ and thus there is no nuclear recoiling

$$\alpha \to 1/m, \quad \eta \to 0 \quad (V_n - E_0)\alpha / \frac{1}{2}\, V_p (1+n)^2 \to 0$$

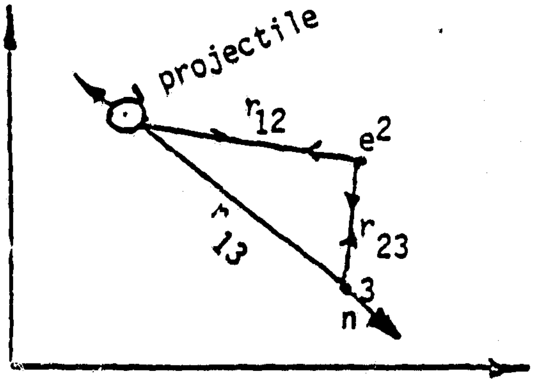
hence $\Delta K_{max} = 2 V_p m$

Therefore, for relatively low energy case, we have two corrections; one is from nuclear recoiling momentum, and another correction is from the initial energy of electron. For most cases the first correction is more important.

From the formula for ΔK_{max}, we can see ΔK_{max} depends on $1+\eta$ or depends on nuclear recoiling momentum P_n which extends the upper limit and will cause an additional stopping power.

In formula $$1+\eta = \sqrt{\frac{\Delta P_e^2 + 2\Delta \bar{P}_e \bar{P}_n + P_n^2}{P_e^2}} \qquad (24)$$

All these $\Delta\bar{P}_e$, $\bar{P}_n$, and $\bar{P}_e$ are numerical results of three body problem. Now let us establish fundamental equations.



we denote projectile by 1, electron by 2, and nucleus by 3.

For simplifying the calculations we established a two dimension model. It is not a bad approach because we are interested in nuclear recoiling effects in which the main contribution is due to the columb interactions between projectile and nucleus. This is partly due to the symmetry and partly due to our interest in obtaining average values.

Equations of motion for projectiles are as follows:

$$M\ddot{Y}_1 = -\frac{e^2(Y_1 - Y_2)}{r_{12}^3} + \frac{e^2(Y_1 - Y_3)}{r_{13}^3}$$

$$M\ddot{X}_1 = \frac{e^2(X_2 - X_1)}{r_{12}^3} - \frac{e^2(X_3 - X_1)}{r_{13}^3}$$

$$Y_1\Big|_{t=to} = b \qquad \dot{Y}_1\Big|_{t=to} = 0$$

$$X_1\Big|_{t=to} = 4a_0 \qquad \dot{X}_1\Big|_{t=to} = Vp$$

Where M is the mass of projectile which in our case is a proton. We took the integration time as projectile moved from $-4a_0$ to $4a_0$ for the standard gas state given the average distances between molecules are about the order of 10A and b is the impact parameter.

For the electron we have the following equations:

$$m\ddot{Y}_2 = \frac{e^2(Y_1 - Y_2)}{r^3_{12}} - \frac{e^2(Y_2 - Y_3)}{r^3_{23}} \qquad Y_2\Big|_{t=to} = \sin\phi \qquad \dot{Y}_2\Big|_{t=to} = Vo\sin\phi$$

$$m\ddot{X}_2 = \frac{e^2(X_3 - X_2)}{r^3_{23}} - \frac{e^2(X_2 - X_1)}{r^3_{12}} \qquad X_2\Big|_{t=to} = -\cos\phi \qquad \dot{X}_2\Big|_{t=to} = Vo\cos\phi$$

where ϕ is the initial phase of electron orbit

Equations of motion of nucleus are:

$$M_n\ddot{Y}_3 = \frac{e^2(Y_2 - Y_3)}{r^3_{23}} - \frac{e^2(Y_1 - Y_3)}{r^3_{13}} \qquad Y_3\Big|_{t=to} = 0 \qquad \dot{Y}_3\Big|_{t=to} = 0$$

$$M_n\ddot{X}_3 = \frac{e^2(X_3 - X_2)}{r^3_{23}} - \frac{e^2(X_3 - X_1)}{r^3_{13}} \qquad X_3\Big|_{t=to} = 0 \qquad \dot{X}_3\Big|_{t=to} = 0$$

