where

$$R_{\rm III}=2\|\Delta_u\psi\|, \quad S_{\rm III}=\|V_{12}\psi\|. \tag{B.13}$$

In order to find an upper bound $C_{\rm II}$ corresponding to $H_{\rm II}$, let us note the following inequality:

$$\left|\int d\tau\Delta_1\psi\Delta_2 f\right| \leq \left[\int d\tau\Delta_1\psi\Delta_2\psi\right]^{\frac{1}{2}}\left[\int d\tau\Delta_1 f\Delta_2 f\right]^{\frac{1}{2}}, \tag{B.14}$$

which can be proved using Schwartz's inequality in a slightly modified manner. From this it follows that $C_{\rm II}$ may be chosen as

$$C_{\rm II}=\alpha^2[bS_{\rm II}+\tfrac{1}{4}b^2], \tag{B.15}$$

where

$$S_{\rm II}=\frac{1}{2}\left[\int d\tau\Delta_1\psi\Delta_2\psi\right]^{\frac{1}{2}}. \tag{B.16}$$

The last term $H_{\rm V}$ may be treated completely differently from the others, being proportional to the kinetic energy K. In this case, the left-hand side of (3.1) becomes

$$(1-\eta^2)(\psi_0,H_{\rm V}\psi_0)-(\psi,H_{\rm V}\psi) = -\tfrac{1}{2}\alpha^2E_0[\lambda-E_0(1-\eta^2)], \tag{B.17}$$

where it is assumed that the trial function ψ satisfies the virial theorem. Since this is the case for ψ's considered here,[21] the accuracy of $(\psi,H_{\rm V}\psi)$ is obviously just as good as that of the variational calculation of the nonrelativistic energy eigenvalue λ. We may therefore regard $(\psi_0,H_{\rm V}\psi_0)$ as exactly known and omit it from our considerations.

Collecting the results obtained, one may therefore choose

$$C_{\rm rel}=\alpha^2[aR+bS+(9/2)ab+\tfrac{1}{4}b^2], \tag{B.18}$$

with

$$\begin{aligned} R&=R_{\rm I}+R_{\rm III}+R_{\rm IV},\\ S&=S_{\rm II}+S_{\rm III}, \end{aligned} \tag{B.19}$$

as an upper bound for the error in the expectation value of the entire relativistic correction $H_{\rm rel}$.

[21] This is because our trial functions are always chosen so that the upper bound λ is minimized with respect to the scale parameter k. For details, see Sec. 3 of reference 2.

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Classical Theory of Electronic and Ionic Inelastic Collisions

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A classical theory of inelastic atomic collisions is given. It is shown that inelastic scattering, ionization, excitation, and other interactions between charged particles and atoms are due to the Coulomb interaction with atomic electrons and depend in a first approximation on their binding energy and momentum distribution. All cross sections can easily be calculated by means of differential cross sections $\sigma(\Delta E)$ and $\sigma(\Delta E,\vartheta)$ derived in the binary encounter approximation. Numerical calculations have been made for several cases and are in very good agreement with the experimental results.

I. INTRODUCTION

THE difficulty of explaining on the basis of classical mechanics some experimental facts observed in atomic collisions and the sufficiently good results obtained by wave mechanics have been viewed as proof of the nonvalidity of classical mechanics for processes involving the interaction of charged particles with the atomic shell.[1,2] Consequently the explanation of all such processes has been sought by using wave mechanics without investigating the possibilities of a classical interpretation of these phenomena. The slowing down of charged particles in a medium had also been treated in this way. In a recent paper[3] the author analyzed this process on the basis of classical mechanics and showed that the disagreement between the first classical theories[4,5] and experiment, particularly in the low-energy range, was the result of an approximation which neglected the orbital motion of the atomic electrons. It was noted that the effect of the interactions in a Coulomb field varies as the fourth power of the *relative* velocity.

The excellent agreement of the classical stopping theory given by the author with experiment automatically gave rise to the suggestion that other processes occurring in atomic collisions, which, after all, make up the stopping process, should be treated in this way. Thus, employing the results of Chandrasekhar[6] and Williamson and Chandrasekhar[7] on the collisions of gravitational masses, we shall construct in the binary

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encounter approximation a classical theory of inelastic atomic collisions.

II. TRANSFER OF MOMENTUM AND SCATTERING OF PARTICLES INTERACTING THROUGH A COULOMB FIELD

Consider the encounter between particles with charges q_1, q_2, masses m_1, m_2, and velocities $\mathbf{v}_1$ and $\mathbf{v}_2$, respectively, interacting with each other through a Coulomb field. All results are also valid for bodies interacting through gravitation if we take $q_1=m_1\sqrt{G}$ and $q_2=m_2\sqrt{G}$, where G is the gravitational constant.

If we idealize each encounter as a two-body problem, then the parameters defining such an encounter in laboratory frame of reference are (see Fig. 1): (i) the angle θ between the two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$, (ii) the azimuthal angle φ referred to a system of coordinates in which the z-axis coincides with the direction of $\mathbf{v}_2$, (iii) the impact parameter D, and (iv) the angle Θ between the orbital plane and the fundamental plane containing the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$.

As a result of the encounter, the directions and the magnitudes of vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ are changed. These changes, which can be measured experimentally, are given by the relations

$$h_{\Delta E}\equiv\Delta E+\frac{K_{12}}{1+x^2}\{E_2-E_1+\tfrac{1}{2}v_1v_2[(m_1-m_2)\cos\theta+(m_1+m_2)\sin\theta\cos\Theta x]\}=0, \quad (1)$$

$$h_\vartheta\equiv-\vartheta+\frac{1}{(1+\Delta E/E_2)^{\frac{1}{2}}}\left\{\left(1+\frac{1}{2}\frac{\Delta E}{E_2}\right)-2\left(\frac{m_1}{m_1+m_2}\right)\left(\frac{V}{v_2}\right)^2\frac{1}{1+x^2}\right\}=0, \quad (2)$$

where ΔE is the change in energy of particle 2, ϑ is the change in the direction of velocity of particle 2, E_1 and E_2 are the energies of particles 1 and 2 before the collision, $V=(v_1^2+v_2^2-2v_1v_2\cos\theta)^{\frac{1}{2}}$ is the relative velocity, μ is the reduced mass, and

$$x=D(\mu/q_1q_2)V^2, \quad K_{12}=4m_1m_2/(m_1+m_2)^2. \quad (3)$$

Equations (1) and (2) have been derived using the results of the Chandrsekhar and Williamson[6,7] (Appendix).

