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Stopping Power of a Medium for Heavy, Charged Particles

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It is shown that the orbital motion of electrons in the molecules of a medium is important for the stopping power of slow charged particles. This is due to the strong dependence of the momentum transfer in a Coulomb field on the relative velocity. Equations for determining the absolute stopping power of an arbitrary medium are derived on the basis of classical mechanics for the entire nonrelativistic energy range. For the high-energy range this equation corresponds to Bethe's formula, and for low energies, to the Fermi-Teller formula. It is concluded, from this equation and from the experimental data, that electron capture is not important in the slowing down of protons. It starts being important for α particles and is decisive for particles of higher charge. The stopping power of H, H_2, and A for protons and of H_2 for α particles is calculated. Good agreement with the experimental data is obtained.

I. INTRODUCTION

THE theoretical formulation of the ionization loss of slow heavy particles is a very difficult problem. Theories of the stopping power for charged particles have been worked out by Bohr,[1] Bethe,[2] and others. These theories give quite good agreement with experiment at high energies, but in the low-energy region they break down completely. The capture and the loss of electrons was interpreted by Rutherford[3] and Kapitza[4] as the main reason for this lack of agreement. These explanations were only qualitative. There were some semiempirical attempts to estimate this effect,[5] but no good quantitative theory has yet been presented.[6] In 1949 Warshaw[7] pointed out that the discrepancy between the calculated and the observed curves for beryllium cannot be explained by the electron capture effect.

It therefore seems reasonable to analyze all the previously neglected factors which might influence the process of stopping charged particles. Since the cross section for the momentum transfer in a Coulomb field decreases with the fourth power of the relative velocity, the orbital velocity of electrons in the atom should be most important at low energies (where the existing theory breaks down). In taking this effect into account, we shall derive the equations for the stopping power of the medium on the basis of classical mechanics. The validity of the classical arguments is shown by Bell[8] who worked out a similar problem—the capture and loss of electrons by fission fragments.

II. THEORY

Consider the slowing down of a particle of charge q_A, mass m_A, and velocity v_A with respect to an assembly of other particles of charge q_B, mass m_B, and velocity v_B (the velocity distribution being isotropic, with $N(v_B)dv_B$ denoting the number of particles/cc having velocity v_B to v_B+dv_B). This problem was solved by Chandrasekhar[9] for bodies interacting through gravitation. Because of the same radial dependence of both fields (Coulomb and gravitational), Chandrasekhar's equation may readily be rewritten for electrically charged particles:

[1] N. Bohr, Phil. Mag. **25**, 10 (1913); **30**, 581 (1913).
[2] H. A. Bethe, Ann. Physik **5**, 325 (1930).
[3] E. Rutherford, Phil. Mag. **47**, 277 (1924).
[4] P. Kapitza, Proc. Roy. Soc. (London) **106**, 602 (1924).
[5] K. L. Kaila, Indian J. Phys. **38**, 479 (1955).
[6] A. Dalgarno and G. W. Griffing, Proc. Roy. Soc. (London) **A232**, 423 (1955).
[7] S. D. Warshaw, Phys. Rev. **76**, 1759 (1949).
[8] G. I. Bell, Phys. Rev. **90**, 549 (1953).
[9] S. Chandrasekhar, Astrophys. J. **93**, 285 (1941).

$$(dE_A/dx)_{v_B} = -N(v_B)\frac{\pi(q_Aq_B)^2}{\mu v_A{}^2}\left\{\frac{1}{2v_B}\int_{|v_B-v_A|}^{|v_B+v_A|}\left[\frac{v_B{}^2-v_A{}^2}{v^2}-\frac{m_A-m_B}{m_A+m_B}\right]\ln(1+g^2v^4)dv\right\}. \quad (1)$$

