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FOR VERY LOW ENERGY IONS

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ABSTRACT

The energy loss by quasi-elastic stopping of very low energy ions passing through matter is discussed and the concept of close and distant collisions is introduced. The expression of the stopping cross-sections is derived and agrees well with the results of previous authors as far as the nuclear effect is concerned. However, the agreement is only partial for the electronic effect.
I. INTRODUCTION

When the velocity of a charged particle passing through matter greatly exceeds the velocity of the atomic electrons of the medium, the energy loss proceeds chiefly through inelastic collisions leading to the ionization or excitation of the atom.

The derivation of the stopping power formula for this effect has been done in first order perturbation theory using the Born approximation. The basic step is the calculation of the matrix element of the Coulomb interaction between the charged particle and the electron:

\[
\int \psi_{\text{final}}(\vec{r}, \vec{R}) \frac{Z_1 e^2}{|\vec{R} - \vec{r}|} \psi_{\text{initial}}(\vec{r}, \vec{R}) \, d\vec{r} \, d\vec{R}.
\] (1)

\( \vec{r} \) and \( \vec{R} \) denote the position of the particle-electron system, and \( Z_1 e \) is the charge of the projectile.\(^1\),\(^2\)

However, when the velocity of the projectile decreases to the order of magnitude of that of the most bound electrons, the Born approximation will no longer be valid for the following reasons.

The wave function of the projectile will be distorted by the field of the atomic electrons.

The electron orbit may be polarized by the field of the approaching particle.\(^3\) Moreover, the capture and loss of electrons experienced by the projectile becomes significantly important and the effective charge \( Z_1 e \) is now a decreasing function of the velocity.

In that case, the magnitude of the stopping power may be approximated quite satisfactorily by the "shell-corrections" method,\(^4\),\(^5\) at least for the K and L shells.
The modified Bethe's relation will generally take the form,

$$\frac{dE}{dx} = \frac{4\pi Z^2 e^4}{m v^2} N \left[ Z_2 \ln \left( \frac{2M_1 v^2}{I_{\text{ave}}} \right) - \sum_{i=k,l} C_i (v) \right],$$  \hspace{1cm} (2)

in which $Z_2 e$ is the charge of the atom of the medium, $M_1$, $m$ are the masses of the projectile and the electron, $C_i$ is a shell correction factor depending on the velocity $v$, and $N$ is the number of atoms per unit volume. $I_{\text{ave}}$ is the average ionization potential, which for large velocities may be determined by Bloch's method\(^6\) using the Thomas-Fermi model of the atom. However, for $v$ comparable to the electronic velocities, the theoretical estimation of $I_{\text{ave}}$ is difficult and in practice, one usually extracts it from experimental data.

If $v < (I_{\text{ave}}/2M_1)^{1/2}$, which, for example, corresponds to an energy of about 6 keV for the stopping of protons in hydrogen gas, the magnitude of the inelastic process becomes very small compared to the elastic and quasi-elastic process, consisting in the transfer of the projectile energy to the electrons and atoms of the medium.

The theoretical treatment of such cases is more difficult, especially for heavy ions, since the interaction is no longer confined to the particle-electron system but must be generalized to the two-atomic systems, including the interatomic forces and the binding forces of the electrons.

While for medium and low velocities, a quantum mechanical approach to the problem is desirable, N. Bohr however first pointed out the "orbital" picture, which, under some restrictive conditions, may be convenient and sufficient to get useful information and give reasonable predictions of the stopping power.\(^7\) This question has been analyzed further by Nielsen\(^8\) and by Lindhard and collaborators.\(^9\)
In a general discussion of the orbit of a particle in the field of various types of potentials\textsuperscript{10} it seems that some of the results obtained may be extended to this question in order to supplement those of the previous authors and to discuss some aspects of the quasi-elastic collision.

As a matter of fact, we shall conform in the following to the notations given in N. Bohr's work.

II. THE QUASI-ELASTIC APPROXIMATION

As was stated above, in the region of velocity whose boundary will be specified later, one must consider the collision between the atomic system of the projectile and the atom of the medium.

Roughly speaking, this may be described as the collision of two semi-penetrable spheres in which the interacting forces are of electrostatic origin.