Now, the cross section for the encounter defined by θ, φ, Θ, and D is

$$\frac{1}{4\pi}f(\theta)d\theta\times d\varphi\times\frac{d\Theta}{2\pi}\times 2\pi DdD, \quad (4)$$

where $f(\theta)$ is the relative angle distribution function between vectors $\mathbf{v}_1$ and $\mathbf{v}_2$. Integrating over the range for which condition (1) is fulfilled, we obtain the cross section for a collision in which particle 2 undergoes a

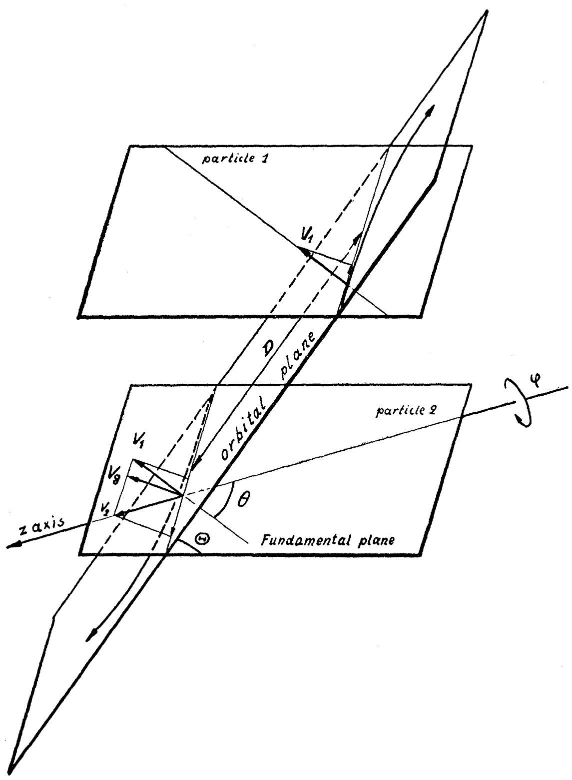

FIG. 1. Space diagram for encounter between charged particles. The fundamental plane is defined by the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ representing the velocities of the two particles before the encounter. The velocity of the mass center denoted by V_g, remains constant during the encounter. In a frame of reference in which the center of gravity is at rest, the two particles describe hyperbolas or parabolas in the orbital plane which, in general, is inclined at some definite angle Θ to the fundamental plane.

change in energy ΔE,

$$\sigma(\Delta E)=\frac{1}{4\pi}\int\int\int\int f(\theta)\delta[h_{\Delta E}(\theta,\Theta,D)]\times d\theta d\varphi\frac{d\Theta}{2\pi}2\pi DdD. \quad (5)$$

In a similar way, the cross section for the scattering of particle 2 in the direction θ with the change of energy ΔE is

$$\sigma(\Delta E,\vartheta)=\frac{1}{4\pi}\int\int\int\int f(\theta)\delta[h_\vartheta(\theta,\Theta,D)]\times d\theta d\varphi\frac{d\Theta}{2\pi}2\pi DdD. \quad (6)$$

Since

$$\int_a^b f(x)\delta[\varphi(x)]dx=\sum_s\frac{f(x_s)}{|\varphi'(x_s)|},$$

where the sum is taken over all roots of the equation $\varphi(x)=0$ in the interval a, b, we obtain, after integrating

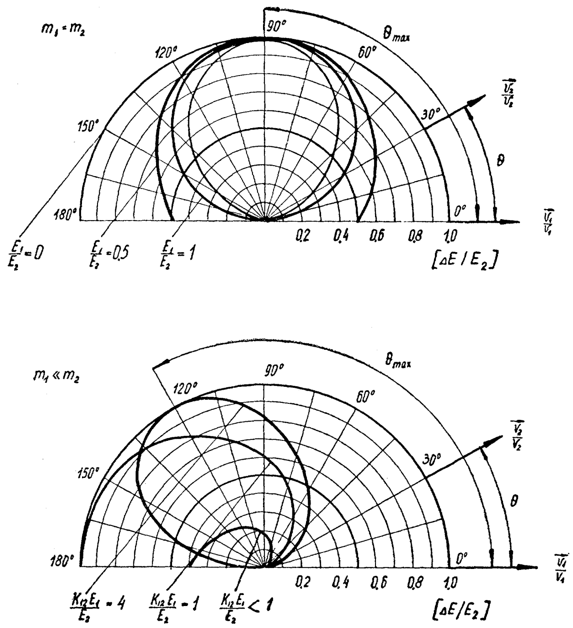

FIG. 2. The loss of energy of impinging particle as the function of the energies and masses of colliding particles and the collision angle θ.

Eq. (5) over the angles φ and Θ,

$$\sigma(\Delta E)=\frac{1}{2}\left(\frac{q_1q_2}{\mu}\right)^2 \times\int\int\frac{f(\theta)}{V^4}d\theta\frac{x^2+1}{\{4a^2x^2-[b+\Delta E(1+x^2)]^2\}^{\frac{1}{2}}}d(x^2). \quad (7)$$

In the last expression we have introduced the symbols

$$\begin{aligned} a&=\mu v_1v_2\sin\theta,\\ b&=K_{12}[E_2-E_1+\tfrac{1}{2}(m_1-m_2)v_1v_2\cos\theta]. \end{aligned} \quad (8)$$

Since the differential cross section must always be real, the integration over x^2 must be performed over the range for which

$$4a^2x^2-[b+\Delta E(1+x^2)]^2\geqslant 0. \quad (9)$$

As a result, we obtain

$$\sigma(\Delta E)=\frac{\pi}{2}\left(\frac{q_1q_2}{\mu}\right)^2\frac{1}{\Delta E^2}\int_{\theta_1}^{\theta_2}\frac{f(\theta)}{V^4}\left(\frac{2a^2}{\Delta E}-b\right)d\theta. \quad (10)$$

By Eqs. (3) and (8), the condition (9) may be readily rewritten:

$$-\frac{K_{12}E_1E_2}{\Delta E^2}\cos^2\theta-2\frac{m_1-m_2}{m_1+m_2}\frac{(K_{12}E_1E_2)^{\frac{1}{2}}}{\Delta E}\cos\theta +\left(\frac{K_{12}E_1E_2}{\Delta E^2}+\frac{K_{12}E_1}{\Delta E}-\frac{K_{12}E_2}{\Delta E}-1\right)\geqslant 0. \quad (11)$$

Therefore the limits of integral (10) are

$$\begin{aligned} \theta_{1,2}&=(x_0\pm x_1) && \text{if } -1\leqslant x_0\pm x_1\leqslant 1\\ &=0 && \text{if } \quad 1\leqslant x_0\pm x_1\\ &=\pi && \text{if } -1\geqslant x_0\pm x_1, \end{aligned} \quad (12)$$

where

$$x_0\pm x_1=-\frac{m_1-m_2}{m_1+m_2}\frac{\Delta E}{(K_{12}E_1E_2)^{\frac{1}{2}}} \pm\left[\left(1-\frac{\Delta E}{E_1}\right)\left(1+\frac{\Delta E}{E_2}\right)\right]^{\frac{1}{2}}. \quad (13)$$