The variable of integration, v, is the relative velocity of particles A and B, and

$$g = D_{\max}\mu/q_Aq_B, \quad (2)$$

μ is the reduced mass, $D_{\max}$ is the maximum impact parameter. After integration, we obtain

$$(dE_A/dx)_{v_B} = -N(v_B)\frac{4\pi(q_Aq_B)^2}{\mu v_A{}^2}G[d,\lambda], \quad (3)$$

where

$$G[d,\lambda] = \frac{1}{4d}\left\{\frac{b-sr}{\sqrt{2}}\left[\arctan\left(\frac{\sqrt{2}s}{1-s^2}\right)-\arctan\left(\frac{\sqrt{2}|r|}{1-r^2}\right)\right]+\frac{b+sr}{\sqrt{2}}\left[\ln\left(\frac{s^2+\sqrt{2}s+1}{(1+s^4)^{\frac{1}{2}}}\right)-\ln\left(\frac{r^2+\sqrt{2}|r|+1}{(1+r^4)^{\frac{1}{2}}}\right)\right]\right.$$
$$\left.+\tfrac{1}{2}(r+bs)\ln(1+s^4)-\tfrac{1}{2}\left(\frac{rs}{|r|}+b|r|\right)\ln(1+r^4)-2b(s-|r|)\right\}. \quad (4)$$

In the last expression we have introduced the symbols,

$$r = g^{\frac{1}{2}}v_B(1-v_A/v_B) = d(1-\lambda),$$
$$s = g^{\frac{1}{2}}v_B(1+v_A/v_B) = d(1+\lambda), \quad (5)$$
$$b = (m_A-m_B)/(m_A+m_B),$$

where $d = g^{\frac{1}{2}}v_B$ and $\lambda = v_A/v_B$. Equation (3) represents the energy loss of particle A per unit path length as a result of scattering by particles B of velocity v_B. On carrying out the integration over the energy distribution of particles B, one obtains the total stopping power of the medium:

$$(dE_A/dx) = -\frac{4\pi(q_Aq_B)^2}{\mu v_A{}^2}\times\int_0^\infty N(v_B)G[d(v_B);\lambda(v_B)]dv_B. \quad (6)$$

Equation (6) contains implicitly the undetermined maximum impact parameter $D_{\max}$. In general, this impact parameter is a function of v_A, v_B, m_A, m_B, q_A, q_B as well as the external fields. In each problem this parameter must be determined separately.

For the special case of the slowing down of heavy particles by electrons, $m_A \gg m_B = m$, $\mu = m$, $b = 1$, $q_B = e$, $q_A = Z_Ae$. Substituting these into Eq. (6), we have

$$(dE_A/dx) = -\frac{4\pi e^4}{mv_A{}^2}Z_A{}^2\int_0^\infty N(v_e)G[d(v_e);\lambda(v_e)]dv_e, \quad (7)$$

and now

$$G[d,\lambda] = \frac{1}{4d}\left\{\frac{1-sr}{\sqrt{2}}\left[\arctan\left(\frac{\sqrt{2}s}{1-s^2}\right)-\arctan\left(\frac{\sqrt{2}|r|}{1-r^2}\right)\right]+\frac{1+sr}{\sqrt{2}}\left[\ln\left(\frac{s^2+\sqrt{2}s+1}{(1+s^4)^{\frac{1}{2}}}\right)-\ln\left(\frac{r^2+\sqrt{2}|r|+1}{(1+r^4)^{\frac{1}{2}}}\right)\right]\right.$$
$$\left.+d\left[\ln(1+s^4)\pm\ln(1+r^4)\right]\begin{matrix}-4\\-4\lambda\end{matrix}\right\}\begin{matrix}\text{if } v_A>v_e\\ \text{if } v_A<v_e\end{matrix}. \quad (8)$$

This function is plotted in Fig. 1 for various values of d.

Since the electrons in a medium are bound in atoms (molecules), the minimum value of energy that may be transferred to electrons is the excitation energy of the first excitation state (U_1). This condition determines the maximum value of the impact parameter[10]:

$$D_{\max} = Z_Ae^2/U_1 \approx 2Z_Ae^2/U_j, \quad (9)$$

where U_j is the ionization energy of the ground state. Substituting (9) into (2) and taking into account the fact that $U_j = E_{\text{kin}}{}^{\text{el}}$, we obtain

$$g = 4/v_e{}^2 \quad \text{and} \quad d = 2. \quad (10)$$

Using Eqs. (7), (8), and the above criterion for determining $D_{\max}$, we may compute the stopping power of an arbitrary medium. If the momentum distribution is not known directly, it can be computed from the radial density $D(r)$ of electrons in the atom (molecule), which may, in turn, be computed by the Hartree-Fock method. Equation (7) may also be written in terms of $D(r)$ as

[10] In a more exact theory we would have to determine the maximum impact parameter more precisely.