The condition for the validity of the classical approximation is

\[ v \ll 2 Z_1 Z_2 V_0 \]  

where \( V_0 = \frac{e^2}{\hbar} = 0.52 \times 10^{-8} \) cm is the electron velocity of the hydrogen atom.

This condition is derived for a Coulomb potential but for a non-Coulomb potential it must be slightly modified.

The presence of the electrons within these two systems creates a "screening effect" which modifies the scattering field.

Many types of potentials may be used to take into account this effect, such as the "Hartree" potential \( V(r) = -Z_r(r) \frac{e^2}{r} \), in which \( Z_r(r) \) is essentially an exponentially decreasing function of the distance \( r \), or the Thomas-Fermi potential.
\[ V(r) = \frac{Z_1 Z_2 e^2}{2} \phi\left(\frac{r}{a}\right), \]

\( \phi(r/a) \) being the Fermi function and \( a \), the screening parameter.

We feel, however, that it is more convenient to use the screening potential

\[ V(r) = \frac{Z_1 Z_2 e^2}{r} e^{-r/a}, \quad (4) \]

where \( a \) has the dimension of a length. This potential covers in fact most of the cases which we shall consider in the following.

According to N. Bohr, with the "screening effect" the condition for a classical approach to the problem is less restrictive, namely

\[ \lambda \ll a, \]

in which \( \lambda \) is the wave length of the projectile.

Let us define \( \chi \) by

\[ \chi = \frac{b}{a} \]

where

\[ b = \frac{2Z_1 Z_2 e^2}{M_0 V^2} \quad \text{and} \]

\( M_0 \) is the reduced mass of the system.

Then the case \( \chi \ll 1 \) will correspond to a very small screening effect.

In fact the scattering law is essentially of the Rutherford type in this region.
For $X > 1$, the screening will be important and one may expect significant deviations from this law.

Introducing the minimum distance of approach $\rho$ defined by

$$\rho = \frac{\chi e^{-\rho/a}}{a},$$

we see that the first case is equivalent to the condition $\rho/a < 1$. We may call this the close collision in which the trajectory of the projectile will be strongly affected by the screening field.

In the second case, $\rho/a$ may be larger than unity and the effect of the field is expected to be less important. This is the distant collision case.

It is well known that the potential $(4)$ may be replaced by a potential of simpler form,

$$V(r) = \frac{b_n}{r^n} \quad (5)$$

when the parameters $b_n$ and $n$ satisfy the following conditions,

$$n = 1 + \frac{r}{a} \quad (6)$$

$$k_n = Z_1 Z_2 e^2 a^{n-1} \left( \frac{n-1}{e} \right)^{n-1}$$

The case $n=1$ correspond of course to the Coulomb potential while for $n=2$, the region of the field which is effective for the scattering of the projectile is around $r=a$ (Thomson scattering).
The case \( n > 2 \) corresponds to distant collisions and it is generally assumed that as \( n \) increases the angular distribution would tend to be nearly isotropic.

We feel, however, that this point still needs to be clarified in the case of the stopping of heavy ions in matter, especially where a relatively accurate estimation of the stopping cross-section is needed.

In the next section we shall investigate this case and derive general expression for the differential cross-section.

### III. THE DIFFERENTIAL CROSS SECTION

We shall use the impact parameter formalism, if \( p \) is the impact parameter,

\[
\frac{d\sigma}{d\Omega} = \pi d(p^2)
\]

Let \( \theta \) be the scattering angle in the c.m. system. Then, for a given potential \( V(r) \), the connection between \( p \) and \( \theta \) is given by Kennard's equation,

\[
\theta = \pi - 2p \int_{p}^{\infty} \frac{dr}{r^2 \left[ 1 - \frac{V(r)}{E} - \frac{p^2}{r^2} \right]^{1/2}}
\]  

(7)

in which \( \rho \) is the minimum distance of approach for a given \( p \) and \( E = 1/2 M_0 v^2 \). \( \rho \) is the solution of the equation

\[
1 - \frac{V(r)}{E} - \frac{p^2}{\rho^2} = 0
\]  

By noting that

\[ \pi = 2p \int_0^\infty \frac{dr}{r\sqrt{r^2 - \rho^2}} \]

Kennard's equation may be transformed to

\[ \theta = 2p \int_0^\infty \frac{V(\rho) - V(r)}{D} \, dr \]

where the denominator \( D \) is found to be

\[ D(r) = B(r^2 - \rho^2)^{3/2} \left\{ 1 + \frac{\rho^2 V(r) - r^2 V(\rho)}{B(r^2 - \rho^2)} + \left[ 1 + \frac{\rho^2 V(\rho) - r^2 V(r)}{B(r^2 - \rho^2)} \right] \frac{1}{E} \right\} \]

If we evaluated the total cross-section by integrating from 0 to \( \pi \),

\[ \sigma_{\text{total}} = \pi \int_{p^2(\pi)}^{p^2(0)} dp^3 \]

the result would diverge for a long range force.