As is well known numerically high order differential equations can be reduced to a first order equation such as:

$$Y^{(m)}=f(x,Y,Y',y',\ldots y^{(m-1)})$$

Let $Y=Y_1$, $Y'=Y_2$, $Y''=Y_3,\ldots Y^{(m-1)}=Y_m$ then this will reduce to

$$\begin{cases} Y_1{}'=y_2 \\ Y_2{}'=y_3 \\ \cdot \\ \cdot \\ \cdot \\ Y_m{}'=f(x,Y_1,Y_2,\ldots Y_m) \end{cases}$$

So our six second order differential equations are reduced to twelve first order equations. The electron is assumed initially to be in the first Bohr orbit. Since we took laboratory coordinates the nucleus is initially at rest in the position of origin. We emphasize here, the difference from the usual treatment. Here we took the impact parameter b as the vertical distance from the projectile to the nuclei's initial position and not the vertical distance from the projectile to the electrons initial position, as is usually done. To apply classical mechanics to the microscale system, the most serious difficulty is that the electron can eventually drop into positive ions columb potential well. It also caused numerical difficulties in practice because we need infinitesimal steps to keep acceptable accuracy.

To prevent this difficulty it looks as though we need to introduce somewhat semi-quantum condition. In 1951 David Bohm suggested an interruption of quantum theory in terms of "hidden variables." [45] Bohm proved that quantum mechanics can be explained as some modification to classical mechanics. Schordinger's equation can be expressed as:

$$m \frac{d^2\bar{r}}{dt^2} = - \nabla \left\{ V(\bar{r}) - \frac{h^2}{2m} \frac{\nabla^2 R}{R} \right\}$$

Where R is the real part of wave function or $R^2 = |\psi(\bar{r})|^2$

So the equation of motion for quantum mechanics can be expressed as using classical potential plus a quantum mechanical potential which is correction to classical theory.

Following Bohm we got some hint that this semi-quantum mechanics treatment prevents the electron from dropping into the nucleus. If given an additional semi-quantum potential then we will have an additional force to balance the usual columb force.

For $r \ll a_0$ this force will be greater than columb force. It will prevent electron dropping into the nucleus. For $r > a_0$, this force will vanish. In some sense this additional potential gives explanation of first Bohr orbit. The above discussion is for the bound state. For the scattering state the electron can approach the nucleus. Thus, we will establish a potential somewhat like Fermi distribution which depends on the energy of the electron

$$V_{ed} = \frac{h^2}{2mR^2} \frac{(e^{-10}+1)}{(e^{10E}+1)} \qquad (25)$$

Figure 2 gives the graphics of this potential for $E>1$ $V_{ed} \sim 0$, and for $E<-1$