Equation (11) gives us the maximum change in energy of the colliding particles as a function of the angle between their velocity vectors. Solving (11) with respect to ΔE, we have

$$\frac{\Delta E}{E_2}=\frac{m_1-m_2}{m_1+m_2}\left(\frac{K_{12}E_1}{E_2}\right)^{\frac{1}{2}}\cos\theta-\frac{K_{12}}{2}\left(1-\frac{E_1}{E_2}\right) \pm\left\{\left[\frac{m_1-m_2}{m_1+m_2}\left(\frac{K_{12}E_1}{E_2}\right)^{\frac{1}{2}}\cos\theta +\frac{K_{12}}{2}\left(1-\frac{E_1}{E_2}\right)\right]^2+\frac{K_{12}E_1}{E_2}\sin^2\theta\right\}^{\frac{1}{2}}. \quad (14)$$

The graph of the ratio $\Delta E/E_2$ as a function of the angle θ is given in Fig. 2. The maximum loss of energy of particle 2 is

$$\begin{aligned} \Delta E_{\max}&=-E_2 && \text{if } -1\leqslant\frac{1}{2}\frac{m_1-m_2}{m_1+m_2}\frac{v_2}{v_1}\\ &=-K_{12}E_2(1+v_1/v_2)(1-m_1v_1/m_2v_2) && \text{if } -1\geqslant\frac{1}{2}\frac{m_1-m_2}{m_1+m_2}\frac{v_2}{v_1}, \end{aligned} \quad (15)$$

and the collision angles corresponding to $\Delta E_{\max}$ are respectively,

$$\theta_{\max}=\text{arc}\cos\left(\frac{1}{2}\frac{v_2}{v_1}\frac{m_1-m_2}{m_1+m_2}\right),\quad \theta_{\max}=\pi. \quad (16)$$

In a similar way, by integrating Eq. (6) over φ, Θ, and D, we obtain

$$\sigma(\Delta E,\theta)=\frac{2\pi(q_1q_2)^2}{(m_2v_2^2)^2}\frac{(1+\Delta E/E_2)^{\frac{1}{2}}}{\xi^{\frac{5}{2}}}\left(\frac{m_1}{m_1+m_2}\right)^2\frac{1}{\pi} \times\int\frac{f(\theta)d\theta}{\xi\{4a^2u_1-[4a^2+(b+\Delta Eu_1)^2]\}}, \quad (17)$$

where

$$\xi=1+\frac{1}{2}\frac{\Delta E}{E_2}-\left(1-\frac{\Delta E}{E_2}\right)^{\frac{1}{2}}\cos\vartheta,$$

$$u_1=2(m_1/m_1+m_2)^2(V/v_2)^2(1/\xi).$$

In the case of a particle 2 moving through the collection of particles 1 having an isotropic distribution of velocities the angular distribution function is

$$f(\theta)=(\sin\theta)\,\bar{V}/v_2, \tag{18}$$

and therefore the cross section for the encounter with a change in energy ΔE is

$$\sigma(\Delta E)=\frac{2\pi(q_1q_2)^2}{m_1v_2^2}\left(\frac{1}{\Delta E^2}\frac{\Delta E}{|\Delta E|}\right)g[\Delta,\lambda], \tag{19}$$

$$\begin{aligned}g[\Delta,\lambda]=\frac{1}{2(1+2\lambda x+\lambda^2)}\Bigg\{&(-\tfrac{2}{3}\Delta)(x\lambda)^2\\&+(x\lambda)\left[\tfrac{4}{3}(1+\lambda^2)\Delta+\left(1-\frac{m_1}{m_2}\right)\right]\\&+\left[\left(1-\frac{m_1}{m_2}\right)(1+\lambda^2)+\lambda^2+\tfrac{4}{3}(1+\lambda^2)^2\Delta\right.\\&\left.-2\lambda^2\Delta-\frac{m_1}{m_2}\right]\Bigg\}\\&\times\begin{cases}(x_0+x_1)/|x_0+x_1|\geqslant 1\\(x_0+x_1)/|x_0+x_1|\leqslant 1\\(x_0-x_1)/|x_0-x_1|\leqslant 1\\(x_0-x_1)/|x_0-x_1|\geqslant 1.\end{cases}\end{aligned} \tag{20}$$

In the last expressions we have introduced the symbols $\Delta=E_1/\Delta E$ and $\lambda=v_2/v_1$. Substituting in Eqs. (10) and (17) the mean relative velocity $\bar{V}=(v_1^2+v_2^2)^{\frac{1}{2}}$, we obtain expressions more convenient for further calculations and which lead to a better approximation of the real process of interaction of charged particles with atomic electrons. This is a result of the elimination of collisions with a long interaction time; such collisions do not occur in fact owing to the curvature of the electron track in the field of the nucleus.

In this approximation the function (20) is given by

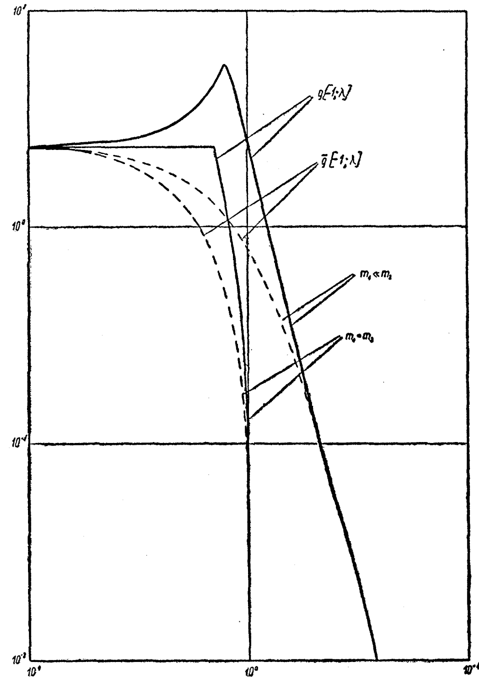

FIG. 3. Values of functions $g[\Delta,\lambda]$ and $\tilde{g}[\Delta,\lambda]$ for $\Delta E=-E_1$, $m_1=m_2$, and $m_1\ll m_2$ *versus* the ratio v_2/v_1.

$$\begin{aligned}\tilde{g}[\Delta,\lambda]=\frac{1}{2}\left(\frac{\lambda^2}{\lambda^2+1}\right)^{\frac{3}{2}}\Bigg\{&(\tfrac{2}{3}\Delta)x^3+\frac{1}{2\lambda}\left(1-\frac{m_1}{m_2}\right)x^2\\&+\left(1-2\Delta+\frac{m_1}{m_2}\frac{1}{\lambda^2}\right)\Bigg\}\\&\times\begin{cases}(x_0+x_1)/|x_0+x_1|\geqslant 1\\(x_0+x_1)/|x_0+x_1|\leqslant 1\\(x_0-x_1)/|x_0-x_1|\leqslant 1\\(x_0-x_1)/|x_0-x_1|\geqslant 1.\end{cases}\end{aligned} \tag{21}$$

The comparison of the exact function $g[\Delta,\lambda]$ with the approximative function $\tilde{g}[\Delta,\lambda]$ for $\Delta E=-E_1$, $m_1=m_2$, and $m_1\ll m_2$ is given in Fig. 3.