However, we are interested here only in the distant collision case and it may be seen that the ratio \( V(\rho)/E \) would be very small compared to unity. In other words, the expression for \( \theta \) may be simplified to

\[ \theta = \frac{p}{E} \int_0^\infty \frac{V(\rho) - V(r)}{B(r^2 - \rho^2)^{3/2}} \, r \, dr \]

In the case \( V(r) = \frac{k}{r^n} \), \( n > 2 \), this becomes
\[ \theta = \frac{k_n}{E \rho^{n-1}} \int_{\rho}^{\infty} \frac{r^n - \rho^n}{r^{n-1}(r^2 - \rho^2)^{3/2}} \, dr \]

and it is possible to show that this integral is convergent.

Introducing a new variable \( \phi \) defined as

\[ \sin \phi = \frac{\rho}{r} \]

and letting the quantity \( K_n \) be

\[ K_n = \int_0^{\pi/2} \frac{1 - \sin^n \phi}{\cos^2 \phi} \, d\phi \]

a straight-forward calculation gives the result

\[ \theta = \frac{k_n}{E \rho^n} K_n \quad . \quad (8) \]

The value of \( K_n \) is given by

\[ K_n = \begin{cases} \frac{\pi}{2} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{2,6} \cdots \frac{n-3}{(n-2)} \right) , & \text{for } n \text{ even} \\ 1 + \frac{2}{3} + \cdots + \frac{2}{1,3} \cdots \frac{n-3}{(n-2)} , & \text{for } n \text{ odd} \end{cases} \]

The differential cross section is then

\[ d\sigma = 2\pi \sigma(\theta) \sin \theta \, d\theta = \pi \, dp^2 \]

or

\[ \sigma(\theta) = \frac{1}{2} \sin \theta \frac{d(p^2)}{d\theta} \quad . \]
The quantity \( \frac{dp^2}{d\theta} \) may be calculated from the equation

\[
p^2 = p_0^2 + \frac{k_n}{E \theta^{n-2}}.
\]

Incidentally, we may note that for \( p=0 \)

\[
|p| = \left( \frac{k_n}{E} \right)^{1/n} \quad (9)
\]

The final result will be

\[
\frac{d\sigma}{d\theta} = \frac{\pi}{n} \left( \frac{k_n}{E \theta} \right)^{2/n} \left( \frac{2}{\theta} + \frac{n-2}{K_n} \right) \quad (10)
\]

This differs slightly from Kennard's relation, which is derived by another method.

However, the above formula is expected to be more accurate since, apart from the same initial assumption of distant collisions, we have made no other approximation in the derivation.

In fact for \( \theta \) small and \( n \) large, (9) agrees with Kennard's relation.
IV. THE STOPPING CROSS-SECTION

The atomic stopping cross-section may be defined as

$$ S = \int_0^{T_m} T \, d\sigma $$

when $T$ is the energy transferred from the projectile to the target. $T_m$ is the maximum energy transfer, and

$$ T = T_m \sin^2 \frac{\theta}{2} $$

For small $\theta$ we have $\theta \approx 2(T/T_m)^{1/2}$. Inserting this result into Eqs. (10) and (11), we finally have, after integration

$$ S_n = \frac{\pi n}{2^{n-2}} \left( \frac{k_n K_n}{n^{2/n}} \right) \left( \frac{1}{n-1} + \frac{n-2}{K_n} \frac{2}{3n-2} \right) \left( \frac{M_1}{M_1+M_2} \right)^{1-2/n} \frac{1}{M_1+M_2} E_0^{1-2/n}, \quad (12) $$

when $E_0$ is the incident energy in the laboratory system.