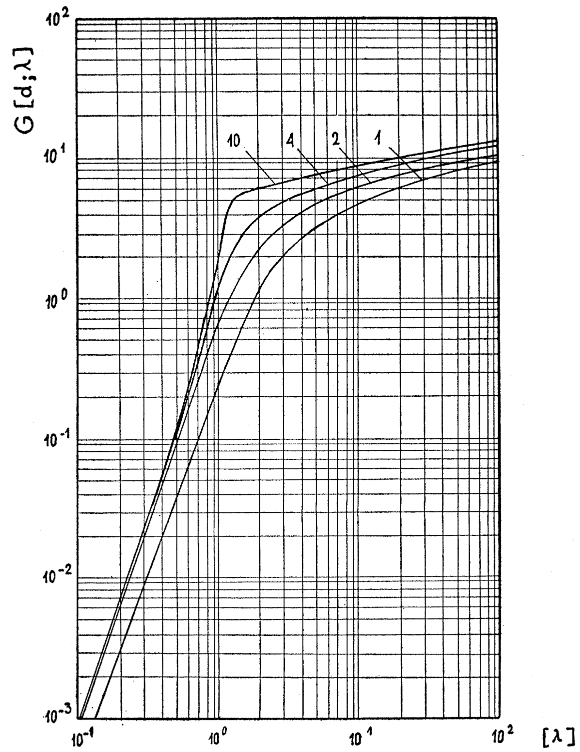

FIG. 1. Plot of the universal stopping power function G as a function of λ for different values of d.

$$(dE_A/dx)=-\frac{4\pi e^4}{mv_A^2}Z_A^2N\int_0^\infty D(r)G[2,\lambda(r)]dr, \quad (11)$$

where N is the number of atoms/cc, and λ depends on r in the following way:

$$\lambda=v_A/v_e(r)=(E_Am/E_{\text{kin}}^{\text{el}}m_A)^{\frac{1}{2}}$$
$$\simeq[2E_Am/E_{\text{pot}}^{\text{el}}(r)m_A]^{\frac{1}{2}}=[2mE_A/m_A\varphi(r)e]^{\frac{1}{2}}. \quad (12)$$

The potential $\varphi(r)$ is given by

$$\varphi(r)=\frac{Ze}{r}-\frac{(Z-1)e}{Z'}\left\{\frac{1}{r}\int_0^r D(r')dr'+\int_r^\infty\frac{D(r')}{r'}dr'\right\}. \quad (13)$$

III. COMPARISON WITH PREVIOUS THEORIES

If we take the asymptotic value of $G[d,\lambda]$ and substitute it into Eq. (7), we obtain

(a) for $v_A \gg v_e$ (i.e., $\lambda \gg 1$)

$$G[d,\lambda]=\ln(d^2\lambda^2), \quad (14)$$

and

$$(dE_A/dx)=-\frac{4\pi e^4}{mv_A^2}Z_A^2\ln\left(d^2\frac{v_A^2}{\langle v_e^2\rangle_{\text{Av}}}\right)\int_0^\infty N(v_e)dv_e.$$

Since $\int_0^\infty N(v_e)dv_e=NZ$, the number of electrons per unit volume, and $m\langle v_e^2\rangle_{\text{Av}}/2=I$ (I is the mean value of the ionization potential of an atom), we obtain Bethe's equation,

$$(dE_A/dx)=-\frac{4\pi e^4}{mv_A^2}Z_A^2NZ\ln\left(\frac{2mv_A^2}{I}\right);$$

(b) for $v_A \ll v_e$ (i.e., $\lambda \ll 1$),

$$G[d,\lambda]\approx\tfrac{2}{3}\lambda^3. \quad (15)$$

Since the momentum distribution for a completely degenerate electron gas is

$$N(v_e)dv_e=\frac{m^3v_e^2}{\pi^2\hbar^3}dv_e, \quad (16)$$

we have

$$(dE_A/dx)=-\frac{4}{3\pi}\left(\frac{2e^4m^2}{\hbar^3}\right)Z_A^2v_A\int_{v_{\min}}^{v_{\max}}dv_e/v_e, \quad (17)$$

observing that $v_{\min}\sim e^2/\hbar$, we obtain

$$(dE_A/dx)=-\frac{4}{3\pi}\left(\frac{2e^4m^2}{\hbar^3}\right)Z_A^2v_A\ln\left(\frac{v_{\max}\hbar}{e^2}\right). \quad (18)$$

This equation is identical with that of Fermi and Teller[11] except for the factor of 4.

