Classical Theory of Atomic Collisions. I. Theory of Inelastic Collisions

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In this paper, a classical theory of inelastic atomic collisions is evolved on the basis of the relations for binary collisions as well as for the Coulomb collisions derived in the laboratory system of coordinates. Built up as an approximation based on the binary collisions, i.e., the independent pair interactions of the individual elements of the colliding systems, the theory, with its immense simplicity, not only permits a clear qualitative interpretation of the atomic collisions, but also describes well their quantitive aspect. In terms of that theory, a majority of basic inelastic processes accompanying the atomic collisions are analyzed. In particular, calculations are made for the following: (i) ionization of atoms and molecules by light particles (electrons), as well as by heavy particles (protons, deuterons), including inner-shell ionization and double ionization; (ii) excitation of single and triplet lines (excitation with exchange and without exchange); (iii) capture of electrons in orbit; (iv) slowing down of heavy charged particles (with consideration of the capture process as well as of the interaction with the Coulomb field of the nucleus); (v) inelastic scattering of electrons on atoms and molecules. According to the theory developed, the "diffraction" of elementary particles on atomic systems is explained on the basis of corpuscular mechanics; it is shown that the discrete energy states of the scatterer electrons—and the anisotropy in the space orientation of their velocities in the case of crystals—are responsible for the main features of the diffraction pattern. Having at our disposal a simple theory without any arbitrary parameters except those describing the target system, we find it a useful tool for the investigation of atomic structures.

I. INTRODUCTION

THE postulation in the twenties of the wave nature of elementary particles, and the imposition of limitations arising from the formalism of wave mechanics upon the scope of applicability of classical mechanics for atomic phenomena, have almost completely checked development of the classical theory of atomic collisions; whereas the sporadic attempts in the direction made in the first period (Bohr[1]), which yielded correct results only in the range of high energies, have been taken to prove the legitimacy of these limitations and the uselessness of further investigations in that direction, the possibility of removing those limitations in the framework of classical mechanics itself being rather uncritically discarded. As has been only recently shown,[2,3] a number of disagreements were the result of mechanical application of the Thompson or Rutherford formula, describing the Coulomb scattering on particles at rest, to atomic collisions, where, after all, we have a dynamic system of charges. From certain previous work,[2,3] as well as from the detailed theory of binary and Coulomb collisions,[4,5] it follows that the effect of interaction between the charged particles depends, first and foremost, on their relative velocity; hence, a description of collision processes based on the Thompson and Rutherford formulas is bound to yield erroneous results if the velocity of the particle scattered on the atom becomes comparable to, or less than, the mean velocity of electrons in the atom.

Another fact disadvantageous for the development of the classical method consisted in overlooking the relationship between the discrete states of electrons in the atomic systems and the "diffraction" phenomenon of scattered particles. That phenomenon rather obviously results from the laws of conservation of energy and momentum (see Papers I and II), which imply, for instance, the observed inverse dependence of the scattering angle on the momentum of the particle scattered. The present paper, as far as the point of the problem is concerned, does not differ from the theory of inelastic atomic and ionic collisions[3] previously published by the author; it only encompasses a considerably larger class of phenomena such as it might again seem could not be interpreted in terms of classical mechanics (exchange collisions, capture of electrons, "diffraction" of inelastically scattered particles). The calculations are made on the basis of extremely simple approximate formulas, owing to which it has been possible to discuss not only qualitatively but also quantitatively almost all basic inelastic processes accompanying the atomic collisions. Application of the methods of classical mechanics, which has the advantage of being an object theory, is of great significance for the proper understanding of atomic collision processes. Having proved that the theory yields good results for atomic structures of known electronic configurations, it will be possible to reverse the problem, and thus from the experimental data for various processes, e.g., from the cross section for ionization, or from the stopping power, to determine the configurations of electrons in complex structures (molecules). The angular measurements in the scattering problem enable one to proceed further than that, and to deduce the form and space orientation of electron orbits in crystal structures.

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[1] N. Bohr, Phil. Mag. **25**, 10 (1913); **30**, 581 (1915).
[2] M. Gryziński, Phys. Rev. **107**, 1471 (1957).
[3] M. Gryziński, Phys. Rev. **115**, 374 (1959).
[4] M. Gryziński, first preceding paper, Phys. Rev. **138**, A305 (1965), hereafter cited as I.
[5] M. Gryziński, preceding paper, Phys. Rev. **138**, A322 (1965), hereafter cited as II.

II. INELASTIC ATOMIC COLLISIONS IN THE TWO-BODY APPROXIMATION

If we consider the Coulomb interaction of the elementary particle with a complex system of charges in a state of dynamic equilibrium, which the atom presents, then we can divide that interaction into two parts:

(a) interaction with the unperturbed field of the whole system, which does not lead to change of its internal energy (elastic collision);

(b) interaction with the individual elements of the system (electrons), which may lead to change of its internal energy (inelastic collision).

According to this division, two different methods of treatment can be applied to describe approximately the complex phenomenon of atomic collision. Process (b) may be analyzed in terms of binary Coulomb collisions, whereas to describe process (a) an appropriate approximation should be found (the expansion in multipole moments seems to be most hopeful).

Since the type of inelastic collision is specified by the change of energy and momentum of the electrons of the scattering system, the problem, in view of Papers I and II, will consist in calculating the cross section for definite collisions between the incident particle and the respective electrons of this system.

In the case of scattering on unoriented atoms and of the inelastic collisions defined by a change of state of only one of the electrons of the atom, the calculating procedure will be comparatively simple.

Denoting by $p_k(v_e,r)$ the probability that at a distance r from the nucleus an electron of a velocity v_e belonging to the shell k can be found, and by σ the cross section for a given change of dynamic variables of that electron, we can determine the cross section relating to the whole atom:

$$\sigma^{\text{atom}}=\sum n_e^k\int_0^\infty\int_0^\infty p_k(v_e,r)\sigma[v_e,v_q(r)]4\pi r^2 dr dv_e\,, \quad (1)$$

where n_e^k is the number of electrons in the shell k, while the summation is extended over all shells of the atom, and $v_q(r)$ is the velocity of the incident particle, which, in general, depends on the averaged potential of the whole system, and hence, is a function of the distance from the nucleus:

$$v_q(r)=\{(2/m_q)[E_q-\varphi(r)q]\}^{1/2}, \quad (2)$$

while E_q is the kinetic energy of an incident particle with a charge q and a mass m_q outside the atom, and $\varphi(r)$ describes the averaged potential of the atom. Expression (1) together with expression (2) would describe the collision process exactly only if the interaction forces between the particle bombarding a given atomic system and its electrons were not Coulomb forces, but had the form of a $\delta(r-r_0)$ function with the radius of interaction r_0 approaching zero; nevertheless, we can assume such a model to be a first approximation of the real collision process, which in fact is an insoluble many-body problem. Errors resulting from the approximation will depend on the structure of the colliding systems and their velocities. (In general, the errors will decrease with increasing velocity and will vary with the type of processes under consideration.) Their influence upon the final results will be discussed when considering definite problems. Assuming that between the kinetic energy of the electron and its distance from the nucleus there exists a unique relationship, which is to be expected from the laws of classical physics, the expression (1) may be rewritten as follows:

$$\sigma^{\text{atom}}=\sum_k n_e^k\int p_k(r)\sigma[v_e(r)v_q(r)]4\pi r^2 dr \quad (3a)$$

or in the alternative form:

$$\sigma^{\text{atom}}=\sum_k n_e^k\int f_k(v_e)\sigma[v_e,v_q(v_e)]dv_e\,, \quad (3b)$$

where $f_k(v_e)$ is the momentum distribution of electrons in the orbit k. Expressions (3a) and (3b) are equivalent if collisions of large energy exchange between the impinging particle and atomic electrons are considered; they are not equivalent for collisions of very small energy exchange, and then expression (3a) must be used. Since in inelastic atomic collision processes the amount of energy transferred to an atomic electron is usually greater than its mean kinetic energy, we are entitled to use the more convenient relation (3b) in calculations. Neglecting the influence of the averaged field of the atom on the motion of the bombarding particle, while putting $\varphi(r)=0$ into (3b), we obtain

$$\sigma^{\text{atom}}=\sum_k n_e^k\int f_k(v_e)\sigma(v_e)dv_e\,; \quad (4)$$

or proceeding still further and operating with the mean velocity of the electron in the orbit, we have

$$\sigma^{\text{atom}}=\sum_k n_e^k\sigma(\bar{v}_e^k)\,. \quad (5)$$

Therefore, the nature and the quantitative aspect of the collision process are determined, first and foremost, by occupation of the atomic levels with electrons, the mean velocities of electrons on these levels and obviously the spectrum of energy levels which otherwise defines the kind of inelastic process.

If we assume $\frac{1}{2}m_e(\bar{v}_e^k)^2$ to be approximately equal to the binding energy of the electron in the orbit k, the atomic cross section becomes in first approximation a function of occupation of levels and of the binding energies of electrons only. The formulas quoted above relate to an isotropic distribution of electron velocities, and so to a system of unoriented atoms; for a system of

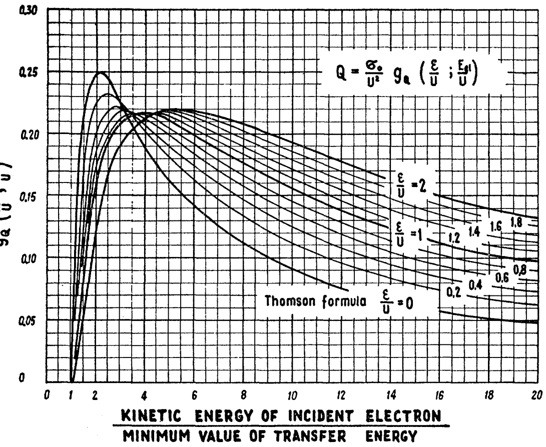

FIG. 1. Plot of the function g_Q which determines the cross section for collision with loss of energy greater than the fixed value U, in the case of equal masses of the colliding particles (electron-electron collisions).

oriented atoms, e.g., in the crystal, the cross sections will have another form depending on the angular relations. In such cases the procedure of introducing corrections with respect to the averaged field of the atom will be rather complicated, and it will depend strongly on the particular problem solved.

III. ADAPTATION OF COULOMB-COLLISION FORMULAS TO THE THEORY OF ATOMIC COLLISIONS

Taking into consideration that the elements of the colliding atomic system interact through a Coulomb field, our theory will be based on the relations of Paper II, but, due to the bound motion of electrons in the atom as well as to the relatively strong mutual interaction between its elements, application of the exact formulas of that theory is of no avail. Exact formulas yield exceedingly high values for cross sections because in those cross sections account has been taken of the collisions of small relative velocities and thus of long collision time which, for the above reasons, do not exist in the real physical process.

Analyzing the experimental data for the inelastic processes, we arrive at the conclusion that in the atomic systems we have to do with the continuous velocity distribution of the electrons; this is, *inter alia*, evidenced in the agreement of the results of Papers I and II with the fact that the cross sections for ionization or excitation by heavy particles lack a threshold. On the other hand the asymptotic form of these cross sections reveals the presence of a logarithmic term, which not only testifies to a continuous distribution of electron velocity, but also determines the high-energy part of that distribution. On the basis of the theory of Coulomb collisions it is thus possible to deduce that the probability of the atomic electron having velocity v_e decreases with increase of that velocity as the inverse third power of v_e. This result is roughly confirmed by the energy dependence of the cross section for inelastic processes for heavy-charged-particle impacts at very small velocities.

Consequently, formulas (50)–(58) of Paper II can be used for the description of inelastic atomic processes, although we must keep in mind that due to the approximate character of the theory, the high-energy part of the velocity distribution that is slightly different from $1/v_e^3$ cannot be excluded.

We introduce somewhat different symbols for the quantities appearing in these formulas:

$$\bar{v}_1\to\bar{v}_e\quad \mathcal{E}_1\to\mathcal{E}=m\bar{v}_e^2/2\quad m_1\to m_e$$
$$v_2\to v_q\quad E_2\to E_q\quad m_2\to m_q.$$

ΔE relates to the absolute value of the loss of energy only. Omitting the symbol of averaging over the velocity distribution of field particles (target-system electrons), we shall rewrite some expressions of Paper II in a modified form:

$$\sigma=\frac{\sigma_0}{\Delta E^2}\frac{1}{\Delta E}\times g_\sigma\left(\frac{\mathcal{E}}{\Delta E};\frac{E_q}{\Delta E}\right)\quad\text{for}\quad m_q=m_e$$
$$=\frac{\sigma_0}{\Delta E^2}\frac{1}{\Delta E}\times G_\sigma\left(\frac{\mathcal{E}}{\Delta E};\frac{v_q}{\bar{v}_e}\right)\quad\text{for}\quad m_q\gg m_e,\tag{6}$$

$$Q=\frac{\sigma_0}{U^2}\times g_Q\left(\frac{\mathcal{E}}{U};\frac{E_q}{U}\right)\quad\text{for}\quad m_q=m_e$$
$$=\frac{\sigma_0}{\sigma_2}\times G_Q\left(\frac{\mathcal{E}}{U};\frac{v_q}{\bar{v}_e}\right)\quad\text{for}\quad m_q\gg m_e,\tag{7}$$

$$S=\frac{\sigma_0}{U}\times g_S\left(\frac{\mathcal{E}}{U};\frac{E_q}{U}\right)\quad\text{for}\quad m_q=m_e$$
$$=\frac{\sigma_0}{U}\times G_S\left(\frac{\mathcal{E}}{U};\frac{v_q}{\bar{v}_e}\right)\quad\text{for}\quad m_q\gg m_e,\tag{8}$$

where the functions g, G have the forms:

(a) For light particles (electrons, positrons—$m_q\simeq m_e$)

$$g_\sigma\left(\frac{\mathcal{E}}{\Delta E};\frac{E_q}{\Delta E}\right)=f_{\bar{v}}\left\{\frac{\Delta E}{\mathcal{E}}+\frac{4}{3}\left(1-\frac{\Delta E}{\mathcal{E}}\right)\ln\left[2.7+\left(\frac{E_q-\Delta E}{\mathcal{E}}\right)^{1/2}\right]\right\}\left(1-\frac{\Delta E}{E_q}\right)^{\mathcal{E}/(\mathcal{E}+\Delta E)},\tag{9}$$

$$g_Q\left(\frac{\mathcal{E}}{U};\frac{E_q}{U}\right)=f_{\bar{v}}\left\{\frac{U}{\mathcal{E}}+\frac{2}{3}\left(1-\frac{U}{2\mathcal{E}}\right)\ln\left[2.7+\left(\frac{E_q-U}{\mathcal{E}}\right)^{1/2}\right]\right\}\left(1-\frac{U}{E_q}\right)^{1+\mathcal{E}/(\mathcal{E}+U)},\tag{10}$$

$$g_S\left(\frac{\mathcal{E}}{U};\frac{E_q}{U}\right)=f_{\bar{v}}\left\{\frac{U}{\mathcal{E}}\left(1-\frac{U}{E_q}\right)\ln\frac{E_q}{U}+\frac{4}{3}\left(1-\frac{U}{E_q}\right)\ln\left[2.7+\left(\frac{E_q-U}{\mathcal{E}}\right)^{1/2}\right]\right\}\left(1-\frac{U}{E_q}\right)^{\mathcal{E}/(\mathcal{E}+U)}.\tag{11}$$