Similarly, in the approximation given above, for $f(\theta)$ given by Eq. (18) and for particles of equal mass $m_1=m_2$, we obtain the cross section for the scattering of particle 2 at the angle θ with a change in energy ΔE,

$$\sigma(\Delta E,\vartheta)=\frac{2\pi(q_1q_2)^2}{(m_2v_2^2)^2}\frac{1}{2\sqrt{2}}\frac{1}{m_1v_1v_2}\begin{cases}\dfrac{(1+\Delta E/E_2)^{\frac{1}{2}}}{\xi^{\frac{5}{2}}}\dfrac{1}{(1-2(v_2/\bar{V})^2\xi)^{\frac{1}{2}}} & \text{if } 1-2\left(\dfrac{v_2}{\bar{V}}\right)^2\xi\geqslant\dfrac{1}{2}\left(\dfrac{v_2}{\bar{V}}\right)^2\xi\dfrac{1}{E_2E_1}\left[E_2-E_1+\dfrac{1}{2}\Delta E\left(\dfrac{\bar{V}}{v_2}\right)^2\dfrac{1}{\xi}\right]^2\\ 0 & \text{if } 1-2\left(\dfrac{v_2}{\bar{V}}\right)^2\xi<\dfrac{1}{2}\left(\dfrac{v_2}{\bar{V}}\right)^2\xi\dfrac{1}{E_2E_1}\left[E_2-E_1+\dfrac{1}{2}\Delta E\left(\dfrac{\bar{V}}{v_2}\right)^2\dfrac{1}{\xi}\right]^2.\end{cases} \tag{22}$$

In two limiting cases, $m_1=m_2$ and $m_1 \ll m_2$, where $\Delta E<0$, the explicit expressions for $\sigma(\Delta E)$ are

$$m_1=m_2 \quad \sigma(\Delta E)=\frac{2\pi(q_1q_2)^2}{m_1v_2^2}\frac{1}{\Delta E^2}\left(\frac{v_2^2}{v_2^2+v_1^2}\right)^{\frac{3}{2}}\begin{cases} 1-\dfrac{E_1}{E_2}+\dfrac{4}{3}\dfrac{E_1}{\Delta E} & \text{if } \Delta E\leqslant E_2-E_1 \\ \dfrac{1}{3}\left(1+4\dfrac{E_1}{\Delta E}+2\dfrac{\Delta E}{E_2}-\dfrac{E_1}{E_2}\right)\left[\left(1+\dfrac{\Delta E}{E_1}\right)\left(1-\dfrac{\Delta E}{E_2}\right)\right]^{\frac{1}{2}} & \text{if } \Delta E\geqslant E_2-E_1, \end{cases} \tag{23}$$

$$m_1 \ll m_2 \quad \sigma(\Delta E)\approx\frac{2\pi(q_1q_2)^2}{m_1v_2^2}\frac{1}{\Delta E^2}\left(\frac{v_2^2}{v_2^2+v_1^2}\right)^{\frac{3}{2}}\begin{cases} 1+\dfrac{4}{3}\dfrac{E_1}{\Delta E} \quad \text{if } \Delta E\leqslant K_{12}E_2(1-v_1/v_2) \\ \dfrac{1}{2}\left[\left(1+\dfrac{\Delta E}{E_1}\right)^{\frac{1}{2}}\left(\dfrac{1}{3}+\dfrac{4}{3}\dfrac{E_1}{\Delta E}-\dfrac{4\Delta E}{K_{12}E_2}\right)+\left(1+\dfrac{4}{3}\dfrac{E_1}{\Delta E}\right)\right. \\ \qquad \left.+3\dfrac{\Delta E}{(K_{12}E_1E_2)^{\frac{1}{2}}}+\dfrac{5}{6}\dfrac{v_1}{v_2}\dfrac{\Delta E^2}{K_{12}E_1E_2}\right] \quad \text{if } \Delta E\geqslant K_{12}E_2(1-v_1/v_2). \end{cases} \tag{24}$$

In the last two expressions and henceforth ΔE indicates the absolute value of the energy loss.

The cross section for a collision with energy loss greater than U is

$$Q(U)=\int_U^{\Delta E_{\max}}\sigma(\Delta E)d(\Delta E), \tag{25}$$

or in explicit form in the case $m_1\cong m_2$

$$Q(U)=\frac{\sigma_0}{U^2}g_j[E_2/U;E_1/U], \tag{26}$$

where

$$g_j[E_2/U;E_2/U]=\left(\frac{v_2^2}{v_2^2+v_1^2}\right)^{\frac{3}{2}}\begin{cases} \dfrac{2}{3}\dfrac{E_1}{E_2}+\dfrac{U}{E_2}\left(1-\dfrac{E_1}{E_2}\right)-\left(\dfrac{U}{E_2}\right)^2 & \text{if } U+E_1\leqslant E_2 \\ \dfrac{2}{3}\left[\dfrac{E_1}{E_2}+\dfrac{U}{E_2}\left(1-\dfrac{E_1}{E_2}\right)-\left(\dfrac{U}{E_2}\right)^2\right]\left[\left(1+\dfrac{U}{E_1}\right)\left(1-\dfrac{U}{E_2}\right)\right]^{\frac{1}{2}} & \text{if } U+E_1\geqslant E_2, \end{cases} \tag{27}$$

and $\sigma_0=(m_2/m_1)(Z_1Z_2)^2\times 6.56\times 10^{-14}$ cm^2 ev^2. The function $g_j[E_2/U;E_1/U]$ is plotted in Fig. 4.

Similarly, the cross section for an encounter with loss of energy in the interval $U_1\leqslant\Delta E\leqslant U_2$ is

$$Q(U_2;U_1)=\int_{U_1}^{U_2}\sigma(\Delta E)d(\Delta E)=Q(U_2)-Q(U_1), \tag{28}$$

if $(U_2-U_1)/U_1\ll 1$, the last expression may be rewritten in the form

$$Q(U_1,U_2)\simeq\sigma(\Delta E)(U_1-U_2), \tag{29}$$

where $\Delta E=U_1$.