IV. COMPARISON WITH EXPERIMENT

To test the theory, we shall calculate the stopping power of some gases for protons and α particles.

(a) Stopping Power of Hydrogen for Protons

The velocity distribution of electrons in hydrogen is:

for atomic hydrogen, $N_{\text{H}}(v_e)=N_{\text{H}}\delta(v_e-v_0^{\text{H}})$,

for molecular hydrogen, $N_{\text{H}_2}(v_e)=N_{\text{H}_2}\delta(v_e-v_0^{\text{H}_2})$,

where N is the electron density and v_0^{H} ($v_0^{\text{H}_2}$) is the velocity in the ground states of atoms (molecules). Using these expressions in Eq. (7) we obtain the atomic stopping cross section in ev-atom^{-1} cm^2:

$$\frac{1}{N}\left(\frac{dE_p}{dx}\right)=-2.39\times10^{-10}G[2;\lambda(E_p)]/E_p(\text{ev}), \quad (19)$$

where E_p is the proton energy,

$$\lambda_{\text{H}}=v_p/v_0^{\text{H}}=[E_p(\text{kev})/24.8]^{\frac{1}{2}} \quad (20)$$

and

$$\lambda_{\text{H}_2}=v_p/v_0^{\text{H}_2}=[E_p(\text{kev})/28.3]^{\frac{1}{2}}. \quad (21)$$

Computing the values of the function $G[2,\lambda]$, we obtain the slowing down curves for protons in atomic and molecular hydrogen (Fig. 2). The theoretical results for molecular hydrogen are in good agreement with the experimental data of Reynolds,[12] Philips,[13] and Weyl.[14]

[11] E. Fermi and E. Teller, Phys. Rev. **72**, 399 (1947).
[12] Reynolds, Dunbar, Wenzel, and Whaling, Phys. Rev. **92**, 742 (1953).
[13] J. A. Philips, Phys. Rev. **90**, 532 (1953).
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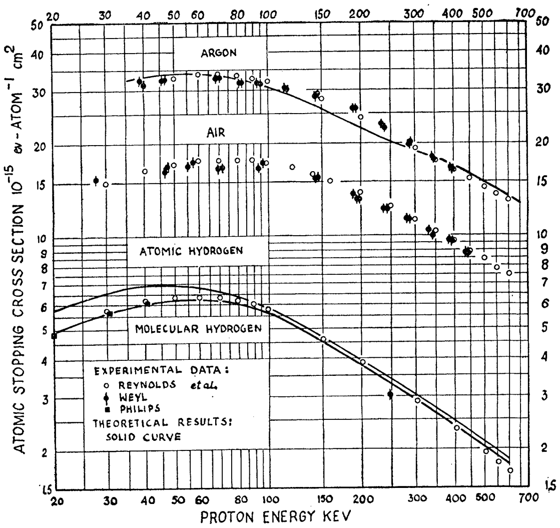

FIG. 2. Comparison of the theoretical calculations of the stopping power of some gases for protons with experimental data.

(b) Stopping Power of Argon for Protons

The stopping power of argon is computed with the help of Eqs. (11), (12), (13) and the radial density of electrons taken from Hartree and Hartree.[15] Here we cannot take the velocity distribution in direct form as in the case of hydrogen, because in A there are eliptical orbits, and therefore the velocity of each electron is not constant. Throughout the energy region, the theoretical curve is in agreement with the experimental data to an accuracy of $\sim 15\%$ (see Fig. 2). A slight hump is observed both in the experimental data and in the theoretical curve at a proton energy of 300–600 kev. This is due to the increase in the relative contribution of the L electrons in the slowing-down process. The contribution of the particular shells in the process is shown in Fig. 3. It is seen that 2–3 outer electrons are most important in the energy range ~ 50 kev. The absolute values of the stopping power and its dependence on energy are very sensitive to the shape of $D(r)$ especially in the external region [e.g., the stopping power of argon as computed from $D(r)$ without exchange is too high by 20%].

V. ROLE OF ELECTRON CAPTURE IN THE SLOWING-DOWN PROCESS

From Eq. (9), taking into account $U_j \sim e^2/2a_0$, we obtain $D_{\max} \approx 4a_0 Z_A$. If the effective field is screened by captured electrons, $D_{\max}$ is smaller than $4a_0 Z_A$.