(b) For heavy particles ($m_q \gg m_e$)

$$G_\sigma\left(\frac{\mathcal{E}}{|\Delta E|};\frac{v_q}{\bar{v}_e}\right)=f_{\bar{v}}\left[\frac{v_q^2}{v_q^2+\bar{v}_e^2}\frac{\Delta E}{\mathcal{E}}+\frac{4}{3}\ln\left(2.7+\frac{v_q}{\bar{v}_e}\right)\right]\left[1-\left(\frac{\Delta E}{\Delta E_{\max}}\right)^{1+v_q^2/\bar{v}_e^2}\right], \tag{12}$$

$$G_Q\left(\frac{\mathcal{E}}{U};\frac{v_q}{\bar{v}_e}\right)=f_{\bar{v}}\left[\frac{v_q^2}{v_q^2+\bar{v}_e^2}\frac{U}{\mathcal{E}}+\frac{2}{3}\left(1-\frac{U}{\Delta E_{\max}}\right)\ln\left(2.7+\frac{v_q}{\bar{v}_e}\right)\right]\left(1-\frac{U}{\Delta E_{\max}}\right)\left[1-\left(\frac{U}{\Delta E_{\max}}\right)^{1+v_q^2/\bar{v}_e^2}\right], \tag{13}$$

$$G_S\left(\frac{\mathcal{E}}{U};\frac{v_q}{\bar{v}_e}\right)=f_{\bar{v}}\left[\frac{v_q^2}{v_q^2+\bar{v}_e^2}\frac{U}{E}\ln\frac{\Delta E_{\max}}{U}+\frac{4}{3}\left(1-\frac{U}{\Delta E_{\max}}\right)\ln\left(2.7+\frac{v_q}{\bar{v}_e}\right)\right]\left[1-\left(\frac{U}{\Delta E_{\max}}\right)^{1+v_q^2/\bar{v}_e^2}\right]. \tag{14}$$

To present a full picture, we also recall that

$$f_{\bar{v}}=\left(\frac{\bar{v}_e}{v_q}\right)^2\left(\frac{v_q^2}{v_q^2+\bar{v}_e^2}\right)^{3/2}, \tag{15}$$

$$\Delta E_{\max}=\mathcal{E}\times 4\left(\frac{v_q}{\bar{v}_e}\right)^2\left(1+\frac{\bar{v}_e}{v_q}\right)=\mathcal{E}\times\alpha. \tag{16}$$

For small velocities of heavy particles $v_q \ll \bar{v}_e$, in correspondence with the formulas (II.50), (II.51), (II.52), the functions G_σ, G_Q, G_S will take the form:

$$G_\sigma=\frac{64}{9}\left(\frac{\mathcal{E}}{\Delta E}\right)^3\left(\frac{v_q}{\bar{v}_e}\right)^4, \tag{17}$$

$$G_Q=\frac{32}{15}\left(\frac{\mathcal{E}}{U}\right)^3\left(\frac{v_q}{\bar{v}_e}\right)^4, \tag{18}$$

$$G_S=\frac{128}{45}\left(\frac{\mathcal{E}}{U}\right)^3\left(\frac{v_q}{\bar{v}_e}\right)^4. \tag{19}$$

The magnitude $\sigma_0=\pi e^4 Z_q^2$ appearing in the above formulas, if ΔE or U is expressed in electron volts, has the value

$$\sigma_0=Z_q^2\, 6.56\times 10^{-14}\ \mathrm{eV}^2\ \mathrm{cm}^2, \tag{20}$$

where Z_q is the charge of the bombarding particle in units of elementary charge e. The graphs of the functions g_Q, G_Q, G_S most commonly used in the theory of atomic collisions are plotted in Figs. 1–3. The relations quoted above do not take into account the influence of the Coulomb field of the nucleus, which field not only modifies the cross sections derived (since the bombarding particle moving in that field changes both its energy and the direction of its motion), but in certain cases plays a decisive role, and is the cause of a definite physical process. Owing to the positive charge of the nucleus, the collision process with atomic electrons is influenced differently for the negative and for the positive impinging particles; whereas in the case of bombarding by electrons the identity of the colliding particles is especially significant. Now, starting with the simplest system, the atom, we shall proceed to make an analysis of the phenomena in both cases.

(a) Impact of Electrons

Neglecting the influence of the nuclear field upon the electron-electron collision process, the following will appear as effects of the first order:

(1) ionization process—when, in a collision, the atomic electron acquires an energy greater than its binding energy,

(2) excitation process—when the electron acquires an energy less than the binding energy, but greater than the energy of excitation.

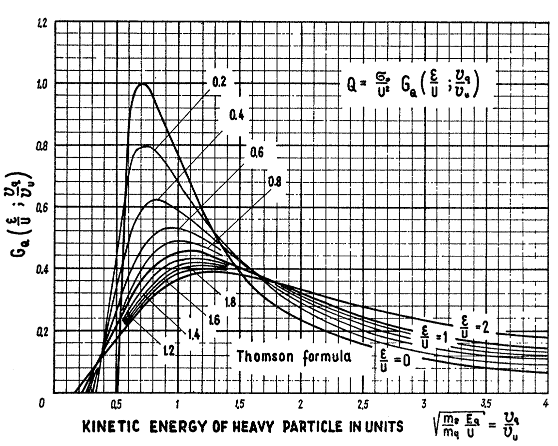

FIG. 2. Plot of the function G_Q which determines the cross section for collision with loss of energy greater than U, in the case of a heavy test particle.

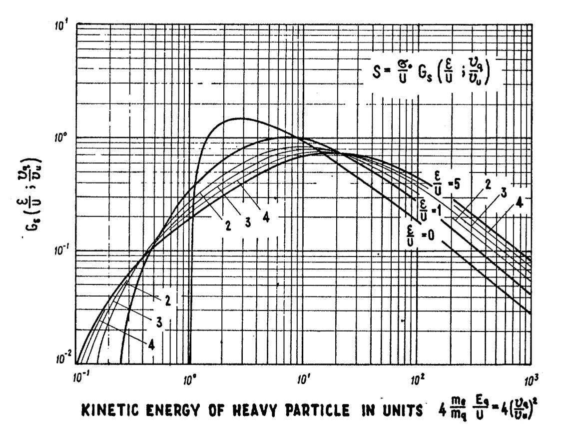

FIG. 3. Plot of the stopping-power function G_S as a function of the kinetic energy of a heavy particle for different values of the kinetic energy of a light field particle.

In such an approximation, the class of phenomena is limited to these two cases only. The presence of the positively charged nucleus immediately leads to the appearance of the exchange process as well as to the formation of negative ions. In this case, the collision of the incident electron should be considered as a collision inside the potential hole created by the Coulomb field of the nucleus. Therefore, if the collision has taken place at a certain distance from the nucleus, to which there corresponds a definite depth of the potential hole, while the external electron as a consequence of the collision has an energy less than the hole depth at the place of collision, then the electron will not be able to leave the nuclear field. As a result, a negatively charged ion may be created if the energy transferred to the atomic electron has been less than the ionization potential of the new system, or the exchange process may occur if it is greater.

The class of phenomena increases in number when we consider the collisions of electrons with heavy atoms. For instance, in the case of helium, new phenomena appear as, e.g., double ionization if the initial electron collides successively with two electrons, transferring to them energies exceeding their binding energies. The process of double ionization may also take a different course in that the initial electron collides with only one electron of the atom, and it is only the latter that causes the other to be ejected. A process similar to the preceding is, furthermore, the cause of excitation of terms with two excited electrons. The exchange process is also inseparably connected with the excitation of singlet and triplet terms. For heavier atoms or molecules, the number of combinations increases considerably, and the influence of multiple collisions must be considered separately in every particular case.

(b) Impact of Heavy Particles

The processes of excitation and ionization by positively charged heavy particles, even when neglecting the nuclear field, are changed by the capture process; whence, for instance, results the division into pure ionization with a free electron formed and ionization with the capture of the electron. This fact influences the slowing-down process, to which not only energy losses in the process of excitation and ionization contribute, but also the losses connected with the capture process, which, depending on the concrete systems, may either increase or decrease the resultant stopping power.

The nuclear field plays a principal role in the processes of inelastic collisions at very low energies of the bombarding particles, since, in that case, the value of the cross section is determined by collisions with electrons of sufficiently high velocities, and electron velocities are greatest in vicinity of the nucleus.

The above picture, which is valid for elementary incident particles, may in certain cases be extended to include collisions between complex atomic systems, particularly if the mean velocities of electrons of one of the systems are considerably less than the relative velocity of the systems, and if we operate with the cross sections of the theory of Coulomb collisions in which the dependence on the impact parameter D has been maintained.

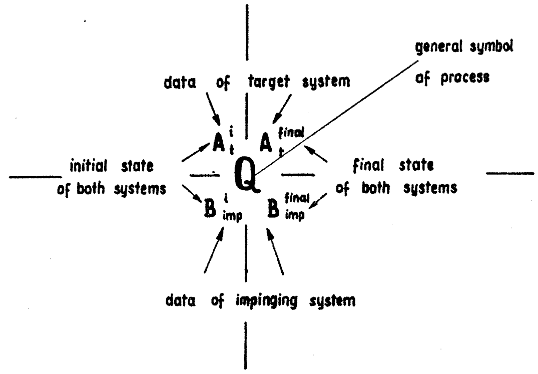

Fig. 4. Sketch illustrating the nomenclature used for atomic collisions.

IV. NOMENCLATURE OF THE THEORY OF ATOMIC COLLISIONS

In proceeding to discuss the various processes of atomic collisions, we think it fit to make some remarks on the notation which will be used. Having the basic symbol of the cross section Q, we shall put down on its left-hand side the data concerning the initial state of the colliding particles, and on its right-hand side those concerning their final state; whereas the superscripts will relate to the target particle, and the subscripts to the bombarding particle. Lack of a symbol in the final state is to be understood to mean a state identical with the initial state, while insertion of several symbols for the final state denotes a cross section corresponding to the sum of those processes. In a number of most typical instances the notation will be some what simplified. The principle of the nomenclature is shown in Fig. 4. Thus, for instance, the full designation of the cross section for single ionization of the argon atom by electrons will be:

$$ {}^{\mathrm{A}}{}_{e}Q^{\mathrm{A}+} \quad \text{or} \quad {}^{\mathrm{A}}{}_{e}Q^{+} \quad \text{or} \quad {}^{\mathrm{A}}{}_{e}Q^{\mathrm{i}}, $$

while the cross section for ionization of argon by protons, both in the pure ionization and in the capture process, may be written as follows:

$$ {}^{\mathrm{A}}{}_{p}Q_{p,\mathrm{H}}{}^{\mathrm{A}+} \quad \text{or} \quad {}^{\mathrm{A}}{}_{p}Q_{p,\mathrm{H}}{}^{+}. $$

By introducing additional symbols, it is possible to show the contribution of the respective shells in the process. So, e.g., the cross section for double ionization of the K shell of nickel by electrons may be written ${}^{K\mathrm{Ni}}{}_{e}Q^{++}$. Speaking in general of a certain class of processes, we shall use the following symbols:

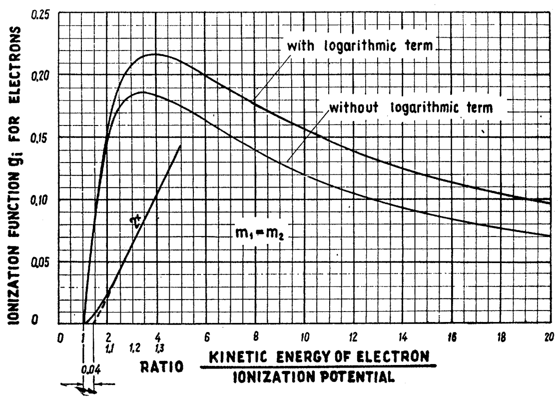

FIG. 5. The ionization function g_i for electrons, with and without the correction for the velocity distribution of atomic electrons.

(a) All cross sections differential with respect to energy exchange will be denoted with the symbol σ, inserting, if necessary, additional symbols, as for example:

$\sigma_{\vartheta,\Delta E}$: cross section for scattering of the impinging particle at an angle ϑ and with the change in energy ΔE.
$\sigma_{\Delta E^+}$: cross section for a collision with the gain of energy ΔE^+.

(b) All cross sections constituting the result of integration of the differential cross sections over a definite range of variable ΔE will be symbolized by the sign Q; thus in the cases of excitation and ionization we shall write Q^{exc} and Q^{i}; insertion of the indexes as superscripts means that we are concerned with the ionization of the target system, while the same done as subscripts indicates the ionization or excitation of the bombarding system.

(c) Cross sections determining the slowing-down process will be marked with the symbol S, the possibility of additional designations included (the slowing down due to the ionization process will therefore be written as S^{i}).

V. SINGLE IONIZATION BY ELECTRON IMPACT

The process of ionization by light particles (electrons) is described by the formulas (7) and (10), which, according to our rough assumption that $\mathcal{E}=U_i$, will assume a very simple form:

$$_eQ^{\mathrm{i}}=(\sigma_0/U_i^2)g_i(x) \tag{21}$$

$$g_i(x)=\frac{1}{x}\left(\frac{x-1}{x+1}\right)^{3/2} \times\left\{1+\frac{2}{3}\left(1-\frac{1}{2x}\right)\ln[2.7+(x-1)^{1/2}]\right\}, \tag{22}$$

where by x we have denoted the ratio of the kinetic energy of the bombarding electron to the binding energy of the orbital electron ($x=E_e/U_i$).

The graph of the function $g_i(x)$ with a logarithmic term resulting from the momentum distribution of the form $f(v_e)\to 1/v_e^3$ for $v_e\gg\bar{v}_e$ and without that term (then $\ln[2.7+(x-1)^{1/2}]\to 1$) is shown in Fig. 5.

The function $g_i(x)$ being at our disposal, the question of calculating the absolute cross section for the ionization of the whole atom, or of some of its shells, remains a completely trivial matter. We shall start the numerical calculations with the simplest case, which is the ionization of atomic hydrogen. Taking into account that the potential of atomic hydrogen is 13.6 eV, relations (21) and (22) immediately yield the absolute value of the ionization cross section:

$$^{\mathrm{H}}{}_eQ^{\mathrm{H}^+}=\frac{6.56\times10^{-14}}{(13.6)^2}g_i\left(\frac{E_e}{13.6}\right)$$
$$=3.54g_i\left(\frac{E_e}{13.6}\right)\quad\text{in Å}^2$$
$$=4.05g_i\left(\frac{E_e}{13.5}\right)\quad\text{in }\pi a_0^2$$
$$=12.5g_i\left(\frac{E_e}{13.6}\right)\quad\text{in cm}^{-1}\text{ (mm Hg)}^{-1}.$$

In the case of molecular hydrogen ($U_i=15.6$ eV), we have immediately:

$$^{\mathrm{H}_2}{}_eQ^{\mathrm{H}_2{}^+}=2\times\frac{6.56\times10^{-14}}{(15.6)^2}g_i\left(\frac{E_e}{15.6}\right)$$
$$=5.40\times10^{-16}g_i\left(\frac{E_e}{15.6}\right)\text{ cm}^2,$$

where the number two is due to the two electrons in the hydrogen molecule (we have assumed both electrons to be in the same energetic state).

Similarly, the ionization cross section of the helium atom is:

$$^{\mathrm{He}}{}_eQ^{\mathrm{He}^+}=2\times\frac{6.56\times10^{-14}}{(24.6)^2}g_i\left(\frac{E_e}{24.6}\right)$$
$$=2.17\times10^{-16}g_i\left(\frac{E_e}{24.6}\right)\text{ cm}^2.$$

Comparison of theoretical and experimental results[6–8] is given in Fig. 6.

At very high energies of the incident electrons ($E_e\gtrsim m_ec^2$) the velocity function $f_V{}^{(0)}$ which determines the cross section Q^{i} [see Eq. (10)], has to be calculated

[6] R. L. F. Boyd and G. W. Green, Proc. Phys. Soc. (London) **71**, 357 (1958).
[7] W. L. Fite and R. T. Brackman, Phys. Rev. **112**, 1141 (1958).
[8] J. T. Tate and P. T. Smith, Phys. Rev. **39**, 270 (1932).