Equation (12) agrees with the result of Lindbard and collaborators\(^{14}\) as far as the dependence on masses and energy is concerned. It differs, however, by a proportionality factor which is dependent on $n$.\(^{*}\)

For $n = 2$, we find

$$ S_2 = \frac{\pi^2}{2} e^2 0.885 a_o \left( \frac{Z_1 Z_2}{Z_1^{2/3} + Z_2^{2/3}} \right)^{1/2} \frac{M_1}{M_1+M_2} $$

\(^{*}\)The power law potential of type $1/n r^n$ used by Lindbard does not correspond exactly to the screening potential we define above.
For convenience it is generally assumed that the nuclear and electronic stopping are two independent effects, with the nuclear stopping independent of the projectiles velocity and the electronic stopping linearly dependent on the velocity of the projectile.

In our description, however, distant collisions are regarded as one of the causes of the electronic stopping. In fact, in such collisions the energy transferred to the target atom would be extremely small and, due to its mass, the stopping atom as a whole will not be displaced by the momentum transfer.

But the projectile which is subjected to the "screening field" may transmit this momentum to the electrons which are loosely bound to the atom. This momentum transfer may provoke the ionization of the atom as well as a very small displacement of the electron which subsequently recovers its initial state due to the equilibrium rearrangement of the atomic system.

This description is similar to the adiabatic process as was first discussed by N. Bohr (Ref. 7, pp. 66-67). From this point of view, the nuclear and electronic stopping effects should not be considered as independent processes but should rather be governed by the same "screening potential" for close and distant collisions.

In fact, for this last eventuality, the energy transferred may be approximated by:

$$T \approx \frac{k}{2M} \frac{1}{p^2 \mu^2},$$

(13)

and this shows that the energy transferred to the electron is more important.
For \( n > 3 \), then, the electronic stopping effect may be taken into account by replacing \( M_2 \) in relation (12) by the electron mass.

In particular, the assumption of a linearity of the electronic stopping cross-section with the velocity \( v \) of the projectile is equivalent to the case \( n = 4 \).

After simplification, the expression of \( S \) for \( n = 4 \) is found to be

\[
S_e(4) = 2.11 \pi e_0^2 \left( \frac{Z_1 Z_2}{Z_1^{2/3} + Z_2^{2/3}} \right)^{1/2} \left( \frac{v}{v_0} \right)^{3/2}.
\]  

Expression (14) looks fairly similar to the semi-empirical formula given by Lindhard and Scharff\(^9\) except that the factor dependent on the atomic number of the target and projectile appears here under the square root sign.

For \( Z_1 \) and \( Z_2 \) small, this does not affect very much the theoretical estimation of the stopping power but for large \( Z_1 \) and \( Z_2 \), one may expect important derivations when compared to Lindhard's formula.

One might find agreement between these two formulas by modifying the initial assumption on the scattering parameter, i.e.

\[
a = (Z_1 Z_2)^{1/3} \frac{0.885 a_0}{\left( Z_1^{2/3} + Z_2^{2/3} \right)}.
\]

but such a modification seems not justified.

Lindhard's relation has been confirmed by many experimental data (see however 14-17).

Nevertheless, it would be interesting to study the variation of the stopping cross section with \( Z_1 \) and \( Z_2 \) systematically in the region where the electronic effect is expected to be important. Although such data are extremely
useful for a qualitative understanding of the stopping mechanism, they are rather scarce at present.

Of course, the charge number $Z_1$ to be taken into account must be the effective charge of the projectile which is a decreasing function of $\nu^{19}$ following the empirical relation

$$Z_{1\text{ eff}} = Z_1(1 - e^{\nu/\alpha})$$

$\alpha$ being a function of $Z_1$.

This brings more complications in the calculation of the range of the ions.

V. CONCLUSION

It seems that the use of a "screening potential" may provide a useful model for the study of the quasi-elastic stopping cross-section for low energy ions within a reasonable theoretical basis.

With the concept of close and distant collisions, the nuclear and electronic effects cannot be considered as independent.

The derivation of the nuclear stopping cross-section is in agreement with previous results while the derivation of relation (16) may be considered as a partial justification of Lindhard's formula for electronic stopping, but it appears however as a particular case with $n = 4$.

It does not claim to replace the Lindbard's formula which has been tested successfully in various experiments, but it may constitute nevertheless a starting point for further investigations.

Finally, this description is, of course, oversimplified and a quantum mechanical approach to this problem would be more appropriate.
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