For protons we have $Z_A = 1$ and $D_{\max} = 4a_0$. If the dipole character of the hydrogen atom (i.e., weak screening of the field of the nucleus) and its dimensions (the distance from the nucleus to the electron being $\sim 2a_0$) is taken into account, the amount of energy loss both for protons and neutral atomic hydrogen is the same to a first approximation.

For α particles $Z_A = 2$ and $D_{\max} = 8a_0$. Since the effective radius of the nuclear field of a neutral He atom is concentrated in the region $1.5a_0$, we obtain a considerable difference between the stopping power of helium ions and neutral atoms. For nuclei of larger Z_A this difference will increase quickly and the process of slowing down has to be considered simultaneously with electron capture. By way of illustration, we shall consider the stopping process of α particles in molecular hydrogen.

When a monoenergetic beam of α particles penetrates into gaseous molecular hydrogen, the α particles capture electrons to form neutral atoms and singly charged helium ions. Denoting by σ_{He^0}, σ_{He^+}, and $\sigma_{\mathrm{He}^{++}}$ the atomic stopping cross section of the respective components, and by p_{He^0}, p_{He^+}, and $p_{\mathrm{He}^{++}}$ the fractional content of the constituents of the beam, the actual stopping power is given by

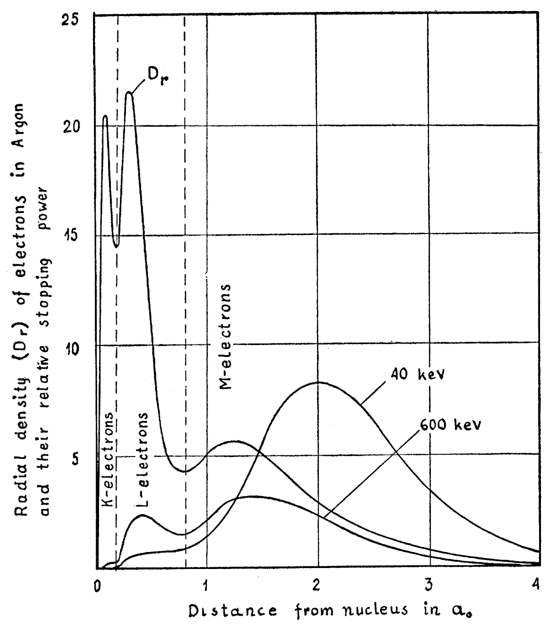

FIG. 3. The radial density of electrons in an argon atom, and their relative contribution to the stopping power for protons in the low- and high-energy ranges.

$$\sigma = p_{\mathrm{He}^0}\sigma_{\mathrm{He}^0} + p_{\mathrm{He}^+}\sigma_{\mathrm{He}^+} + p_{\mathrm{He}^{++}}\sigma_{\mathrm{He}^{++}}, \tag{22}$$

where

$$\sigma_{\mathrm{He}^0} = -38.2\times 10^{-10} G[0,7;\lambda]/E_\alpha(\mathrm{ev}), \tag{23a}$$

$$\sigma_{\mathrm{He}^{++}} = -38.2\times 10^{-10} G[2;\lambda]/E_\alpha(\mathrm{ev}), \tag{23b}$$

$$\sigma_{\mathrm{He}^+} = \sigma_{\mathrm{He}^0} + 9.6\times 10^{-10} \times\{G[0,7;\lambda] - G[2,\lambda]\}/E_\alpha(\mathrm{ev}). \tag{23c}$$

In the last expression we take into account the fact that, for He, $D_{\max}$ is 1.5 a_0 [$D_{\max}$ may be determined very easily from the plot of $\varphi(r)$ for the helium atom], and

[15] D. R. Hartree and W. Hartree, Proc. Phys. Soc. (London) **A166**, 450 (1938).