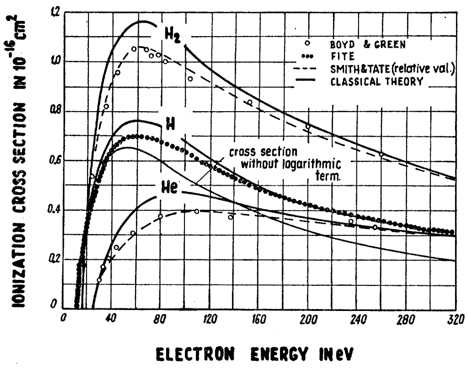

FIG. 6. Ionization cross sections of different gases by electron impact.

using the relativistic formula for the velocities. Denoting $f_V{}^{(0)\mathrm{rel}}/f_V{}^{(0)}=r(U_i/m_ec^2;\,E_e/U_i)$, we can write

$$_eQ^{\mathrm{i}}=\frac{\sigma_0}{U_i^2}g_i\left(\frac{E_e}{U_i}\right)r\left(\frac{U_i}{m_ec^2};\frac{E_e}{U_i}\right),\tag{23}$$

where $f_V{}^{(0)\mathrm{rel}}$ is given by (II.59). Clearly, in the nonrelativistic energy range $r=1$.

If the ionization potential is not too high ($U_i\leqslant m_ec^2$) and the velocity of the ionizing electron is much greater than the mean velocity of the atomic electron, the ionization cross section given by (23) will take the form

$$_eQ^{\mathrm{i}}=\frac{\sigma_0}{U_i^2}2\frac{U_i}{m_ec^2}\frac{(1+m_ec^2/E_e)^2}{1+2(m_ec^2/E_e)}\left(1+\frac{1}{3}\ln\frac{E_e}{U_i}\right)$$

$$\rightarrow\frac{\sigma_0}{U_i^2}\frac{2}{3}\frac{U_i}{m_ec^2}\ln\frac{E_e}{U_i}\qquad\text{for}\quad E_e\gg m_ec^2$$

$$\rightarrow\frac{\sigma_0}{U_i^2}\frac{U_i}{E_e}\left(1+\frac{2}{3}\ln\frac{E_e}{U_i}\right)\quad\text{for}\quad E_e\ll m_ec^2.\tag{24}$$

Using the above formulas, the ionization cross section

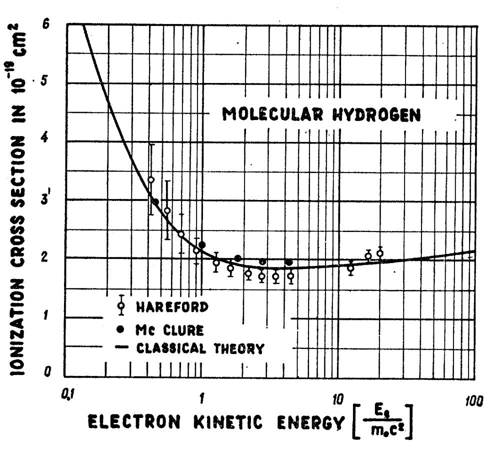

FIG. 7. Ionization cross section of molecular hydrogen for relativistic electrons.

of the molecular hydrogen for relativistic electrons has been calculated as

$$^{\mathrm{H}_2}{}_eQ^{\mathrm{i}}=5.40\times10^{-16}g_i\left(\frac{E_e}{15.6}\right)r\left(\frac{15.6}{5.11}\times10^{-5};\frac{E_e}{15.6}\right)\,\mathrm{cm}^2,$$

and has been compared with the experimental data of Hareford[9] and McClure[10] (see Fig. 7).

The validity of the approximate formula (23) has also been proved in two other cases in which the target electrons are of relativistic energies. These are the inner-shell ionization of Ni and Ag by electrons. Taking into account that the respective ionization potentials are $U_i{}^{\mathrm{Ni}K}=8.350$ eV and $U_i{}^{\mathrm{Ag}K}=25\,500$ eV (these ionization potentials have been taken from the tables given by Cauchois[11,12]), we have

$$^{\mathrm{Ni}K}{}_eQ^{\mathrm{i}}=18.8\times10^{-22}g_i\left(\frac{E_e}{U_i{}^{\mathrm{Ni}K}}\right)r\left(\frac{U_i{}^{\mathrm{Ni}K}}{m_ec^2};\frac{E_e}{U_i{}^{\mathrm{Ni}K}}\right)\,\mathrm{cm}^2,$$

$$^{\mathrm{Ag}K}{}_eA^{\mathrm{i}}=2.02\times10^{-22}g_i\left(\frac{E_e}{U_i{}^{\mathrm{Ag}K}}\right)r\left(\frac{U_i{}^{\mathrm{Ag}K}}{m_ec^2};\frac{E_e}{U_i{}^{\mathrm{Ag}K}}\right)\,\mathrm{cm}^2.$$

The theoretical results with and without the relativistic correction are plotted in Fig. 8; those with the relativistic correction are in very good agreement with the experimental data.[13–16]

Now, we shall pass on to more complicated cases, namely, the elements of greater atomic number with several groups of electrons of different binding energies. The simplest atom having electrons of different binding energies is lithium. It has two electrons of binding

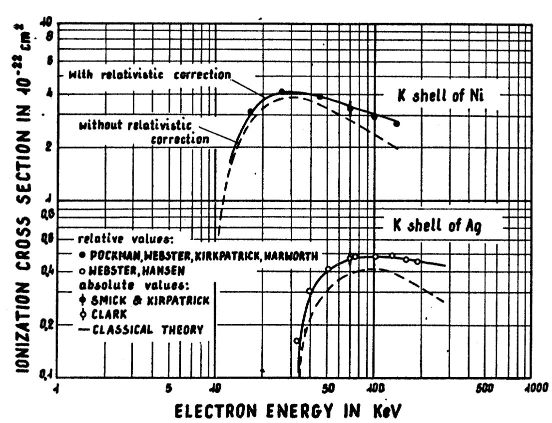

FIG. 8. Inner-shell ionization, with and without relativistic correction, by electron impact.

[9] F. L. Hareford, Phys. Rev. **74**, 574 (1948).
[10] G. W. McClure, Phys. Rev. **90**, 796 (1953).
[11] Y. Cauchois, J. Phys. Radium **13**, 113–121 (1952).
[12] Y. Cauchois, J. Phys. Radium **16**, 153–262 (1955).
[13] A. E. Smick and P. Kirkpatrick, Phys. Rev. **67**, 1153 (1945).
[14] L. T. Pockman, D. L. Webster, P. Kirkpatrick, and K. Harworth, Phys. Rev. **71**, 330 (1947).
[15] D. L. Webster, W. W. Hansen, and F. B. Duveneck, Phys. Rev. **43**, 839 (1933).
[16] I. C. Clark, Phys. Rev. **48**, 30 (1935).

energy 55 eV (1s electrons), and one electron of binding energy 5.4 eV (2s electron).

According to our approximate method, the total ionization cross section is the sum of the ionization cross sections of the individual shells. Thus, we have:

cross section for ejection of the 2s electron:

$$ {}^{\mathrm{Li2}s}{}_{e}Q^{\mathrm{i}}=1\times\frac{6.56\times10^{-14}}{5.4^2}g_i\left(\frac{E_e}{5.4}\right)\mathrm{cm}^2 $$

$$ =22.5\times10^{-16}g_i\left(\frac{E_e}{5.4}\right)\mathrm{cm}^2; $$

cross section for ejection of one of the two 1s electrons:

$$ {}^{\mathrm{Li1}s}{}_{e}Q^{\mathrm{i}}=2\times\frac{6.56\times10^{-14}}{55^2}g_i\left(\frac{E_e}{55}\right)\mathrm{cm} $$

$$ =0.44\times10^{-16}g_i\left(\frac{E_e}{55}\right)\mathrm{cm}^2; $$

and finally the total ionization cross section:

$$ {}^{\mathrm{Li}}{}_{e}Q^{\mathrm{i}}={}^{\mathrm{Li2}s}{}_{e}Q^{\mathrm{i}}+{}^{\mathrm{Li1}s}{}_{e}Q^{\mathrm{i}}. $$

In Fig. 9 the theoretical results and relative values obtained by Brink,[17] both normalized at 500 eV, are given. Similarly, in the case of the argon atoms we have:

Group of electrons Shell of an atom		Number of electrons in the shell	Ionization potential of the shell in eV
K	1s	2	3190
L	2s	2	324
L	2p	6	247
M	3s	2	29
M	3p	6	15.7

The ionization cross section of each shell is, respectively:

$$ {}^{\mathrm{A}1s}{}_{e}Q^{+}=1.29\times10^{-20}g_i(E_e/3190)\times r(6.25\times10^{-3};E_e/3190)\ \mathrm{cm}^2, $$

$$ {}^{\mathrm{A}2s}{}_{e}Q^{+}=1.25\times10^{-18}g_i(E_e/324)\times r(6.34\times10^{-4};E_e/324)\ \mathrm{cm}^2, $$

$$ {}^{\mathrm{A}2p}{}_{e}Q^{+}=6.45\times10^{-18}g_i(E_e/247)\times r(4.84\times10^{-4};E_e/247)\ \mathrm{cm}^2, $$

$$ {}^{\mathrm{A}3s}{}_{e}Q^{+}=1.56\times10^{-16}g_i(E_e/29)r(5.67\times10^{-5};E_e/29)\ \mathrm{cm}^2, $$

$$ {}^{\mathrm{A}3p}{}_{e}Q^{+}=16\times10^{-16}g_i(E_e/17.5)\times r(3.08\times10^{-5};E_e/15.7)\ \mathrm{cm}^2, $$

and the total ionization cross section of an argon atom, being the sum of the partial ionization cross sections, is:

$$ {}^{\mathrm{A}}{}_{e}Q^{+}={}^{\mathrm{A}1s}{}_{e}Q^{+}+{}^{\mathrm{A}2s}{}_{e}Q^{+}+{}^{\mathrm{A}2p}{}_{e}Q^{+}+{}^{\mathrm{A}3s}{}_{e}Q^{+}+{}^{\mathrm{A}3p}{}_{e}Q^{+}. $$

The greatest contribution to the total cross section is that due to the outer shell of the atom, which in the case of argon is of the order of 99%. The contribution

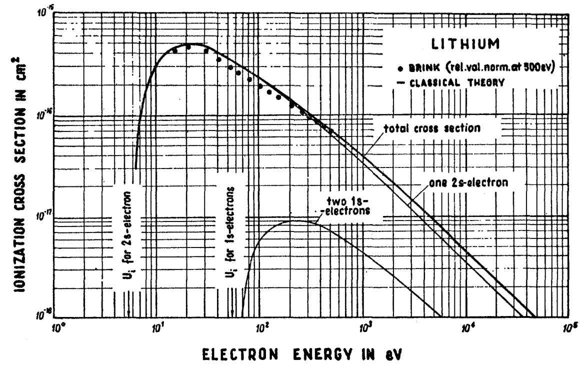

FIG. 9. The ionization cross section of lithium, including the contribution of the K-shell ionization, by electrons.

of the inner-shell electrons to the total ionization is negligibly small (Fig. 10, experimental data of Bleakney[18]).

Taking into account that the maximum value of the function g_i, being independent of U_i, is equal to 0.216, the greatest value of the ionization cross section of a given shell is:

$$ Q_{\mathrm{max}}{}^{\mathrm{i}}=(\sigma_0/(U_i{}^k)^2)\times0.216n_e{}^k. \tag{25} $$

This maximum is attained at energies of incident electrons

$$ E_e\simeq4U_i{}^k. $$

At very high energies, for velocities of the incident electrons much greater than the mean velocity of the K-shell electrons, the atomic cross section can be

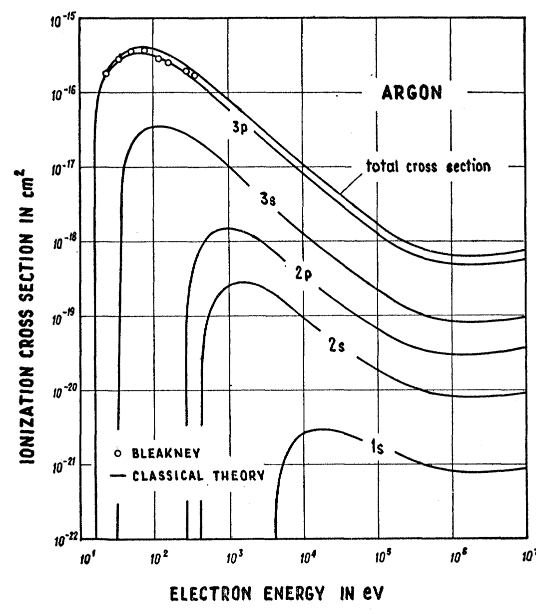

FIG. 10. The cross section for the ionization of different shells and the total ionization cross section of argon for electrons up to relativistic energies.

[17] G. O. Brink, Phys. Rev. 127, 1209 (1962).

[18] L. Bleakney, Phys. Rev. 34, 157 (1929).

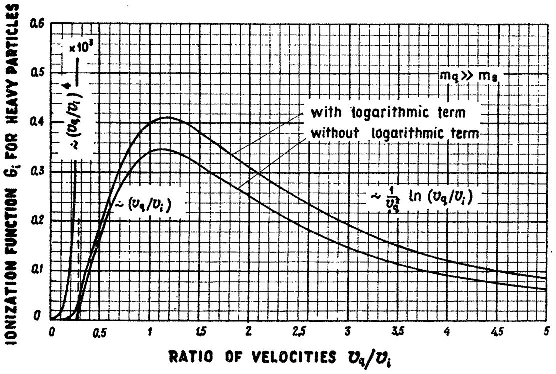

FIG. 11. Ionization function G_i for heavy particles, averaged over the continuous velocity distribution of atomic electrons (with the logarithmic term) and not averaged (without logarithmic term).

expressed by the very simple formula

$$ {}^{\text{atom}}{}_{e}Q^{\mathrm{i}} \simeq \frac{1}{\frac{1}{2}m_e v_e^2}\sum_k n_e^k \frac{\sigma_0}{U_i^k}\left(1+\frac{1}{3}\ln\frac{E_e}{U_i^k}\right), \qquad (26) $$

which shows the contribution of each shell clearly. The contribution of each shell in the first approximation is inversely proportional to the ionization potential of the shell, and is proportional to the number of electrons in the shell.

VI. SINGLE IONIZATION BY HEAVY CHARGED PARTICLES

If the velocity of the ionized particle is much greater then the velocities of electrons in the ionized atoms, no difference exists between ionization by heavy charged particles and by electrons of the same velocity. The difference occurs at the low velocities of the impact particle. As we know from Paper II, the minimum energy of the incident particle at which the amount of energy ΔE can be transferred to the target electron of energy $\mathcal{E}$ is

in the case of electrons,

$$ E_e = \Delta E , $$

in the case of heavy particles, (27)

$$ E_q = \frac{\Delta E}{4m_e/m_q}\left[\left(\frac{\mathcal{E}}{\Delta E}+1\right)^{1/2} - \left(\frac{\mathcal{E}}{\Delta E}\right)^{1/2}\right]. $$

It is necessary here to draw attention to a very common error resulting from the assumption $\mathcal{E}=0$, impermissible for the atomic collisions: At $\mathcal{E}=0$ the threshold energy for ionization by heavy particles, determined from relation (27), amounts to

$$ E_q = \tfrac{1}{4}(m_q/m_e)U_i = U_i/K_{qe} \qquad (28) $$

as against the value

$$ E_q = 0.17 \times U_i/K_{qe} \qquad (29) $$

obtained for $\mathcal{E}=U_i$. Evidently, as a result of the continuous character of the velocity distribution function of the electrons in the atom, the ionization process may also take place at still lower energies, while the threshold for the mean velocity of the electron in the orbit, which we will call the apparent threshold, is only accompanied by a change in energy dependence. According to this the process of ionization by heavy particles may be described in the following way:

$$ Q^{\mathrm{i}} = (\sigma_0/U_i^2)G_i(v_q/v_i) , \qquad (30) $$

where the function G_i has the form:

(a) above the apparent threshold (for $v_q > 0.206 v_i$)

$$ G_i = f_{\bar{v}}\left[\frac{v_q^2}{v_q^2+v_i^2} + \frac{2}{3}\left(1+\frac{1}{\alpha}\right)\ln\left(2.7+\frac{v_q}{v_i}\right)\right] \times\left(1-\frac{1}{\alpha}\right)\left[1-\left(\frac{1}{\alpha}\right)^{1+v_q^2/v_i^2}\right], \qquad (31) $$

(b) below the apparent threshold (for $v_q < 0.206 v_i$)

$$ G_i \simeq 2\frac{2}{15}\left(\frac{v_q}{v_i}\right)^4 . \qquad (32) $$

In the above, v_i denotes the velocity of an electron, corresponding to the ionization potential. The plot of the function $G_i(v_q/v_i)$ is shown in Fig. 11.