The stopping cross section of particle 1 with the minimum excitation energy U is given by

$$\langle(\sigma\Delta E)\rangle_{\text{Av}}=\int_U^{\Delta E_{\max}}\sigma(\Delta E)\Delta E d(\Delta E). \tag{30}$$

For heavy charged particles slowing down on light particles ($m_1\ll m_2$) the stopping cross section is

$$\langle(\sigma\Delta E)\rangle_{\text{Av}}\simeq\frac{\sigma_0}{E_2}\left(\frac{v_2^2}{v_2^2+v_1^2}\right)^{\frac{3}{2}}\begin{cases} \left[2+\ln\dfrac{K_{12}E_2}{U}+\dfrac{4}{3}\dfrac{E_1}{U}-\dfrac{2}{3}\left(\dfrac{v_1}{v_2}\right)^2\right] \quad \text{if } U\leqslant K_{12}E_2(1-v_1/v_2) \\ \left(1+\dfrac{\Delta E}{E_2}\right)^{\frac{1}{2}}\left[-\dfrac{2}{3}\dfrac{E_1}{\Delta E}+\dfrac{1}{3}-\dfrac{1}{3}\left(\dfrac{v_1}{v_2}\right)^2-\dfrac{4}{3}\dfrac{\Delta E}{K_{12}E_2}\right]+\dfrac{1}{2}\ln\left(\Delta E\dfrac{[1+(\Delta E/E_1)]^{\frac{1}{2}}-1}{[1+(\Delta E/E_1)]^{\frac{1}{2}}+1}\right)-\dfrac{2}{3}\dfrac{E_1}{\Delta E} \\ \qquad \left.+\dfrac{3}{2}\dfrac{\Delta E}{K_{12}E_1E_2}+\dfrac{5}{24}\dfrac{v_1}{v_2}\dfrac{\Delta E^2}{K_{12}E_1E_2}\right|_U^{K_{12}E_2(1-v_1/v_2)} \quad \text{if } U\geqslant K_{12}E_2(1-v_1/v_2). \end{cases} \tag{31}$$

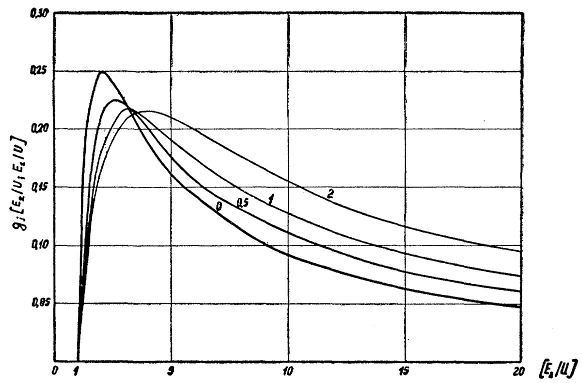

FIG. 4. Plot of the function g_j.

III. INELASTIC COLLISIONS OF CHARGED PARTICLES WITH ATOMS AS A PROCESS OF BINARY ENCOUNTERS WITH ATOMIC ELECTRONS

Now, by means of the calculated $\sigma(\Delta E)$ and $\sigma(\Delta E,\vartheta)$, we can give at once a quantitative interpretation of inelastic collisions as a result of binary encounters with atomic electrons of given binding energies and velocities.

(i) The Ionization and Excitation of Atoms by Charged Particles

Denoting by $N^{(i)}(v_e)$ the velocity distribution of i shell electrons of an atom and by $U_j^{(i)}$ their ionization potential, the ionization cross section of an atom is at once seen to be

$$Q_j^{\mathrm{at}}=\sum_{(i)}\int_0^\infty N^{(i)}(v_e)Q(U_j^{(i)})dv_e, \qquad (32)$$

and the cross section for the excitation of the level n

$$Q_{\mathrm{exc}}{}^n=\sum_{(i)}\int_0^\infty N^{(i)}(v_e)Q(U_{n+1}{}^{(i)};\,U_n{}^{(i)})dv_e, \qquad (33)$$

where $U_n{}^{(i)}$ $(U_{n+1}{}^{(i)})$ is the excitation energy of the level n $(n+1)$ from the shell i.

(ii) The Atomic Stopping Cross Section

The theory of the atomic stopping cross section, obtained in a similar way, was given previously by the author. At present, however, the theory is more consistent. We have eliminated the parameter D which was not very well determined, and the process of slowing down of charged particles is only a special case of the general theory of inelastic collisions. According to the above results, we have

$$\frac{1}{N}(dE/dx)\equiv\langle\sigma\Delta E\rangle_{\mathrm{Av}}{}^{\mathrm{at}}=\sum_{(i)}\int_0^\infty\langle\sigma\Delta E\rangle_{\mathrm{Av}}N^{(i)}(v_e)dv_e. \qquad (34)$$

(iii) The Angular Distribution of Inelastically Scattered Electrons from Atoms

This angular distribution is found at once to be

$$q(\Delta E,\vartheta)=\int_0^\infty \sigma(\Delta E_1\vartheta)N(v_e)dv_e. \qquad (35)$$

In a similar way we can interpret by means of the cross sections $\sigma(\Delta E)$ and $\sigma(\Delta E,\vartheta)$ a number of other phenomena arising during atomic collisions.

IV. COMPARISON WITH EXPERIMENT

To test the theory and illustrate its application we shall give some numerical results.

(i) Velocity Distribution of Ejected and Scattered Electrons of Primary Energy 100 ev from Helium Atoms

If it is recalled that the kinetic energy[8] and the ionization potential of the helium atom are 79 ev and

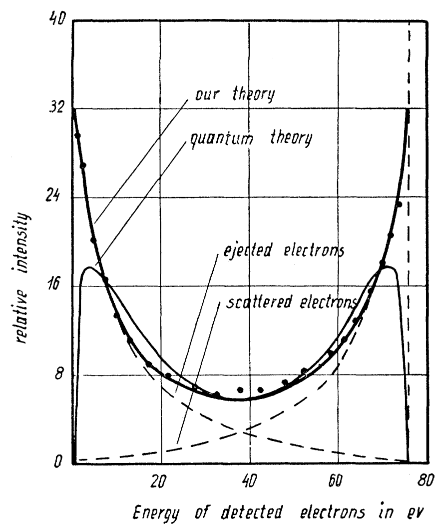

FIG. 5. Velocity distribution of ejected and scattered electrons resulting from ionizing collisions with helium atoms.