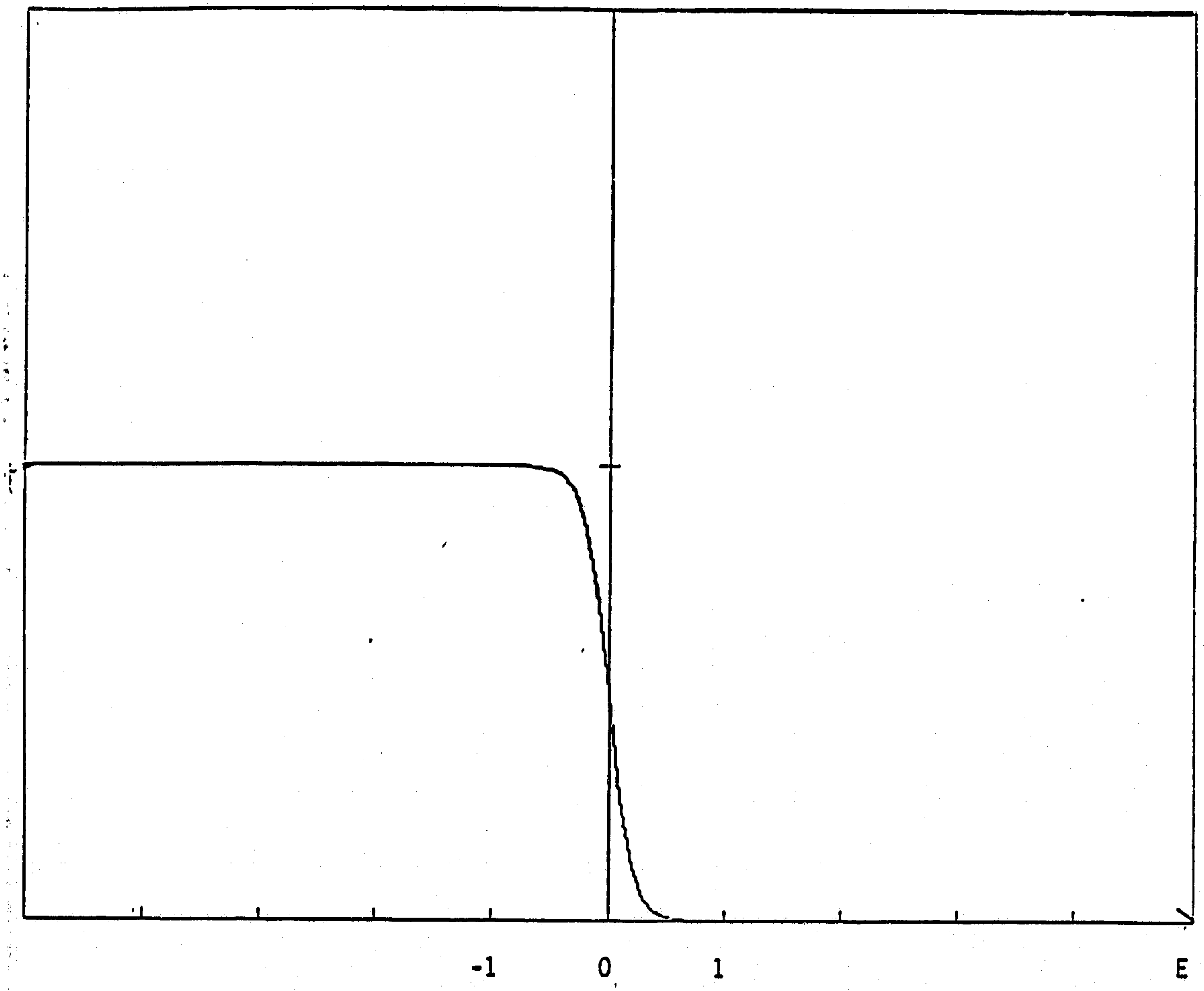


Figure 2.

$V_{ed} \sim \frac{h^2}{2mR^2}$ or we may say for scattering state our model is a classical model but for bound state we have an additional term somewhat semi-quantum term.

We use the expression (25) rather than a potential like

$$V_{ed} = \frac{h^2}{2mR^2} \qquad E<0$$

$$V_{ed} = 0 \qquad E>0$$

merely due to the reason that we need a continuous potential to obey the conservation law accurately. We have some freedom to choose e^{-10} or e^{-12} or e^{-8} in the terms of V_{ed}. The bigger the number we choose in exponential terms the sharper the curve obtained. But as mentioned too sharp a value will cause energy or momentum conservation problems.

We calculated these recoiling momenta and averaged them over phase of the electron orbit and then took the average over impact parameter b. Here as we mentioned earlier, b is the vertical distance from projectile to the initial position of the nucleus. From (23) we have the maximum momentum transfer

$$\Delta K_{max} = V_p \frac{(1+\eta)^2}{\alpha} \left(1 + \sqrt{1 - \frac{(V_n - E_0)\alpha}{\frac{1}{2} V_p^2 (1+\eta)^2}}\right) = \xi \, 2m \, V_p$$

In the stopping number formula instead of $2m\, V_p$ we have $2m\, V_p \xi$ hence we finally obtained the new stopping number formula

$$L = \ln \left(\frac{2m\, V_p^2 \xi}{I}\right)$$

In this two dimension model, there are two parameters, impact parameter b and initial phase. Numerically we calculated P_n, P_e, P_p, $(1+n)$, and finally took the average over ϕ and b. Table 15 shows some examples of P_n, P_e, P_p as functions of initial phase. Table 16 shows some examples of the average of ϕ as a function of impact of parameter b. The correction coefficient of the stopping number involves two factors. One is an additional contribution due to nuclear momentum recoiling. As b is very small this factor is very important, as b becomes larger this effect vanishes. Another factor is mainly due to the velocity of the electron in the initial state. This factor makes negative contribution on correction (make it less than unity) as V_p increases this factor becomes negligible. After an average over ϕ and an average over b, we obtained table 17 as a function of the projectiles energy.