In the region of extremely low energies we cannot neglect the influence of the averaged field of the target atom upon the motion of the heavy incident particle. For positive impacts, the region of radii smaller than the distance of closest approach, as determined by:

$$ M_t/(M_t+m_q)E_q = e\varphi(r)Z_q , $$

where M_t is the mass of the target atom and the other symbols are the same as in (2), is excluded from penetration. Since according to the classical mechanics we can put

$$ e\varphi(r) = E_e(r) , $$

the velocity of the impact in the vicinity of the target nucleus can be written approximately

$$ v_q \simeq \left[\frac{2}{m_q}\left(\frac{M_t}{M_t+m_q}E_q - E_e Z_q\right)\right]^{1/2} . \qquad (33) $$

Using (33) for the calculation of G_i^{thr} (see Sec. VI of Paper II) we have

$$ G_i^{\mathrm{thr}} \simeq \frac{2}{3}\left(\frac{m_e q}{m_q e}\right)^{1/2}\int_{x_1}^{x_2}\frac{(a-x^2)^{1/2}}{x^4} \times\left[1+\frac{A}{x(a-x^2)^{1/2}}\right]\left[1-\frac{A}{x(a-x^2)^{1/2}}\right]^2 dx, \qquad (34) $$

where

$$a=\frac{E_q}{U_i}\frac{M_t}{M_t+m_q}\frac{1}{Z_q}\quad A=\frac{1}{4}\left(\frac{m_q}{m_e}\frac{1}{Z_q}\right)^{1/2}, \tag{35}$$

and x_1 and x_2 are the roots of the equation

$$1-A/x(a-x^2)^{1/2}=0.$$

The lower limit of integration x_1 corresponds to the maximum distance from the nucleus $r_{\max}$, i.e., to the minimum velocity of the target electron at which the ionizing collisions can still take place, while similarly the upper limit of integration x_2 corresponds to the minimum distance and the maximum velocity. As a result, the process of ionizing collisions occurs in the layer between the radii $r_{\max}$ and $r_{\min}$. As the velocity of the heavy particle decreases, the thickness of this layer grows smaller, and at $x_1=x_2$ vanishes, thus determining the threshold for the ionization process by positively charged heavy particles.

$$E_q^{\text{thr}}=\frac{U_i}{2}\left(\frac{m_q}{M_t}+1\right)\left(\frac{m_q}{m_e}\frac{e}{q}\right)^{1/2}. \tag{36}$$

Denoting E_q/E_q^{thr} by x and performing the integration in (34), we finally obtain:

$$G_i^{\text{thr}}=2\frac{2}{15}\left(\frac{v_q}{v_i}\right)^4\left\{1-\frac{19}{12}x^2-\frac{1}{24}x^4+\frac{5}{16}\frac{x^6}{(1-x^2)^{1/2}}\ln\frac{1+(1-x^2)^{1/2}}{1-(1-x^2)^{1/2}}\right\}(1-x^2)^{1/2}. \tag{37}$$

The form of the function G_i having been derived, performing the numerical calculations presents no difficulty. Calculations are identical to those for the case of electrons, provided, obviously, that instead of the function g, we use the function G. Thus the cross sections for the ionization of atomic hydrogen, helium, and argon by protons are

$$^{\text{H}}{}_pQ^{\text{H}^+}=3.54\times10^{-16}G_i(v_p/2.2\times10^8\text{ cm sec}^{-1})\text{ cm}^2,$$

$$^{\text{He}}{}_pQ^{\text{He}^+}=2.17\times10^{-16}G_i(v_p/2.96\times10^8\text{ cm sec}^{-1})\text{ cm}^2,$$

$$^{\text{A}}{}_pQ^{\text{A}^+}={}^{\text{A}3p}{}_pQ^{\text{A}3p^+}+{}^{\text{A}3s}{}_pQ^{\text{A}3s^+}$$
$$=16\times10^{-16}G_i(v_p/2.4\times10^8\text{ cm sec}^{-1})+1.56\times10^{-16}G_i(v_p/3.6\times10^8\text{ cm sec}^{-1}).$$

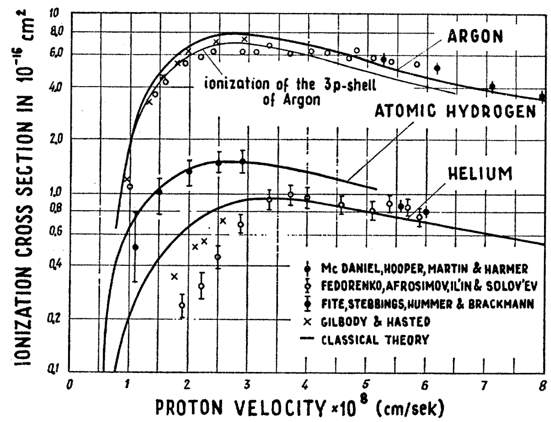

FIG. 12. The ionization cross sections of different gases by protons.

Experimental data[19–22] and the theoretical results are shown in Fig. 12.

Similarly, with the help of (36) and (37), we have calculated cross sections for the inner-shell ionization of some elements (Al, Ti, Zn, Ag, Ni) by low-energy protons and K-shell ionization of Cu by deuterons.

$$^{\text{Al}K}{}_pQ^+=5.4\times10^{-20}G_i(v_p/2.35\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/2.35\times10^9\text{ cm sec}^{-1}),$$
$$^{\text{Ti}K}{}_pQ^+=5.3\times10^{-21}G_i(v_p/4.2\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/4.2\times10^9\text{ cm sec}^{-1}),$$
$$^{\text{Ni}K}{}_pQ^+=1.9\times10^{-21}G_i(v_p/5.5\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/5.5\times10^9\text{ cm sec}^{-1}),$$
$$^{\text{Cu}K}{}_pQ^+=1.6\times10^{-21}G_i(v_p/5.7\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/5.7\times10^9\text{ cm sec}^{-1}),$$
$$^{\text{Zn}K}{}_pQ^+=1.4\times10^{-21}G_i(v_p/5.9\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/5.9\times10^9\text{ cm sec}^{-1}),$$
$$^{\text{Cu}K}{}_dQ^+=1.6\times10^{-21}G_i(v_p/5.7\times10^9\text{ cm sec}^{-1})+G_i^{\text{thr}}(v_p/5.7\times10^9\text{ cm sec}^{-1}).$$

The calculated curves and the experimental data[23–28] are in very good agreement; see Figs. 13–16.

According to (36) we have calculated threshold energies for ionization for various colliding systems including heavy ions and heavy atoms. The theoretical and experimental[29] values are given in Table I.

[19] E. W. McDaniel, J. W. Hooper, D. W. Martin, and D. S. Harmer, *Proceedings of the Fifth Conference on Ionization in Gases, Munich, 1961* (North-Holland Publishing Company, Amsterdam, 1962), pp. 60–68.

[20] N. V. Fedorenko, V. V. Afrosimov, R. N. Il'in, and E. S. Solovev, *Proceedings of the Fourth Conference on Ionization in Gases, Uppsala, 1959* (North-Holland Publishing Company, Amsterdam, 1960), p. 47.

[21] W. L. Fite, *Proceedings of the Fourth International Conference on Ionization in Gases, Uppsala, 1959* (North-Holland Publishing Company, Amsterdam, 1960), Vol. I, p. 23.

[22] H. B. Gilbody and J. B. Hasted, Proc. Roy. Soc. (London) **A240**, 382 (1957).

[23] O. Peter, Ann. Physik **27**, 299 (1936).

[24] P. R. Bevington and E. M. Bernstein, Bull. Am. Phys. Soc. **1**, 198 (1956).

[25] M. S. Livingston, F. Genevese, and E. J. Konopiński, Phys. Rev. **51**, 835 (1937).

[26] H. W. Lewis, B. E. Simmons, and E. Merzbacher, Phys. Rev. **91**, 343 (1953).

[27] B. Singh, Phys. Rev. **107**, 711 (1957).

[28] E. Merzbacher and H. W. Lewis, *Encyclopedia of Physics* (Springer-Verlag, Heidelberg, 1958), Vol. 341, p. 183.

[29] H. S. Massey and B. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Clarendon Press, Oxford, 1952), pp. 455–456.

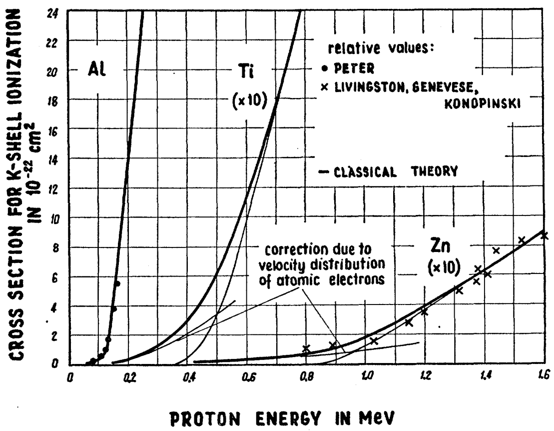

FIG. 13. Ionization cross section of Al, Ti, and Zn for protons at very low energies.

It follows from the comparison given that the experimental value of the threshold energy is several times higher than the theoretical value, this being rather unobjectionable in view of the fact that we do not determine the exact threshold value in the experiment, but one considerably greater by an amount determined by the sensitivity of the measurement method.

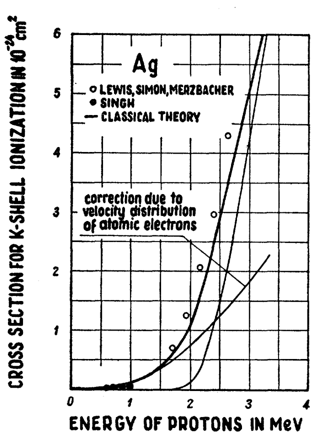

FIG. 14. Ionization cross section of Ag for low-energy protons.

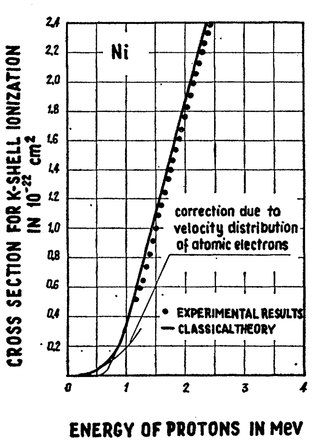

FIG. 15. Ionization cross section of Ni for low-energy protons.

In spite of the fact that the masses of the colliding particles as well as their charges change by several tens of times, and as a result, the threshold energies also change by several hundred times, the ratio of the experimental to the theoretical value changes by only several times, remaining approximately constant within a given group determined by the type of the ionizing particle. From the qualitative agreement obtained between theory and experiment, an inference can be made that in the process of ionization by atoms or heavy ions, at very low energies of the colliding systems, the decisive role is played by the interaction of the electrons of the ionized system with the nucleus of the bombarding system, and at the moment of closest approach of the two.

VII. CHARGE TRANSFER

The capture of an electron, which according to our nomenclature will be written as follows:

$${}^{A}{}_{B^+}Q_{B}{}^{A^+},$$

can be easily explained on the basis of the theory of binary collisions. And thus if we denote by U_i^A the binding energy of the electron in system A, and by U_i^B the ionization energy of the level on which the electron in the B^+ system is captured, then, in order that the capture should occur, any of the electrons of the A system has to gain from the particle B^+ an energy corresponding to its velocity plus the difference $U_i^A - U_i^B$ of binding energies in the two systems; nevertheless, the acquired energy cannot be greater than that corresponding to the translational motion plus the ionization energy of the level on which the electron is captured; or in other words, the energy of the relative motion after collision cannot be greater than the ionization potential of the B system. The capture then occurs if in collsion the electron acquires energy within the limits

$$\tfrac{1}{2}m_e v_{B^+}^2 + U_i^A - U_i^B \leqslant \Delta E \leqslant \tfrac{1}{2}m_e v_{B^+}^2 + U_i^A + U_i^B. \quad (38)$$

Having determined the limits for ΔE, we can estimate the cross section for the process considered:

$$Q_c \simeq \int_{m_e v_{B^+}^2/2 + U_i^A - U_i^B}^{m_e v_{B^+}^2/2 + U_i^A + U_i^B} \sigma_{\Delta E}\, d(\Delta E)$$

or, with the aid of (II.38) and with use of the assumption $\bar{E}_e^A \simeq U_i^A$:

$$Q_c = \frac{\sigma_0}{(U_i^A)^2} \frac{2U_i^B}{U_i^A} G_c\left(\frac{U_i^B}{U_i^A}; \frac{v_{B^+}}{v_i^A}\right), \quad (39)$$

where

$$G_c\left(\frac{U_i^B}{U_i^A}; \frac{v_{B^+}}{v_i^A}\right) = \frac{f_{\bar{v}}(v_{B^+}/v_i^A)}{[1 + (v_{B^+}/v_i^A)^2]^2 - (U_i^B/U_i^A)^2}. \quad (40)$$

From the above relation it follows that if $U_i^A > U_i^B$, the cross section for that process will have its maximum at velocities such that

$$\tfrac{1}{2}m_e v_{B^+}{}^2 \simeq U_i{}^A - U_i{}^B.$$

For $U_i{}^A = U_i{}^B$ (which corresponds to the resonance charge transfer), the cross section increases monotonically with decrease of the particle energy. At very small velocities, since the electron considered is not a free particle for which the theory of binary collisions could be appropriate, but is bound in the atom and has a limited region of motion, the formula (39) is no longer

TABLE I. Experimental and theoretical values of threshold energies for ionization by atoms, molecules, atomic ions and molecular ions.