24.6 ev, respectively, the energy distributions of scattered and ejected electrons are given by the Eq. (23), where we have substituted $E_1=39.5$ ev, $E_2=100$ ev, $U_j=24.6$ ev and $\Delta E=E_2-E_X$ for scattered electrons and $\Delta E=U_j+E_{\mathrm{ej}}$ for ejected electrons. E_X is the energy of the scattered electrons and E_{ej} is the energy of the ejected electrons. The velocity distribution of electrons in a helium atom has been assumed to be $N_{\mathrm{He}}(v_e)=2\delta[v_e-(2E_1/m)^{\frac{1}{2}}]$. The results of the computations are in very good agreement with the experimental data of Goodrick[9] (Fig. 5). The slight asymmetry of the experi-

[8] P. Gombas, *Theorie und Lösungsmethoden des Mehrteilchenproblems der Wellen Mechanik* (Birkhaüser, Basel, 1950), pp. 167, 181.

[9] M. Goodrick, Phys. Rev. **49**, 422 (1936).

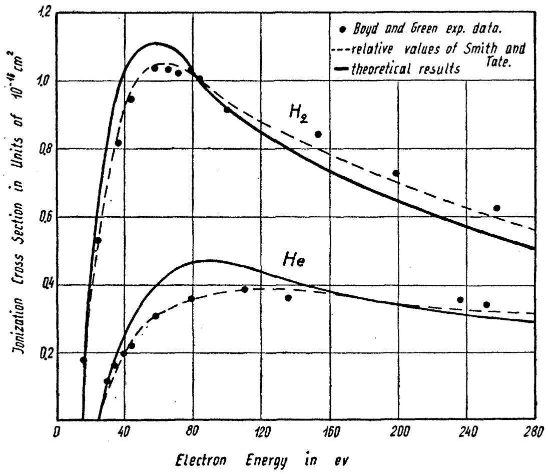

FIG. 6. Ionization cross sections of H_2 and He by electron impact.

mental curve is due to the excited He^+; therefore the number of high-energy electrons decreases and the number of low-energy electrons increases slightly. It should be noted here that quantum mechanics[10] does not give as good agreement with experiment, especially at the extremes of the energy distribution where the disparity is not only of a quantitative character, but of a qualitative nature as well.

(ii) Ionization Cross Sections of H_2 and He for Electrons

The ionization cross sections of H_2 and He for electrons are given by Eqs. (26), (27), (32) where we have substituted $E_1 = U_j = 15.6$ ev and

$$N_{H_2}(v_e) = 2\delta[v_e - (2U_j/m)^{\frac{1}{2}}]$$

for the hydrogen molecule and $E_1 = 39.5$ ev, $U_j = 24.6$ ev,

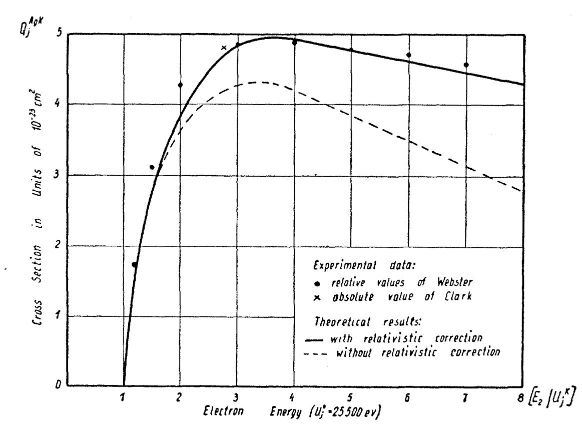

FIG. 7. The ionization cross section of Ag K shell by electron impact.

[10] See reference 2, pp. 236, 237.

$N_{He}(v_e) = 2\delta[v_e - (2E_1/m)^{\frac{1}{2}}]$ for the helium atom.

$$Q_j(H_2) = 5.51 \times 10^{-16} g_j[E_2/15.4; 1] \text{ cm}^2,$$
$$Q_j(He) = 2.20 \times 10^{-16} g_j[E_2/39.5; 1.6] \text{ cm}^2.$$

Comparison of theoretical and experimental results[11,12] are given in Fig. 6.

(iii) K Shell Ionization of Ag and Ni by Electron Impact

We assume that the velocity distribution of K electrons is $N^K(v_e) = 2\delta[v_e - v_e^K]$. Since their kinetic energy (E_1) is equal in the first approximation to the ionizing potential of shell K ($U_j^{AgK} = 25\,500$ ev, $U_j^{NiK} = 8350$ ev), we obtain immediately

$$Q_j^K(Ag) = 202 \times 10^{-22} g_j[E_2/U_j^{AgK}; 1] \times r[E_2/U_j^{AgK}; U_j^{AgK}/mc^2],$$

$$Q_j^K(Ni) = 18.8 \times 10^{-22} g_j[E_2/U_j^{NiK}; 1] \times r[E_2/U_j^{NiK}; U_j^{NiK}/mc^2].$$

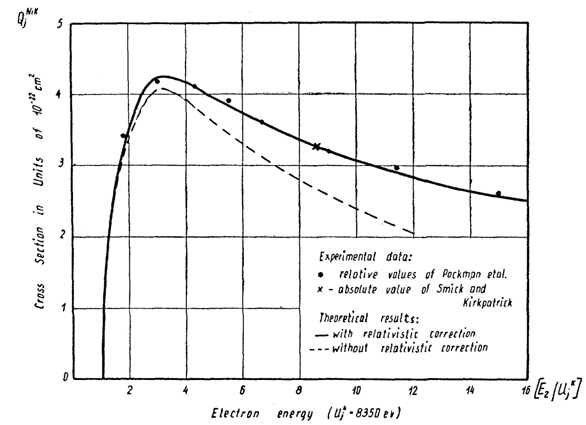

FIG. 8. The ionization cross section of Ni K shell by electron impact.

The function r is due to relativistic effects and is defined as the ratio $Q_{j\,\text{rel}}/Q_j$ where $Q_{j\,\text{rel}}$ is calculated from Eq. (26) using relativistic formula for v_1, v_2, m_1, m_2. Clearly in the nonrelativistic energy range $r \approx 1$. The theoretical results with and without the relativistic correction are plotted in Figs. 7 and 8. There is very good agreement with the experimental data of Webster *et al.*,[13] Clark,[14] Smick and Kirkpatrick,[15] and Pockman *et al.*[16]

[11] P. Smith and J. Tate, Phys. Rev. **39**, 270 (1932).
[12] R. L. F. Boyd and G. W. Green, Proc. Phys. Soc. (London) **71**, 357 (1958).
[13] Webster, Hansen, and Duveneck, Phys. Rev. **43**, 839 (1933).
[14] J. C. Clark, Phys. Rev. **48**, 30 (1935).
[15] A. E. Smick and P. Kirkpatrick, Phys. Rev. **67**, 153 (1945).
[16] Pockman, Webster, Kirkpatrick, and Harworth, Phys. Rev. **71**, 330 (1947).