Table 15. Momentums after collision as a function of the initial phase.

Initial Phase	Momentums after collision		
ϕ	P_p(m_e-Bohr/sec)	P_e(m_e-Bohr/sec)	P_n(m_e-Bohr/sec)
0	3672	1.39	9.28
1.10	3672	1.36	11.47
2.04	3672	1.30	11.27
2.98	3667	2.80	2.86
4.08	3671	1.83	12.31
5.03	3667	4.31	7.65
5.97	3672	2.35	9.67

(a) b =.1 (a_0) E = 100 kev

Initial Phase	Momentums after collision		
ϕ	P_p(m_e-Bohr/sec)	P_e (m_e-Bohr/sec)	P_n(m_e-Bohr/sec)
0	3672	1.47	1.99
1.10	3672	1.37	3.63
2.04	3672	1.21	3.50
2.98	3671	1.73	2.88
4.08	3671	2.15	0.84
4.87	3668	4.72	0.95
5.97	3672	1.25	1.09

(b) b =.5 (a_0) E=100 kev

Table 16. ξ as a function of impact parameters

$b(a_0)$	ξ
0.1	80
0.3	8.84
0.5	2.94
0.7	1.41
1.3	0.852

(a) (E=50 keV)

$b(a_0)$	ξ
0.1	39.2
0.3	3.82
0.5	1.17
0.7	0.9313
0.9	0.9318

(b) (E=100 keV)

$b(a_0)$	ξ
0.1	19.1
0.3	1.161
0.5	0.9660
0.9	0.9665

(c) (E=200 keV)

$b(a_0)$	ξ
0.1	7.5
0.3	0.981
0.5	0.983

(d) (E=400 keV)

Table 17.

E(keV)	50	75	100	200	400	1600
ξ	2.20	1.43	1.19	1.01	0.991	0.996

As we expected when projectiles energy is small that is when the projectile moves slow, it causes significant nuclear momentum recoiling effect. Meanwhile the initial velocity effect is covered by nuclear recoiling effect. As projectile moves fast it can not cause significant nuclear recoiling momentum. We can see that the initial velocity effect however is less important when the projectile moves very fast both effects vanish and there is no correction and we obtain the Bethe's formula.

An approximate useful formula obtained by fitting the values as energy greater than 50 kev, is:

$$\xi = \frac{1}{2}\left(1 + 8.9\left(\frac{V_0}{V_p}\right)^5\right)\left(1 + \sqrt{1 - \left(\frac{V_0}{V_p}\right)^2}\right)$$

Where V_0 is the Bohr velocity and V_p is the velocity of projectile. Numerical results of relative correction of stopping number are also calcued.

L/L_0 as a function of projectiles energy are listed below

E(keV)	50	75	100	200	400	1600
L/L_0	1.398	1.15	1.065	1.0035	0.998	0.9993

From the table we can see that for the hydrogen atom target and for the proton as a projectile of 50 keV nuclear recoiling momentum caused a consid-

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erable correction (40%) on stopping power for 100 kev about 6-7% correction on stopping above 200 kev the correction of stopping power can be negligible.

Argument of Extending to General Material.

Up to now we have calculated the recoiling momentum of hyderogen atom target. Now we will give an argument that this result can be roughly extended to a general case of any other atoms. Let us consider proton projectile passing through material composed of atoms of charge Ze. Then due to the columb interaction between proton and nucleus the momentum transfer is:

$$\Delta P_n = \int_{-\infty}^{\infty} f_y(t)\, dt$$

where $f_y(t)$ is proportional to Zt and is independent of the nuclear mass. Now only for estimating we suppose that all the momentum obtained by nuclei is transferred to the electrons. Thus Z electrons share their additional momentum. Hence on the average each electron obtained momentum independent of Zt and nuclear mass.

Then the additional stopping power is proportional to Zt but the stopping number is independent of Zt and nuclear mass. We can roughly say that the ratio of "additional stopping number" to stopping number of any atom are the same as for the hydrogen atom.