Ionizing	Ionized	Ionization potential in eV	Experimental values in keV	Theoretical values in keV	Ratio of exp. value to theor. value
H^+	He	24.56	2.35	0.66	3.6
He^+	He	24.56	15.0	3.0	5
He	He	24.56	15.0	3.0	5
Be^+	He	24.56	55.0	10.4	5.3
B^+	He	24.56	76.0	14.7	5.15
B^{++}	He	24.56	76.0	14.7	5.15
C^+	He	24.56	90.0	18.0	5.0
C^{++}	He	24.56	90.0	18.0	5.0
Al^+	He	24.56	441.0	77.0	5.7
K^+	He	24.56	260	155.0	1.7
Fe^+	He	24.56	1600	303.0	5.3
Fe^{++}	He	24.56	1600	303.0	5.3
Fe^{+++}	He	24.56	1600	303.0	5.3
Cu^+	He	24.56	2000	384.0	5.2
Cu^{++}	He	24.56	2000	384.0	5.2
Cu^{+++}	He	24.56	2000	384.0	5.2
H^+	Ar	15.75	0.78	0.345	2.25
L^+	Ar	15.75	7.1	1.8	4.0
Ne^+	Ar	15.75	31.0	8.4	3.7
Mg^{++}	Ar	15.75	77.0	10.5	7.3
Ar	Ar	15.75	62.1	18.1	3.45
Ar^+	Ar	15.75	62.1	18.1	3.45
Ar^{++}	Ar	15.75	62.1	18.1	3.45
K^+	Ar	15.75	62.1	18.1	3.45
Rb^+	Ar	15.75	186.0	59.5	3.12
Co^+	Ar	15.75	400.0	125.0	3.2
H_2^+	Ar	15.75	1.6	0.69	2.32
N_2^+	Ar	15.75	37.	9.0	4.1
Li^+	Ne	21.56	13.7	2.84	4.83
Ne	Ne	21.56	58.0	13.1	4.43
Ne^+	Ne	21.56	58.0	13.1	4.43
Ne^+	Ne	21.56	74.0	15.7	4.70
Mg^{++}	Ne	21.56	77.0	17.3	4.45
Ar	Ne	21.56	175.0	37.0	4.73

valid. The maximum impact parameter at which the electron can still be captured into the orbit is determined by the condition

$$e^2 Z_{B^+}/D_{\max} \leqslant U_i{}^A.$$

Denoting by r_A the amplitude of oscillation of the target-atom electron, we can estimate a maximum of the cross section for the capture:

$$Q_c{}^{\text{geom}} \simeq \pi (r_A + D_{\max})^2 = \pi a_0{}^2 \left(\frac{r_A}{a_0} + 2 \frac{U_i{}^H}{U_i{}^A} Z_{B^+} \right)^2. \quad (41)$$

The situation will be analogous for $U_i{}^A < U_i{}^B$, the

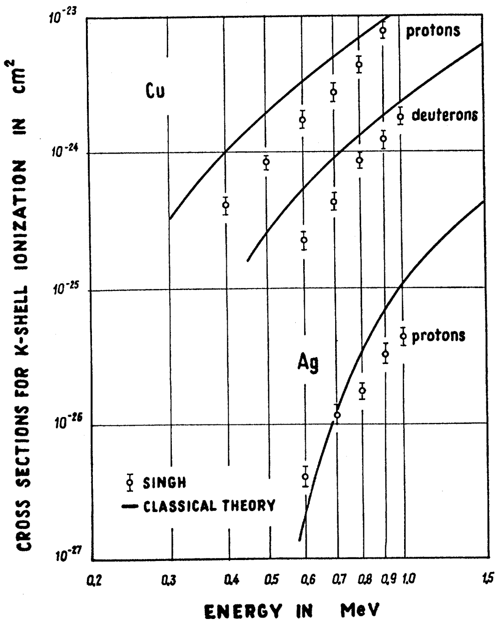

FIG. 16. K-shell ionization of Cu and Ag by low-energy protons and deuterons.

only difference being that the asymptotic value of the cross section corresponding to the geometrical cross section (41) will be reached much earlier, already at energies

$$\tfrac{1}{2}m_e v_{B^+} = U_i{}^B - U_i{}^A,$$

shifting with the increase of $U_i{}^B$ more and more into the region of high energies. The plot of the capture function G_c is shown in Fig. 17, while the qualitative

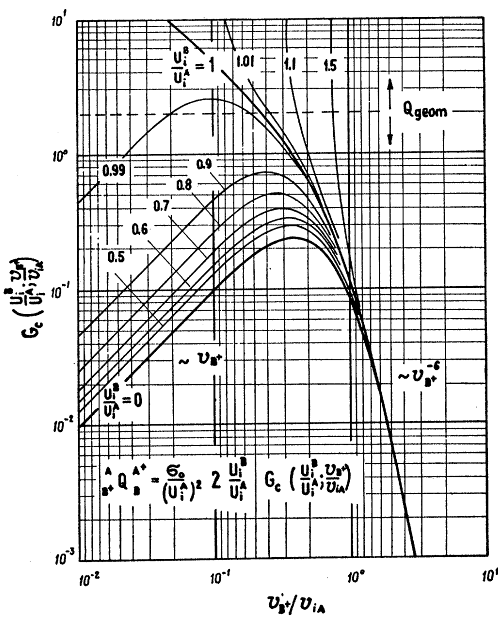

FIG. 17. Graph of the function which determines the capture process.

form of the cross section for the capture process is shown in Fig. 18. To illustrate the considerations, calculations have been made for several cases, using the formula (39):

$$\tfrac{1}{2}\,{}^{H_2}{}_{p}Q_{H}{}^{H_2^+}=\frac{6.56\times10^{-14}}{15.6^2}\,2\,\frac{13.6}{15.6}\,G_c\left(\frac{13.6}{15.6};\, v_p/2.4\times10^8\text{ cm sec}^{-1}\right)=5.05\times10^{-16}G_c(0.87;\, v_p/2.4\times10^8\text{ cm sec}^{-1})\text{ cm}^2,$$

$${}^{He}{}_{p}Q_{H}{}^{He^+}=2.39\times10^{-16}G_c(0.55;\, v_p/2.95\times10^8\text{ cm sec}^{-1})\text{ cm}^2,$$

$${}^{A}{}_{p}Q_{H}{}^{A^+}\simeq{}^{A3p}{}_{p}Q_{H}{}^{A3p^+}+{}^{A3s}{}_{p}Q_{H}{}^{A3s^+}$$

$$=3\times10^{-15}G_c(0.87;\, v_p/2.4\times10^8\text{ cm/sec}^{-1})+2\times10^{-16}G_c(0.5;\, v_p/3.1\times10^8\text{ cm sec}^{-1})\text{ cm}^2,$$

$${}^{H}{}_{p}Q_{H}{}^{H^+}=7.1\times10^{-16}G_c(1;\, v_p/2.2\times10^8\text{ cm sec}^{-1})\text{ cm}^2.$$

The process ${}^{H}{}_{p}Q_{H}{}^{H^+}$ represents the resonance charge transfer; in this case the cross section is deprived of a maximum, increasing to the value of the order of Q_c^{geom} as $v_p\to0$. As is evident from Figs. 19–21, the calculated cross sections indicate qualitatively the nature of the capture process.[30–33] At high velocities the calculated cross section decreases with the sixth power of the impact velocity which is the same dependence as that experimentally found in the region of medium energies; at very high energies, the decrease is too slow.

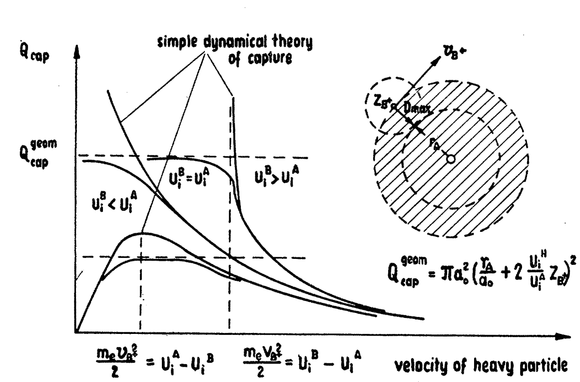

FIG. 18. Sketch illustrating the qualitative form of the capture cross section, and of the role of the geometric cross sections determined by the dimensions of the orbit in the target atom and by the ionization potentials of the atom and the moving ion.

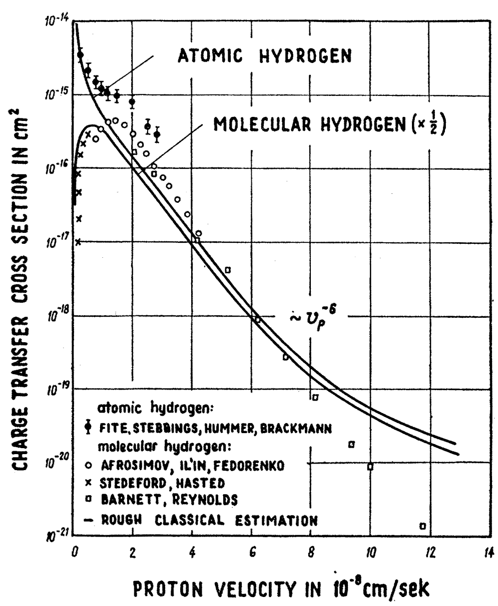

FIG. 19. The capture of electrons by protons in atomic and molecular hydrogen. For atomic hydrogen we have the case of resonance.

The cause of this difference lies in too rough a treatment of the process considered, since the condition (38) is necessary but not sufficient for the target-atom electron to be captured into the orbit of the moving

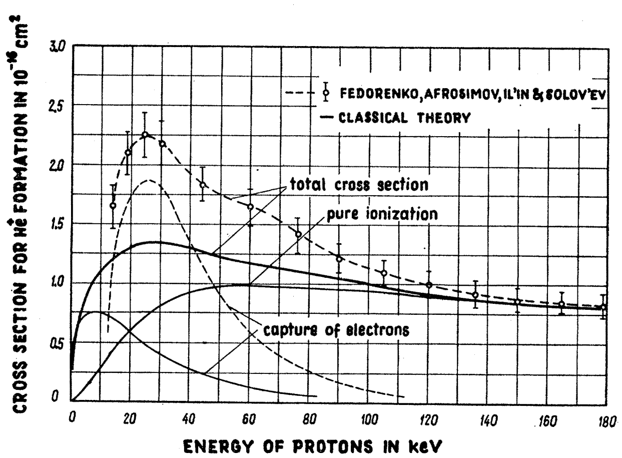

FIG. 20. Cross section for the formation of helium ions by protons, which is the sum of the cross sections for pure ionization and for ionization in the capture process.

particle; moreover, the atomic electron should be ejected in the direction of the velocity vector of the incident particle. Both velocity vectors must be contained in an appropriately small angle which, being a function of energy, rapidly decreases with increase

[30] W. L. Fite, R. F. Stebbings, D. G. Hummer, and R. T. Brackman, Phys. Rev. **119**, 663 (1960).

[31] B. B. Afrosimov, R. N. Il'in, and H. B. Fedorenko, Zh. Eksperim. i Teor. Fiz. **34**, 1398 (1958) [English transl.: Soviet Phys.—JETP **7**, 969 (1958)].

[32] J. B. H. Stedeford and J. B. Hasted, Proc. Roy. Soc. (London) **A240**, 382 (1957).

[33] C. F. Barnett and H. K. Reynolds, Phys. Rev. **109**, 355 (1958).

of the latter, conducing to additional decrease of the cross section.

However, this process may be quite correctly explained in terms of the theory of binary collisions, wherein the calculations become considerably complicated, and in the reasoning the essential role is played by the momentum distribution of the target electrons.

As far as the difference in the region of small energies is concerned, it will be rather difficult to eliminate it on the ground of the two-body approximation; for $v_q \to 0$ and $\Delta E \to 0$, considering that the electrons are bound in the atom, this approximation is not valid any more.

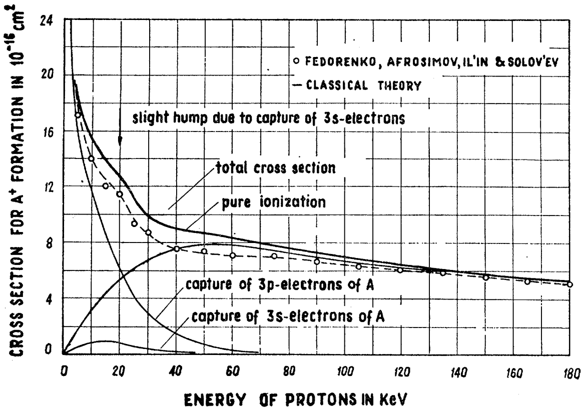

FIG. 21. Cross section for formation of argon ions by protons.

VIII. MULTIPLE IONIZATION

The formation of a multiply ionized atomic system may occur either in the process of successive collisions of the ionizing incident particle with some electrons of the system, or in the process of collision between the electron being ejected and the remaining electrons. The cross section for the transfer of energy ΔE from the incident particle to some of the n_e electrons of the system (we consider the group of electrons as being in the same energy state) is (see Fig. 22) $n_e\sigma_{\Delta E}(E_q)$, and the probability that the primary particle will collide once more with some other electron, transferring to it energy $\Delta E'$, is

$$\sum_{i=1}^{n_e-1} \frac{1}{4\pi}\frac{1}{r_i^2}\sigma_{\Delta E'}(E_q-\Delta E).$$

Therefore the cross section for two successive, collisions

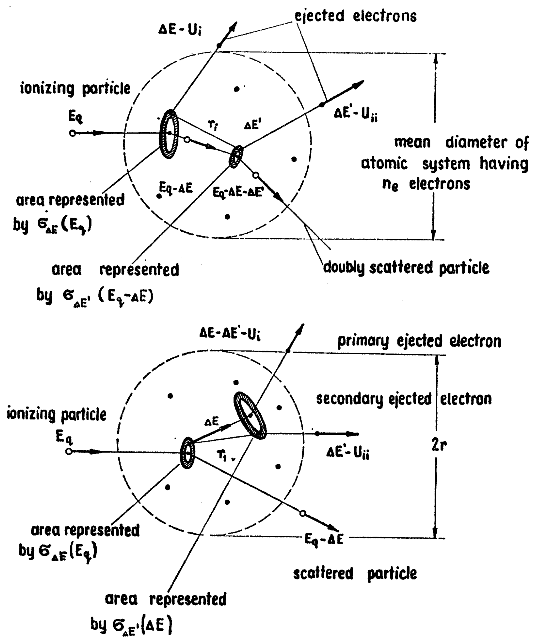

FIG. 22. Two ways of formation of doubly ionized ions in the double ionization process.

in which impact loses energies ΔE and $\Delta E'$ can be written

$$n_e\sigma_{\Delta E}(E_q)\sum_{i=1}^{n_e-1}\frac{1}{4\pi}\frac{1}{r_i^2}\sigma_{\Delta E'}(E_q-\Delta E), \tag{42a}$$

where E_q is the initial energy of the particle, $E_q-\Delta E$ represents the energy left with the particle after the first collision, and r_i is the distance from the electron which has acquired energy ΔE to the ith electron. Assuming that the density of electrons in the shell of the atom is uniform, and denoting the mean distance between electrons by $\bar{r}$, (42a) may be rewritten

$$(1/4\pi)(n_e(n_e-1)/\bar{r}^2)\sigma_{\Delta E}(E_q)\sigma_{\Delta E'}(E_q-\Delta E). \tag{42b}$$

In order to make the first electron leave the system, it is necessary to provide it with an energy greater than the first ionization potential U_i, whereas to eject the next electron, an energy greater than the second ionization potential U_{ii} is needed. Finally, the cross section for double ionization by the primary particle only will be [Fig. 22(a)]

$$Q_{\mathrm{sc}}{}^{\mathrm{ii}}=\frac{n_e(n_e-1)}{4\pi r^2}\int_{U_i}^{\Delta E^{\max}=f(E_q-U_{ii})}\sigma_{\Delta E}(E_q)d(\Delta E)\int_{U_{ii}}^{\Delta E^{\max}=f(E_q-\Delta E)}\sigma_{\Delta E'}(E_q-\Delta E)d(\Delta E'). \tag{43}$$

Analogous reasoning carried out for the ionization by the recoiled electron gives [Fig. 22(b)]

$$Q_{\mathrm{ej}}{}^{\mathrm{ii}}=\frac{n_e(n_e-1)}{4\pi r^2}\int_{U_i+U_{ii}}^{\Delta E^{\max}}\sigma_{\Delta E}(E_q)d(\Delta E)\int_{U_{ii}}^{\Delta E}\sigma_{\Delta E'}(\Delta E)d(\Delta E'). \tag{44}$$

If the primary particle is an electron, then $\Delta E^{\max}=E_q-\Delta E$ and the above relations may be reduced to the form

$$ {}_eQ_{\rm sc}{}^{\rm ii}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i}^{E_q-U_{ii}}\sigma_{\Delta E}(E_q)Q_{U_{ii}}(E_q-\Delta E)d(\Delta E'), \tag{45} $$

$$ {}_eQ_{\rm ej}{}^{\rm ii}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i+U_{ii}}^{E_q}\sigma_{\Delta E}(E_q)Q_{U_{ii}}(\Delta E)d(\Delta E). \tag{46} $$