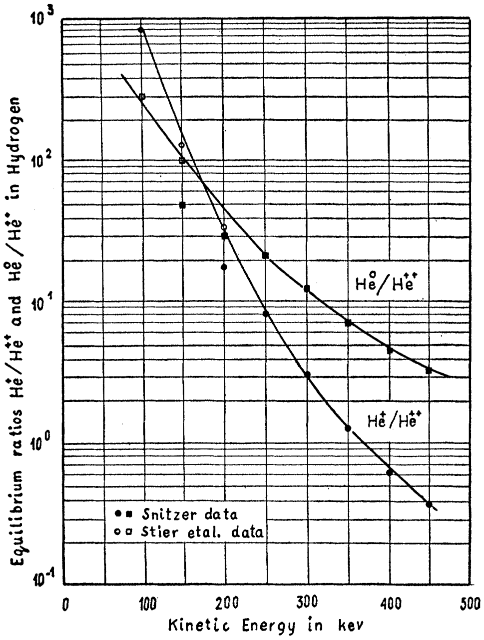

FIG. 4. Ratios He^0/He^+ and He^0/He^{++} for a helium beam in a molecular hydrogen.

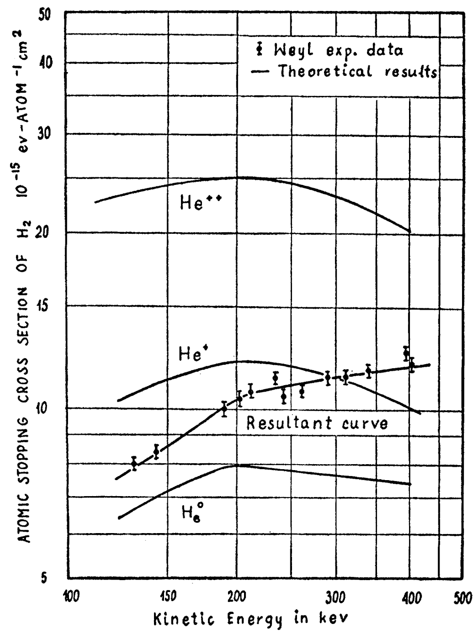

FIG. 5. Theoretical energy loss of helium atoms and helium ions, and the mean energy loss of a helium beam in molecular hydrogen.

the fact that, for He^+ in the region 0–1.5 a_0, the effective charge is $2e$; outside this region, the effective charge is e.

No exact theory of the capture process has yet been presented. Schiff[16] has made theoretical studies of the capture cross section for helium ions traversing gaseous hydrogen, but there is lack of agreement between the theoretical curve and the experimental results obtained by Alleson, Cuevas, and Murphy.[17] Therefore we must take the fractional contents from empirical data. Snitzer[18] and afterwards Stier, Barnett, and Evans[19] have measured the ratio He^+/He^{++} and He^0/He^{++}. If we denote these ratios by r_{12} and r_{02}, respectively, we obtain

$$p_{He^0}=r_{02}/(1+r_{12}+r_{02}),\quad p_{He^+}=r_{12}/(1+r_{12}+r_{02}),\quad p_{He^{++}}=1/(1+r_{12}+r_{02}). \quad (24)$$

The energy loss (per atom of the medium) of helium atoms and helium ions was calculated from (23) and the over-all stopping power was calculated from (22). The values of r_{12} and r_{02} are experimental and are taken from the graph in Fig. 4. The absolute value as well as the shape of the curve is in the good agreement with experimental data (Fig. 5).

[16] H. Schiff, Can. J. Phys. **32**, 393 (1954).
[17] Allison, Cuevas, and Murphy, Phys. Rev. **102**, 1041 (1956).
[18] E. Snitzer, Phys. Rev. **89**, 1237 (1953).
[19] Stier, Barnett, and Evans, Phys. Rev. **96**, 973 (1954).

VI. CONCLUSIONS

The stopping power of a medium depends on the density and the momentum distribution of electrons in the atoms of the medium. Those electrons whose velocities are near the velocity of the slowed-down particle play the decisive role.

In the low-energy region the valence electrons are the most effective in the stopping process. Their energy is strongly dependent on chemical bonds. Bragg's law is therefore not valid (especially below 100 kev). Changes in the state of a medium (density, temperature, etc.) have some influence on the stopping power, if they are accompanied by changes in the configuration of energy levels or momentum distribution of electrons.

On the basis of this theory we can explain at once, such "anomalies" as the very low stopping power of water, and the excessive stopping power of Li and C when compared to the stopping power of Be.

The mean ionization energy of an atom is a good characteristic of the stopping power of a medium only for particles with velocity much greater than the velocity of electrons in the medium. Otherwise, the relative contribution of the electrons to the stopping power varies with the energy, and consequently Bloch's "constant" also varies with the energy. As a result various investigators have obtained different results for Bloch's constant.