(iv) Excitation Cross Sections, $4p\,^1P_1$, of He and, $6p\,^3P_1$, of Hg Levels and the Sodium D Lines, by Electron Impacts

Because the excitation energy of levels $4p\,^1P_1$ and $5p\,^1P_1$ are 23.7 ev and 23.95 ev, respectively, and other data for the helium atom are the same as in (i) we have

$$Q_{\text{exc}}(\text{He }4p\,^1P_1)\simeq 2\{Q(23.7)-Q(23.95)\}.$$

In the excitation of Hg the two outer electrons (6s) of Hg are the most effective because of the strong dependence on the excitation energy ($Q\sim 1/U_{\text{exc}}{}^n$ where $2<n<3$) therefore

$$Q_{\text{exc}}(\text{Hg }6p\,^3P_1)\simeq 2\times[Q(4.86)-Q(5.43)],$$

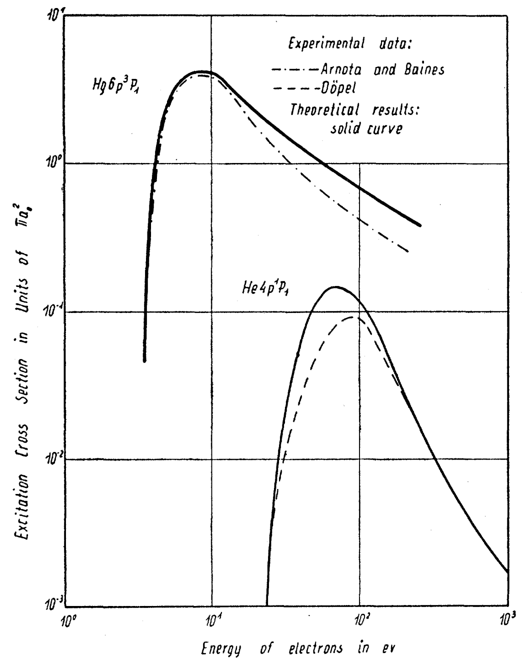

FIG. 9. The excitation cross sections of Hg $6p\,^3P_1$ and He $4p\,^1P_1$ by electron impact.

5.43 ev and 4.86 ev are the excitations energies of levels $6p\,^3P_1$ and $6p\,^3P_2$, respectively.

Taking into account the fact that the majority of transitions from high-energy levels of Na pass through the levels $2p\,^2P_{\frac{3}{2}}$ and $2p\,^2P_{\frac{1}{2}}$, the excitation cross section of the sodium D lines is

$$Q_{\text{exc}}{}^D\simeq 1\times Q(2.1).$$

The theoretical and experimental results[17–20] are plotted in Figs. 9 and 10.

(v) Atomic Stopping Cross Section of Helium for Protons

The atomic stopping cross section of helium for protons is $\langle\sigma\Delta E\rangle_{\text{Av}\,p}{}^{\text{He}}=2\langle\sigma\Delta E\rangle_{\text{Av}}$, where $\langle\sigma\Delta E\rangle_{\text{Av}\,p}$ is

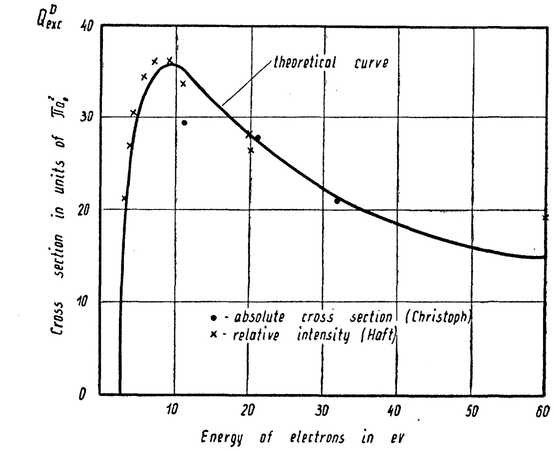

FIG. 10. Excitation of the D lines of sodium by electron impact.

given by (31) and U is the first excitation potential of the helium atom. The experimental data of Reynolds[21] and Weyl[22] are in very good agreement with the theoretical results (Fig. 11).

(vi) Angular Distribution of Inelastically Scattered 200-ev Electrons from H_2

The angular distribution of electrons of energy E_2 scattered by electrons of energy E_1 with the loss of energy ΔE is given by Eq. (22). In our case we have $E_1=15.7$ ev, $E_2=200$ ev, and $\Delta E=150$, 100, and 50 ev. The obtained angular distributions are given in Fig. 12. It is seen that the range of scattering is contained in an angular interval whose value and position depends on E_1, E_2, and ΔE. The above results concern collisions

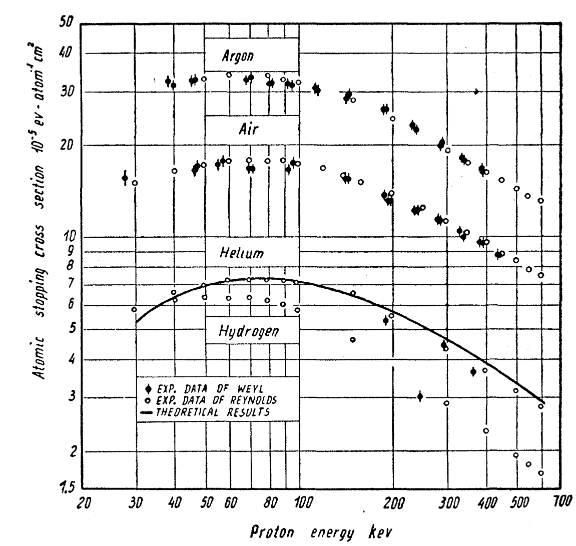

FIG. 11. Comparison of the theoretical calculations of the stopping power of He for protons with experimental data.

[17] R. Döpel, Ann. Physik **16**, 1 (1933).
[18] G. Haft, Z. Physik **82**, 73 (1933).
[19] F. L. Arnota and G. O. Baines, Proc. Roy. Soc. (London) **A151**, 256 (1935).
[20] W. Christoph, Ann. Physik **23**, 51 (1935).
[21] Reynolds, Dunbar, Wenzel, and Whaling, Phys. Rev. **92**, 742 (1953).
[22] P. K. Weyl, Phys. Rev. **91**, 289 (1953).