Taking into account that $\sigma_{\Delta E}(E_q)$ is a rapidly decreasing function of ΔE [$\sigma_{\Delta E}\propto 1/(\Delta E)^{2\text{ to }3}$], (45) can be written approximately

$$ {}_eQ_{\rm sc}{}^{\rm ii}\simeq\frac{n_e(n_e-1)}{4\pi\bar{r}^2}[Q_{U_i}(E_q)-Q_{E_q-U_{ii}}(E_q)]Q_{U_{ii}}(E_q-\langle\Delta E_{\rm sc}\rangle_{\rm av}), \tag{47} $$

where

$$ \langle\Delta E_{\rm sc}\rangle_{\rm av}\simeq\frac{\int_{U_i}^{E_q-U_{ii}}(1/\Delta E^2)\Delta E d(\Delta E)}{\int_{U_i}^{E_q-U_{ii}}(1/\Delta E^2)d(\Delta E)}=\frac{\ln((E_q-U_{ii})/U_{ii})}{1-U_i/(E_q-U_{ii})}. \tag{48} $$

Similarly, (46) yields to

$$ {}_eQ_{\rm ej}{}^{\rm ii}\simeq\frac{n_e(n_e-1)}{4\pi\bar{r}^2}Q_{U_i+U_{ii}}(E_q)Q_{U_{ii}}(\langle\Delta E_{\rm ej}\rangle_{\rm av}), \tag{49} $$

whereas now

$$ \langle\Delta E_{\rm ej}\rangle_{\rm av}\simeq\frac{\int_{U_i+U_{ii}}^{E_q}(1/\Delta E^2)\Delta E d(\Delta E)}{\int_{U_i+U_{ii}}^{E_q}(1/\Delta E^2)d(\Delta E)}=(U_i+U_{ii})\frac{\ln(E_q/(U_i+U_{ii}))}{1-(U_i+U_{ii})/E_q}. \tag{50} $$

Making use of the previously introduced notation, relations (47) and (49) may be rewritten in the following form:

$$ {}_eQ_{\rm sc}{}^{\rm ii}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left(\frac{\sigma_0}{U_i^2}\right)\left(\frac{\sigma_0}{U_{ii}^2}\right)\left[g_Q\left(\frac{\mathcal{E}}{U_i};\frac{E_q}{U_i}\right)-\left(\frac{U_i}{\mathcal{E}-U_{ii}}\right)^2 g_Q\left(\frac{\mathcal{E}}{E_q-U_{ii}};\frac{E_q}{E_2-U_{ii}}\right)\right]g_Q\left(\frac{\mathcal{E}}{U_{ii}};\frac{E_q-\langle\Delta E_{\rm sc}\rangle_{\rm av}}{U_{ii}}\right), \tag{51} $$

$$ {}_eQ_{\rm ej}{}^{\rm ii}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left(\frac{\sigma_0}{U_i^2}\right)\left(\frac{\sigma_0}{U_{ii}^2}\right)\left[\left(\frac{U_{ii}}{U_i+U_{ii}}\right)^2 g_Q\left(\frac{\mathcal{E}}{U_i+U_{ii}};\frac{E_q}{U_i+U_{ii}}\right)g_Q\left(\frac{\mathcal{E}}{U_{ii}};\frac{\langle\Delta E_{\rm ej}\rangle_{\rm av}}{U_{ii}}\right)\right]. \tag{52} $$

The functional dependence of the cross sections obtained on the energy of impact is determined by the expressions within the brackets, while the absolute value of these relations is given by the expression in front of the brackets.

Considering that $U_{ii}\simeq 2U_i$ and $\mathcal{E}\simeq U_i$, the cross section for double ionization is roughly of the same shape for the majority of cases and can be written as follows:

$$ {}_eQ_{\rm tot}{}^{\rm ii}={}_eQ_{\rm ej}{}^{\rm ii}+{}_eQ_{\rm sc}{}^{\rm ii}=Q_0{}^{\rm ii}\,{}_eg^{\rm ii}(E_e/U_i+U_{ii}), \tag{53} $$

where

$$ Q_0{}^{\rm ii}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\frac{\sigma_0}{U_i^2}\frac{\sigma_0}{U_{ii}^2}. \tag{54} $$

The plot of the function ${}_eg^{\rm ii}$ is given in Fig. 23. Thus, we see that in the region of low energies of incident electrons the main contribution to the double ionization is due to the process of double collision of the primary electron, and the cross section for this process decreases as E_q^{-2} (this dependence results from the asymptotic form of the function g_Q) whereas the cross section for ionization by ejected electrons decreases as E_q^{-1}, being decisive in the high-energy range. The E_q^{-1} dependence of the latter results from the fact that the mean energy of recoiled electrons depends slightly on the energy of the primary electron [see Eq. (50)] and the resulting decrease is due to the decrease of the cross section for the first collision.

In the process of ionization by scattered electrons whose energies do not change appreciably in encounter, the cross sections for both collisions, being each proportional to E_q^{-1}, give as a result a $1/E_q^2$ dependence.

Since the relations obtained explicitly include, via the mean distance $\bar{r}$, the dimensions of the atomic system, the problem may be reversed, and knowing the experimental value of the cross section for the double ionization, it is possible to determine the dimensions of the system. Having the experimental value Q_0^{ii} and taking into consideration that ${}_e g_{ii}{}^{\max}=0.058$, we find

$$\bar{r}\simeq\frac{\sigma_0}{U_iU_{ii}}\left(\frac{n_e(n_e-1)}{4\pi}\frac{0.058}{Q_{\max}{}^{\mathrm{ii}}}\right)^{1/2}, \tag{55}$$

and the mean radius of doubly ionized system

$$\bar{R}\simeq\bar{r}n_e{}^{1/3}. \tag{56}$$

Proceeding similarly we can calculate the cross sections for ionization that is threefold, fourfold, etc.

If the primary particle is a heavy one, then considering that the energy of the particle does not change considerably in the ionizing collision process, i.e., $E_q'=E_q-\Delta E\simeq E_q$, we obtain

$${}_qQ_{\mathrm{sc}}{}^{\mathrm{ii}}\simeq\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i}^{\Delta E_{\max}}\sigma(\Delta E,E_q)d(\Delta E)\int_{U_{ii}}^{\Delta E_{\max}}\sigma(\Delta E',E_q)d(\Delta E'), \tag{57}$$

$${}_qQ_{\mathrm{ej}}{}^{\mathrm{ii}}\simeq\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\int_{U_i+U_{ii}}^{\Delta E_{\max}}\sigma(\Delta E,E_q)d(\Delta E)\int_{U_{ii}}^{\Delta E}\sigma(\Delta E',\Delta E)d(\Delta E'). \tag{58}$$

The above relations may be rewritten

$$Q_{\mathrm{sc}}{}^{\mathrm{ii}}=(n_e(n_e-1)/4\pi\bar{r}^2)Q_{U_i}Q_{U_{ii}}, \tag{59}$$

$$Q_{\mathrm{ej}}{}^{\mathrm{ii}}=(n_e(n_e-1)/4\pi\bar{r}^2)Q_{U_i+U_{ii}}Q_{U_{ii}}(\langle\Delta E\rangle_{\mathrm{av}}), \tag{60}$$

where now

$$\langle\Delta E\rangle_{\mathrm{av}}=\frac{\int_{U_i+U_{ii}}^{\Delta E_{\max}}\Delta E(1/\Delta E^2)d(\Delta E)}{\int_{U_i+U_{ii}}^{\Delta E_{\max}}(1/\Delta E^2)d(\Delta E)}=(U_i+U_{ii})\frac{\ln(\Delta E_{\max}/(U_i+U_{ii}))}{1-(U_i+U_{ii})/\Delta E_{\max}}, \tag{61}$$

and finally:

$$Q_{\mathrm{sc}}{}^{\mathrm{ii}}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left(\frac{\sigma_0}{U_i^2}\right)\left(\frac{\sigma_0}{U_{ii}^2}\right)G_i\left(\frac{v_q}{v_i}\right)G_Q\left(\frac{U_i}{U_{ii}};\frac{v_q}{v_i}\right), \tag{62}$$

$$Q_{\mathrm{ej}}{}^{\mathrm{ii}}=\frac{n_e(n_e-1)}{4\pi\bar{r}^2}\left(\frac{\sigma_0}{U_i^2}\right)\left(\frac{\sigma_0}{U_{ii}^2}\right)\left(\frac{U_{ii}}{U_i+U_{ii}}\right)^2G_Q\left(\frac{E_q}{U_i+U_{ii}};\frac{v_q}{v_i}\right)g_Q\left(\frac{E}{U_{ii}};\frac{\langle\Delta E\rangle_{\mathrm{av}}}{U_{ii}}\right). \tag{63}$$

In the above G_i, as we know, is the ionization function for heavy particles, given by (31), while G_Q is determined by (13). Since for atomic electrons $\mathcal{E}\simeq U_i$ and $U_{ii}\simeq 2U_i$, we can make universal graphs for double ionization by heavy particles (Fig. 24).

Analysis of experimental data will be started with

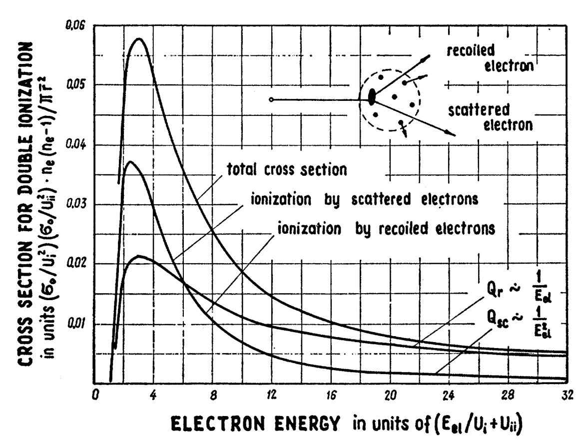

FIG. 23. Plot of the function determining double ionization, showing the contribution of ionization by double scattering of the primary electron and by the recoiled electrons.

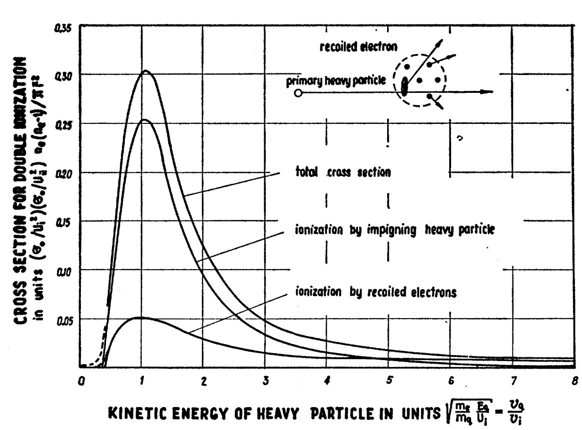

FIG. 24. The double-ionization function for heavy charged particles.

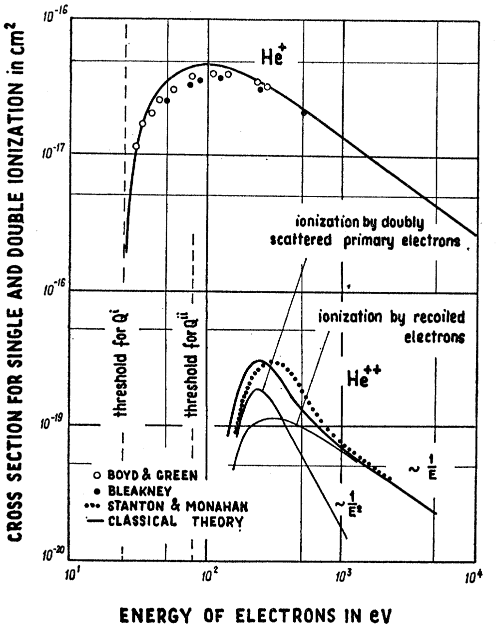

FIG. 25. Cross sections for the single and double ionization of helium.

the simplest case, which is the double ionization of the helium atom.

For helium we have $U_i=24.6$ eV, $U_{ii}=54.4$ eV, $n_e=2$, and the experimentally found maximum value of the cross section for double ionization,[34] is 2.4×10^{-19} cm^2. Using (55) and (56), we find the radius of the helium atom to be $R^{\mathrm{He}}=1.18\times10^{-8}$ cm, while the gas-kinetic radius of the helium atom is 0.95×10^{-8} cm.

Similarly, having for the argon atom:

$$n_e=8,\quad U_i{}^{\mathrm{A}}=15.7\text{ eV},\quad U_{ii}{}^{\mathrm{A}}=27.6\text{ eV},\quad {}^{\mathrm{A}}{}_eQ^{\mathrm{ii}}=0.308\times10^{-16}\text{ cm}^2,$$

and neglecting the small contribution of inner shells to the double ionization, the radius of the argon atom has been estimated. The calculated value is $R^{\mathrm{A}}=1.3\times10^{-8}$ cm as against the gas-kinetic radius 1.5×10^{-8} cm. Using the derived relations, the cross section for the double ionization of the helium atom by electrons has been calculated and compared with the ratio ${}^{\mathrm{He}}{}_eQ^{\mathrm{i}}/{}^{\mathrm{He}}{}_eQ^{\mathrm{ii}}$ found experimentally.[34] See Figs. 25 and 26.

The formulas of this chapter can automatically be applied to the problem of excitation of x-ray satellites; knowing the cross-sections, it is possible with the use of the theory to estimate the dimensions of inner orbits.

IX. EXCITATION OF ATOMS AND MOLECULES BY ELECTRONS AND IONS

Denoting by U_n and U_{n+1} the excitation energy of the levels n and $n+1$, respectively, the excitation cross section of the level n per electron of the excited shell is at once seen to be

$$Q^{\mathrm{exc}}(U_n;U_{n+1})=\int_{U_n}^{U_{n+1}}\sigma_{\Delta E}d(\Delta E)$$
$$=Q\left(\frac{U_i}{U_n};\frac{E_q}{U_n}\right)-Q\left(\frac{U_i}{U_{n+1}};\frac{E_q}{U_{n+1}}\right),\qquad(64)$$

where the function Q is given by (7), (10), and (13). (See also Figs. 1 and 2.) For $U_n/U_{n+1}\rightarrow1$ we obtain

$$Q^{\mathrm{exc}}\simeq\sigma_{\Delta E=U_n}\times(U_{n+1}-U_n).\qquad(65)$$

This simple picture of excitation is strongly deformed in the low-energy range by the capture process in the case of positively charged particles, and to a lesser extent by the exchange process in the case of electrons.

The capture of electrons influences the excitation process in this way: Some of the electrons which have gained the amount of energy necessary for excitation are removed from the atom by the positive potential hole of the moving heavy ion. As a result, the real excitation cross section decreases by a certain amount:

$$Q_{\mathrm{resultant}}{}^{\mathrm{exc}}\simeq Q^{\mathrm{exc}}-k\cdot Q_c,\qquad(66)$$

where Q_c is the total cross section for capture and k is of the order of

$$k\sim(U_{n+1}-U_n)/(\tfrac{1}{2}mv_q{}^2+U_i{}^A).\qquad(67)$$

The influence of the capture process on the excitation cross section is negligibly small at high energies of the incident particle, because Q^{exc} is inversely proportional to E_q, and Q_c is inversely proportional to the cube of E_q; but it is dominant at low energies.

To illustrate the problem, the excitation of helium by protons has been calculated. Because the excitation energies of helium levels with $n=4$ and $n=5$ are 23.70 and 23.95 eV, respectively, the excitation cross section

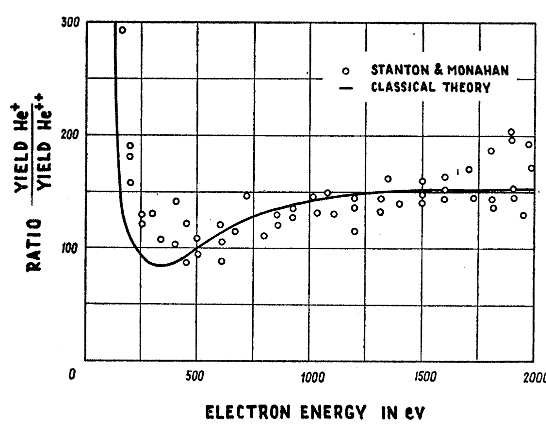

FIG. 26. The ratio of the cross section for single ionization to that for double ionization of helium as a function of the energy of incident electrons.

[34] H. E. Stanton and J. E. Monahan, Phys. Rev. 119, 711 (1960).

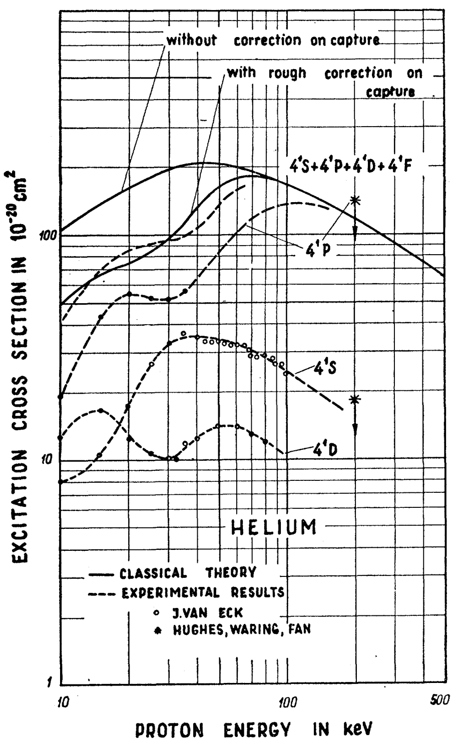

FIG. 27. Excitation of helium levels by proton impact.

is simply

$$ {}^{\rm He}{}_{p}Q^{\rm He(4s+4p+4d+4f)} \simeq 2\frac{\sigma_0}{23.7^2}\,\frac{0.25}{23.7}\,G_\sigma\!\left(\frac{24.6}{23.7};\frac{v_p}{v_i^{\rm He}}\right) - \frac{0.25}{24.6+mv_p^2/2}\,Q_c^{\rm He}(v_p). $$

Using the experimental data for the capture process, shown in Fig. 27, the correction due to this process according to formulas (66) and (67) has been also estimated. Results of calculations and some experimental data[35–37] are given in Fig. 27.

The exchange process can be quite easily explained on the basis of the theory of two-particle collisions if the Coulomb field of the nucleus is taken into account. As has been mentioned before, the kinetic energy of the incident electron increases in the potential field of the nucleus; therefore, a possibility exists of collision with the loss of energy greater than the initial energy of the electron. If this happens, the electron will not be able to escape from the "potential hole" of the nucleus. On the other hand, the atomic electron gaining the amount of energy greater than its binding energy can be ejected from the atom. In order to estimate the cross section for this process, we assume the atomic electron to have zero velocity and to be confined within a potential hole with a depth equal to the binding energy of the atomic electron. Therefore, the initial kinetic energy E_e of the incident electron increases inside the potential to the value E_e+U_i. The incident electron, depending on the amount of energy lost in the collision with the atomic electron, can escape from the potential hole if $|\Delta E|<E_e$, or be captured if $|\Delta E|>E_e$. If the energy of the primary electron after the collision is in the interval U_n-U_{n+1} then the above is equivalent to the excitation of the level n of the target atom in the exchange process. Using formula (II.10) and substituting $E=E_e+U_i$ we obtain at once the excitation cross section due to the exchange process:

$$ Q_{\rm exch} \simeq \frac{\sigma_0}{E_e+U_i}\int_{E_e+U_i-U_n}^{\epsilon^\pm}\frac{d(\Delta E)}{\Delta E^2}. \tag{68} $$

The double upper limit

$$ \begin{aligned} \epsilon^\pm &= U_i && \text{if } E_e+U-U_{n+1}<U_i \\ &= E_e+U_i-U_{n+1} && \text{if } E_e+U_i-U_{n+1}>U_i \end{aligned} $$

in the above integral appears because the minimum gain of energy needed by the atomic electron to be ejected is equal to its binding energy. Performing a simple integration, we finally obtain

$$ Q_{\rm exch} = \frac{\sigma_0}{U_n^2}\,\frac{U_{n+1}-U_n}{U_n}\,g_{\rm exch}\!\left(\frac{U_i}{U_n};\frac{U_i}{U_{n+1}};\frac{E_e}{U_n}\right), \tag{69} $$

$$ \begin{aligned} g_{\rm exch} &= \frac{U_n^2}{(E_e+U_i)(E_e+U_i-U_n)}\times\frac{U_n}{U_i}\,\frac{E_e-U_n}{U_{n+1}-U_n} && \text{if } E_e<U_{n+1} \\ &= \frac{U_n^2}{(E_e+U_i)(E_e+U_i-U_n)}\times\frac{U_n}{E_e+U_i-U_{n+1}} && \text{if } E_e>U_{n+1}. \end{aligned} \tag{70} $$

Assuming U_n to equal zero and U_{n+1} to equal the ionization potential of the atom, (68) represents the total cross section for the exchange process. As can be easily shown, the exchange cross section decreases very rapidly with increase of energy:

$$ Q_{\rm exch} \propto 1/E_e^3. $$

Now, we shall again proceed to calculate concrete cases.

[35] J. Van Eck, thesis, University of Amsterdam, 1964 (unpublished).
[36] R. Hughes, R. Waring, and C. Fan, Phys. Rev. **122**, 525 (1961).
[37] R. Döpel, Ann. Physik **16**, 1 (1933).

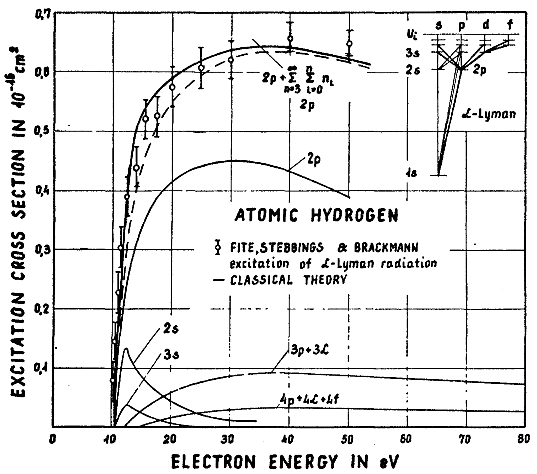

FIG. 28. Theoretical cross sections for the excitation of different levels of atomic hydrogen and experimental values for the excitation of Lyman α radiation by electrons.

(a) Excitation of atomic hydrogen levels. Taking into account that the excitation energies of the first three levels of atomic hydrogen are 11.2, 12.1, and 12.7 eV, the respective cross sections for excitation will be

$${}^{\mathrm{H}}{}_{e}Q^{\mathrm{H}2p}=6.35\times10^{-16}g_Q(1.34;E_e/10.2)-4.48\times10^{-16}g_Q(1.12;E_e/12.1),$$

$${}^{\mathrm{H}}{}_{e}Q^{\mathrm{H}(3p+3d)}=4.48\times10^{-16}g_Q(1.12;E_e/12.1)-4.08\times10^{-16}g_Q(1.07;E_e/12.7),$$

whereas the excitation of the S levels may take place by the exchange process only (direct excitation is impermissible according to the selection rules). Thus using formula (66), we obtain

$${}^{\mathrm{H}}{}_{e}Q^{\mathrm{H}2s}=1.26\times10^{-16}g_{\mathrm{exch}}\left(\frac{13.6}{12.1};\frac{13.6}{12.1};\frac{E_e}{10.2}\right),$$

$${}^{\mathrm{H}}{}_{e}Q^{\mathrm{H}3s}=0.223\times10^{-16}g_{\mathrm{exch}}\left(\frac{13.6}{12.1};\frac{13.6}{12.7};\frac{E_e}{12.1}\right),$$

and, analogically, we can calculate the cross sections for the excitation of the higher levels. The results of the numerical calculations have been shown in Fig. 28, where the experimentally found cross section for the excitation of the Lyman α series[38] is presented, which cross section, considering the negligibly small probability of $np\rightarrow ls$ transitions for $n>2$, is approximately equal to the cross section for the excitation of all levels of atomic hydrogen.

Similarly, taking into account the fact that the majority of transitions from high-energy levels of Na pass through the levels $2p^2P_{3/2}$ and $2p^2P_{1/2}$, we have calculated the cross section for the excitation of the D lines of sodium,

$${}^{\mathrm{Na}}{}_{e}Q^{\mathrm{Na}D}=1.48\times10^{-14}g_Q\left(2.45;\frac{E_e}{2.10}\right)-0.25\times10^{-14}\times g_Q\left(1;\frac{E_e}{5.12}\right)+2.12\times10^{-14}g_{\mathrm{exch}}\left(2.45;1;\frac{E_e}{2.1}\right),$$

where the last term represents the contribution of excitation due to exchange. (See Fig. 29, experimental data of Christoph[39] and Haft.[40])

Proceeding to the excitation of the energy levels of helium, we can, in view of a relatively small difference of energies between the levels, avail ourselves of relation (63). Thus we obtain successively

$${}^{\mathrm{He}}{}_{e}Q^{3^1P}=7.3\times10^{-18}g_\sigma\left(1.1;\frac{E_e}{23.1}\right),$$

$${}^{\mathrm{He}}{}_{e}Q^{4^1P}=2.5\times10^{-18}g_\sigma\left(1.04;\frac{E_e}{23.1}\right),$$

$${}^{\mathrm{He}}{}_{e}Q^{5^1P}=0.47\times10^{-18}g_\sigma\left(1.02;\frac{E_e}{23.1}\right),$$

where the function $g_\sigma(U_i/U_n;E_e/U_n)$ is given by (9).

If we take the classical approach to the problem in assuming that the probability that after the exchange the spins of the electrons will be parallel is the same as the probability that their spins will be antiparallel, the cross sections for the excitation of triplet levels of helium will be

$${}^{\mathrm{He}}{}_{e}Q^{4^3S}=1.87\times10^{-18}g_{\mathrm{exch}}(1.05;1.03;E_e/23.5),$$

$${}^{\mathrm{He}}{}_{e}Q^{2^3S}=2.45\times10^{-17}g_{\mathrm{exch}}(1.24;1.08;E_e/19.8),$$

$${}^{\mathrm{He}}{}_{e}Q^{2^1S}=1.90\times10^{-17}g_{\mathrm{exch}}(1.20;1.08;E_e/20.5).$$

In Fig. 30 we have drawn theoretically calculated cross sections for the excitation of various levels, and relative

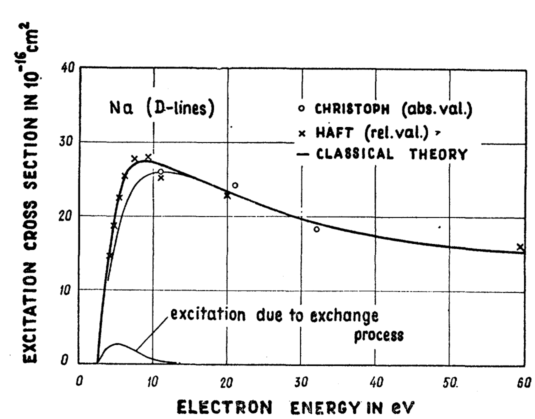

FIG. 29. Excitation of the D lines of sodium by electron impact.

[38] W. L. Fite, R. F. Stebbings, and R. T. Brackman, Phys. Rev. **116**, 356 (1959).

[39] W. Christoph, Ann. Physik **23**, 51 (1935).

[40] G. Haft, Z. Physik **82**, 73 (1933).

values of the excitation of lines n^1P-2^1S measured by Thieme[41] and Lees[42] normalized at the maximum of line 2^1S-3^1P, as well as the cross section for the excitation of the triplet level of $n=4$ and the relative intensity of the triplet level of $n=4$ and the relative intensity of the line 2^3P-4^3S.

Recently, St. John *et al.*[43] measured the excitation cross section of the 3^1P level of helium; their result is nearly the same as calculated.

Quite good agreement is shown by the calculated maximum value of the cross sections for the excitation levels 2^1S and 2^3S with the experimental results obtained by Maier-Leibnitz[44] by the electron collision method.

	theor.	expt.
${}^{\mathrm{He}}{}_eQ_{\max}{}^{\mathrm{He}2^1S}$	3.8×10^{-18} cm^2	2.7×10^{-18} cm^2
${}^{\mathrm{He}}{}_eQ_{\max}{}^{\mathrm{He}2^3S}$	4×10^{-18} cm^2	4.8×10^{-18} cm^2.

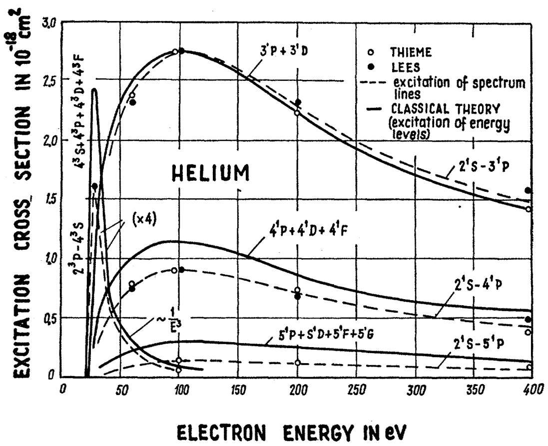

FIG. 30. Excitation of singlet and triplet lines of helium by electrons.

X. STOPPING POWER OF MEDIUM FOR CHARGED PARTICLES

A charged particle moving in the medium loses energy because of:

(i) interaction with atomic electrons (excitation and ionization losses),

(ii) interaction with the Coulomb field of a nucleus screened by atomic electrons,

(iii) scattering by nuclear forces (elastic and inelastic nuclear collisions),

(iv) interaction due to magnetic moments of the colliding particles,

(v) radiation losses.

In the moderate- and high-energy range, if the energy of the particle is not extremely high, the most important (excluding, of course, special conditions existing in high-temperature plasmas[45] or inside some kinds of stars[46]) are the ionization and excitation losses.

At very low energies of heavy particles the interaction with the averaged field of the atom cannot be neglected. For light particles (electrons and positrons) at energies of a few MeV, the radiation losses must be taken into account.

The losses related to the interaction with atomic electrons are determined by the excitation energies of the lowest levels of all shells of the atom ($U_{\mathrm{exc}}{}^k$). According to the relations derived in Paper II which have been adopted for atomic collisions (see relations at the beginning of the paper), we can write simply

$$
\begin{aligned}
{}^{\mathrm{atom}}S&=\sum_k n_e{}^k\frac{\sigma_0}{U_{\mathrm{exc}}{}^k}\times g_s\left(\frac{\mathcal{E}^k}{U_{\mathrm{exc}}{}^k};\frac{E_e}{U_{\mathrm{exc}}{}^k}\right) \quad \text{for light particles}\\
&=\sum_k n_e{}^k\frac{\sigma_0}{U_{\mathrm{exc}}{}^k}\times G_s\left(\frac{\mathcal{E}^k}{U_{\mathrm{exc}}{}^k};\frac{v_q}{\bar{v}_e}\right) \quad \text{for heavy ions}, \qquad (71)
\end{aligned}
$$

where g_S and G_S are given by (11) and (14). At high energies the losses due to excitation and ionization are well described by the asymptotic expression:

$$
\begin{aligned}
{}^{\mathrm{atom}}S&=\sum_k n_e{}^k\frac{\sigma_0}{U_{\mathrm{exc}}{}^k}\left(\frac{\bar{v}_e{}^k}{v_q}\right)^2\left[2\frac{U_{\mathrm{exc}}{}^k}{\mathcal{E}^k}\ln\frac{v_q}{\bar{v}_e{}^k}\left(\frac{\mathcal{E}^k}{U_{\mathrm{exc}}{}^k}\right)^{1/2}+\frac{4}{3}\ln\frac{v_q}{\bar{v}_e{}^k}\right] \quad \text{for light particles}\\
&=\sum_k n_e{}^k\frac{\sigma_0}{U_{\mathrm{exc}}{}^k}\left(\frac{\bar{v}_e{}^k}{v_q}\right)^2\left[2\frac{U_{\mathrm{exc}}{}^k}{\mathcal{E}^k}\ln2\frac{v_q}{\bar{v}_e{}^k}\left(\frac{\mathcal{E}^k}{U_{\mathrm{exc}}{}^k}\right)^{1/2}+\frac{4}{3}\ln\frac{v_q}{\bar{v}_e{}^k}\right] \quad \text{for heavy ions}. \qquad (72)
\end{aligned}
$$

If we insert in the above relations $U_i{}^k$ instead of $U_{\mathrm{exc}}{}^k$ we shall obtain the losses S^i due to the ionization process. Subtracting S^i from S we will have the losses connected with the excitation process only.