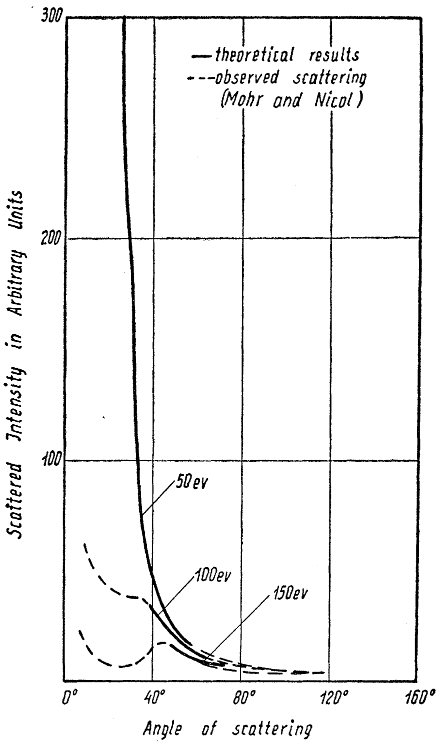

FIG. 12. The angular distribution of inelastically scattered electrons from H_2 for various loss of energy (50,000, and 150 ev).

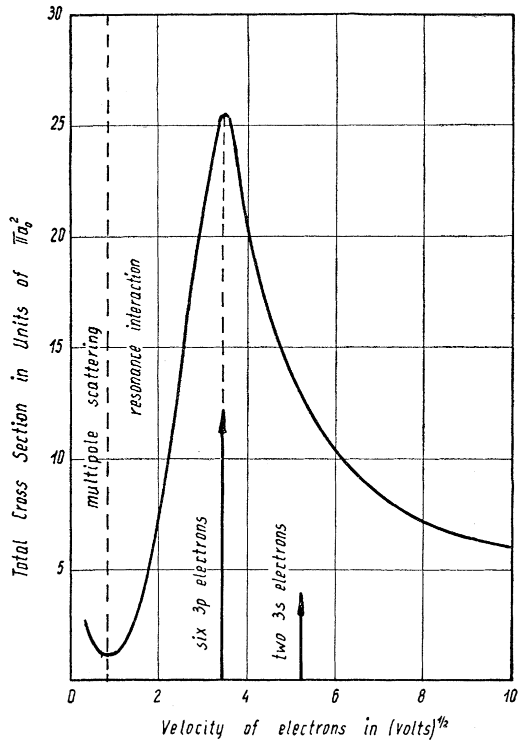

FIG. 13. The total cross section of argon for electrons and velocities of its outer electrons.

with free electrons. In scattering on electrons bound in a molecule or atom the distribution is strongly deformed by the field of the nucleus, but the character of the curve and the position of the maximum on the theoretical curve coincide, in principle, with the experimental data.[23]

The above examples do not exhaust all the possibilities of the theory presented here nor is there a claim to great accuracy, although in many cases the accuracy may be considerably improved by a careful analysis of each problem.

V. CONCLUSIONS

From comparison of the theory with experimental results, it follows that the interaction of charged particles with the atomic shell can be interpreted solely on the basis of classical mechanics; the binary encounter approximation is sufficiently good to describe the majority of inelastic processes and compares favorably with experiment. The approximation is relatively inaccurate for describing the angular distributions of inelastically scattered particles; this is because of the strong influence of elastic scattering in the field of the entire atom which does not change the energy distribution strongly affects the angular distribution. The above theory, however, can be used to explain the diffraction pattern of scattered electrons.

In a similar way, the theory of elastic collisions can be built on the basis of classical mechanics. It should be noted that the scattering of charged particles by an atom cannot be treated as scattering by the static field of the atom, but this process must be treated dynamically. With such an approach to the problem it is clear that the occurrence of maxima in the scattering curve is the result of mechanical resonance of the impinging particles with atomic electrons of the same velocity.

Probably the Ramsauer effect is due to such mechanical resonance, but not due to the wave nature of interaction process. Figure 13, where the total scattering cross section of argon for electrons and the velocities of its $6s$ and $6p$ electrons are shown, is very impressive. The lack of, or very weak, Ramsauer effect in the case of scattering by e.g., H_2 or He is the result of a large asymmetry in the charge distribution of the atom and the resulting large cross section for multipole scattering, which masks the Ramsauer effect.

APPENDIX

Equation (1) of our paper can be easily obtained by means of the relations given by Chandrasekhar.[6] According to Chandrasekhar, the change in energy ΔE suffered by a star as a result of an encounter is

$$\Delta E = -2\mu V_g V \cos(\phi - \psi) \cos\psi \cos i. \qquad \text{(I 16)}$$

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

Also

$$\cos^2\psi = 1/[1+D^2V^4/G^2(m_1+m_2)^2], \qquad \text{(I 5)}$$

$$\cos\phi \cos i = \cos\Phi, \quad \sin\phi \cos i = \sin\Phi \cos\Theta, \qquad \text{(I 27)}$$

$$V_g^2 = \frac{1}{(m_1+m_2)^2}(m_1^2v_1^2 + m_2^2v_2^2 + 2m_1m_2v_1v_2 \cos\theta), \qquad \text{(I 30)}$$

$$V^2 = v_1^2 + v_2^2 - 2v_1v_2 \cos\theta, \qquad \text{(I 31)}$$

$$\cos\Phi = [m_2v_2^2 - m_1v_1^2 + v_1v_2(m_1-m_2) \cos\theta]/V_gV(m_1+m_2), \qquad \text{(I 33)}$$

$$\sin\Phi = (v_1v_2/V_gV) \sin\theta. \qquad \text{(I 36)}$$

Hence Eq. (I 16) may readily be rewritten

$$\Delta E = -4\frac{m_1m_2}{(m_1+m_2)^2}\frac{1}{1+[D^2V^4/G^2(m_1+m_2)^2]} \times\left\{\frac{m_2V_2^2}{2} - \frac{m_1V_1^2}{2} + \frac{1}{2}v_1v_2\left[(m_1-m_2)\cos\theta + (m_1+m_2)\sin\theta\cos\Theta\frac{DV^2}{G(m_1+m_2)}\right]\right\},$$

which is our Eq. (1).

Similarly, it follows from the results of Williamson and Chandrasekhar[7] that the change in the direction of the star resulting from the encounter is:

$$\cos 2\Psi = \frac{2m_1(v_2 - v_1\cos\theta)\cos^2\psi + 2m_1v_1\sin\theta\sin\psi\cos\psi\cos\Theta - (m_1+m_2)v_2}{\{(m_1+m_2)^2v_2^2 - 4m_1[(m_2v_2^2 - m_1v_1^2) + (m_1-m_2)v_1v_2\cos\theta]\cos^2\psi - 4m_1(m_1+m_2)v_1v_2\sin\theta\sin\psi\cos\psi\cos\Theta\}^{\frac{1}{2}}}. \qquad \text{(II 30)}$$

Solving Eq. (1) for $\cos\Theta$, substituting in Eq. (II 30) and taking into account Eq. (I 5), we obtain Eq. (2) of our paper where we have replaced 2Ψ by ϑ.