Using (II.13) we can estimate the stopping power

[41] O. Thieme, Z. Physik **86**, 646 (1933).

[42] J. H. Lees, Proc. Roy. Soc. (London) **A137**, 173 (1932).

[43] R. M. St. John, C. J. Broncs, and R. G. Fowler, J. Opt. Soc. Am. **50**, 28 (1960).

[44] H. Maier-Leibnitz, Z. Physik **95**, 499 (1935).

[45] M. Gryziński, Phys. Rev. **111**, 900 (1958).

[46] M. Gryziński, Phys. Rev. **115**, 1087 (1959).

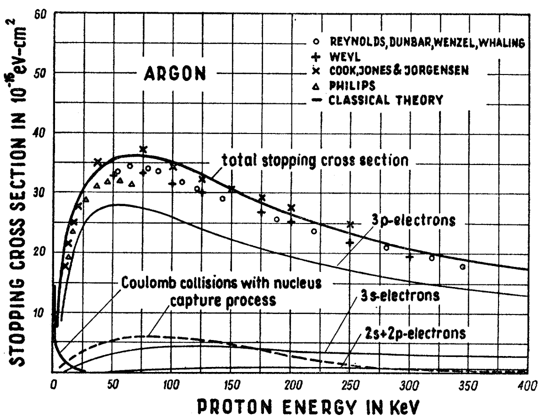

FIG. 31. Stopping cross section of argon for protons.

due to the Coulomb interaction with the nucleus:

$$S_D=\frac{2\pi e^4}{M_q v_q^2}Z_q^2Z_t^2\ln\left[1+\left(\frac{m_qM_t}{m_q+M_t}\frac{v_q^2D}{e^2}\frac{1}{Z_qZ_t}\right)^2\right], \quad (73)$$

where we have assumed the target atom to be at rest and the maximum impact parameter to be of the order of the radius of the atom. In the above equation Z_t denotes the charge of the target nucleus in units of elementary charge, and M_t its mass.

In the case of the positively charged particles, especially of large q, the capture process must be taken into account. As a result of the capture, the Coulomb field of the moving particle is screened, and the losses can decrease; on the other hand, the capture process permits losses of energy to atomic electrons in amounts smaller than necessary for excitation of the lowest level, increasing the slowing-down force.

The influence of the capture on the slowing down can easily be taken into account if the stopping power is discussed in terms of the function G_d in which the dependence on the maximum impact parameter has been retained (as in the author's earlier paper[2]). The increase of the stopping power which is predominant for particles of small charge, as for instance for protons, can be easily estimated, too.

According to the results of Sec. VII, the mean loss of energy in one cycle of capture and loss of the electron by a moving particle is of the order of $\frac{1}{2}m_ev_q^2$; therefore the contribution to the stopping cross section due to this process is

$$S=(m_e/m_q)(Q_cQ_l/Q_c+Q_l)E_q, \quad (74)$$

where Q_c is the cross section for the capture, and Q_l is the cross section for the loss of the electron.

Using derived formulas, the total stopping cross section of some gases for protons have been calculated. The contribution of S_C in the total stopping cross section of argon and helium has been estimated, using for Q_c and Q_l the experimental data of Federenko and others.[17] It has been found that the contribution of S_c is greatest at energies of some tenths of keV, being, in agreement with the previous estimate by Allison,[47] the order of 15 to 20%. The results of calculations and experimental data[48–52] are shown in Figs. 31 and 32.

Having found the stopping cross section, it presents no difficulty to calculate the ranges of charged particles in matter, although the analytical formula can be found (approximately) only in the very special case of one kind of stopping electrons. Considering only the losses due to interaction with electrons as given roughly by (II.41), we can write

$$R_q\simeq\frac{1}{N_e}\int_0^{E_q^0}\frac{dE_q}{(\sigma_0/\mathcal{E})f_{\bar{v}}\ln\{1+4(\mathcal{E}/U_{\mathrm{exc}})^2[1+(v_q/\bar{v}_e)^2]^2\}}, \quad (75)$$

where R_q is the range of a heavy particle of initial kinetic energy E_q^0 in the medium having N_e electrons, with mean velocity $\bar{v}_e$ and excitation energy U_{exc} per unit of volume.

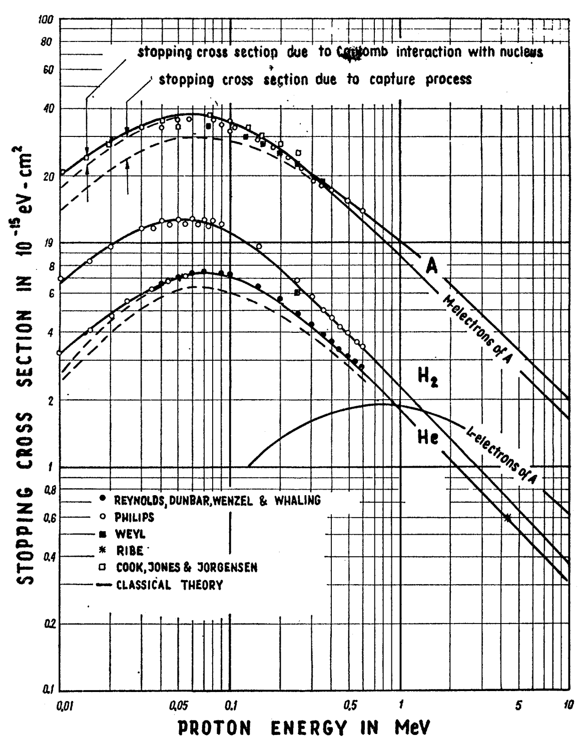

FIG. 32. Stopping cross section of molecular hydrogen, helium, and argon for protons.

[47] S. K. Allison, Rev. Mod. Phys. **30**, 1137 (1958).
[48] L. Reynolds, D. Dunbar, W. A. Wentzel and W. Whaling, Phys. Rev. **92**, 742 (1953).
[49] P. K. Weyl, Phys. Rev. **91**, 289 (1953).
[50] C. J. Cook, E. Jones, and T. Jorgensen, Phys. Rev. **91**, 1417 (1953).
[51] J. A. Philips, Phys. Rev. **97**, 404 (1955).
[52] F. Ribe, Phys. Rev. **85**, 1217 (1951).

The above relation may be written approximately,

$$R_q \simeq \frac{1}{N} \frac{\mathcal{E}^2}{\sigma_0} \frac{M_q}{m_e \ln\{1+4(\mathcal{E}/U_{\text{exc}})^2[1+\frac{1}{2}(v_q^0/\bar{v}_e)^2]^2\}} \times \int_0^{(v_q^0/\bar{v}_e)^2} \frac{dx}{1/x(x/(1+x))^{1/2}}; \quad (76)$$

or, after the integration has been performed,

$$R_q = \frac{1}{N} \frac{\mathcal{E}^2}{\sigma_0} \frac{M_q}{m_e} \times f_R\left(\frac{\mathcal{E}}{U_{\text{exc}}}; \frac{v_q^0}{\bar{v}_e}\right), \quad (77)$$

where by $f_R(\mathcal{E}/U_{\text{exc}}; v_q^0/\bar{v}_e)$ we have denoted the function

$$f_R\left(\frac{\mathcal{E}}{U_{\text{exc}}}; \frac{v_q^0}{\bar{v}_e}\right) = \frac{1}{4} \frac{(v_q^0/\bar{v}_e)[1+(v_q^0/\bar{v}_e)^2]^{1/2}[\frac{5}{2}+(v_q^0/\bar{v}_e)^2]+3 \arcsin(v_q^0/\bar{v}_e)}{\ln\{1+4(\mathcal{E}/U_{\text{exc}})^2[1+\frac{1}{2}(v_q^0/\bar{v}_e)^2]^2\}}. \quad (78)$$

At high energies we find that

$$f_R\left(\frac{\mathcal{E}}{U_{\text{exc}}}; \frac{v_q^0}{\bar{v}_e}\right) \sim \frac{(v_q^0)^4}{\ln(v_q^0/\bar{v}_e)}$$

in agreement with the dependence found experimentally. Making use of formula (77), the range of protons in molecular hydrogen has been calculated, and the results compared with the experimental data[53] (see Fig. 33).

XI. THE SCATTERING PROBLEM IN ATOMIC COLLISIONS

The scattering problem in the general case of atomic collisions is a many-body problem, for which the solution can be only approximate. A method for solution of elastic scattering will be quite different from that for inelastic scattering. The latter can be solved in the binary-encounter approximation; but in the case of scattering, the dependence on the space orientation of the averaged fields of colliding atomic systems and on the velocity distribution of electrons is much greater than in the case of pure energy exchange processes. Nevertheless if we use cross sections averaged over velocity distribution of atomic electrons, a two-body approximation enables the main features of inelastic scattering to be obtained correctly.

On the basis of the relations derived in Paper II we can proceed at once to numerical examples.

We shall start our calculations with the inelastically scattered electrons suffering a given loss of energy in molecular hydrogen. The angular distribution of electrons of energy E_e scattered by electrons of mean velocity $\bar{v}_e$ with loss of energy ΔE is given by (II.80) (we use the formula for isotropically oriented atoms, which is the case for a gaseous scatterer). In our particular instance we have $\mathcal{E}=15.6$ eV, $E_e=200$ eV, and $\Delta E=50$, 100, 125, and 150 eV. The results of calculations and the experimental data of Mohr and Nicoll,[54] both normalized at the maximum of the curve for $\Delta E=125$ eV, are given in Fig. 34. It is seen that, as a result of the assumed velocity distribution of the form (II.45) with $n=3$, good agreement with the experimentally observed angular distribution has been achieved (cf. the results of the paper[3] where the velocity distribution of the form of the δ function has been used).

The slight deviation between theory and experiment is probably due to the influence of the nuclear Coulomb field which increases the back scattering, as well as to the contribution of ejected electrons not having been taken into account. The existence of the maximum in the angular distribution of the inelastically scattered particles, as seen in Fig. 34, may be interpreted as a corpuscular explanation of the diffraction pattern of inelastically scattered particles.

The angular distribution of particles scattered in "ionizing collisions," i.e., scattered inelastically with a loss of energy greater than the ionization potential, also has the form of a diffraction ring, although it is not so distinct, and more diffuse (see Fig. II.15). In the case of scattering on atomic systems with electrons of different binding energies, a corresponding number of diffraction rings will occur in the diffraction pattern. The continuous background of inelastically scattered

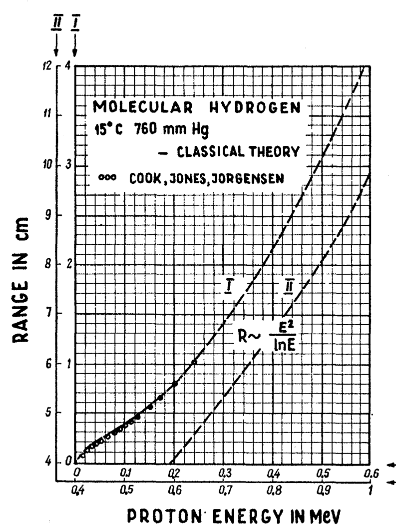

FIG. 33. The range of protons in molecular hydrogen.

[53] C. J. Cook, E. Jones, and T. Jorgensen, Phys. Rev. 91, 1417 (1953).

[54] C. B. O. Mohr and F. H. Nicoll, Proc. Roy. Soc. (London) A138, 469 (1932).

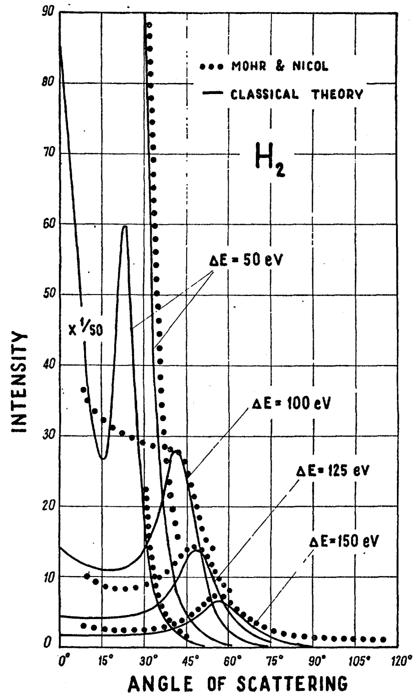

FIG. 34. The angular distribution of inelastically scattered electrons on molecular hydrogen.

particles varies as

$$1/(1-\cos\vartheta)^2,$$

which can be easily proved on the basis of Paper II.

It has been observed that fast electrons passing through solids experience discrete energy losses which are practically independent of the energy of the primary particles. Later Watanabe[55] found that some of the characteristic energy losses are associated with the diffraction pattern of the scattered particles, and the empirical formula for the characteristic energy loss ΔE and the scattering angle ϑ can be extimated:

$$\Delta E/E_e = \Delta E_0/E_e + a\vartheta^2,$$

where the constants ΔE_0 and a depend slightly on the scatterer used. The above formula is the same as the approximate formula of Paper II for the diffraction maximum of inelastically scattered particles, provided we have

$$\Delta E_0 = \mathcal{E}, \quad a = 1.$$

Taking into account that $\mathcal{E}$ is of the order of the ionization potential of the atom of the scatterer, we can confirm the theoretical formula of Paper II (see Table II).

TABLE II. Experimental and rough theoretical values for $\Delta E_0/E_e$ and a. (The accelerating voltage is 25 keV.)

	$\Delta E_0/E_e$		a(radian^{-2})	
Scatterer	expt.	theor.	expt.	theor.
Be	7.6×10^{-4}	3.8×10^{-4}	0.84	1
Mg	4.2×10^{-4}	3.0×10^{-4}	1.24	1
Al	6.0×10^{-4}	2.4×10^{-4}	1.00	1
Ge	6.6×10^{-4}	3.2×10^{-4}	1.66	1

The results obtained are in fairly good agreement with those found experimentally, especially if we take into consideration that the theoretical values concern free atoms, and the experimental values concern solids.

Going on to the crystal structures, we may expect a strong anisotropy in the velocity distribution of their electrons. It is evident that this anisotropy has to be related to the orientation of the main crystallographic axes and planes; therefore, the spatial orientation of electron velocities is determined by plane or axis indices which in our formalism relate to the discrete values of the angles θ and φ.

For the polycrystalline structures oriented relative to the plane, as in the case of thin sheets of metals evaporated onto films, there exists a set of discrete values for the angle θ while the orientation with respect to the angle φ is isotropic. As a result, the diffraction pattern will have the form of sharp rings.

In the case of monocrystals, there is a set of discrete values both for the angle θ and for angle φ which results in a diffraction pattern of spot form.

On the basis of the anisotropic velocity distribution of electron velocities in the crystals, the spatial distribution of ejected electrons can be explained, as well as the classical experiment of Davisson and Germer.

[55] H. Watanabe, *Proceedings of the Gatlinburg Conference on Penetration of Charged Particles in Matter, Tennessee, 1958* (National Academy of Science, Washington, D. C., 1960), p. 152.