

Dispersion Relations in Atomic Scattering Problems*

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Dispersion relations appropriate to the scattering of electrons by hydrogen atoms are deduced, and applied to actual measurements in the 0–10 eV energy range. Two such experiments exist, yielding quite different results. Dispersion relations indicate that only certain angular distributions at low energy are consistent with these low-energy total cross-section measurements; this suggests experiments which could be used as checks on the accuracy of the existing measurements.

I. INTRODUCTION

ALTHOUGH dispersion relations—expressions which relate the real and the imaginary parts of a scattering amplitude—have long been used by workers in meson physics to help analyze the results of high-energy nuclear scattering experiments, their possible utility in investigations of atomic scattering processes has been unexplored. In atomic scattering problems spin-orbit forces generally are negligible, so that the forces can be supposed wholly Coulombic, ergo known. Thus applications of dispersion relations to atomic reactions will not be hampered by difficulties, common in nuclear applications, stemming from inadequate understanding of the forces involved. Moreover, even in the simplest atomic reactions, e.g., the collisions of electrons with atomic hydrogen, it is not yet practical to compute exactly the expected cross sections from the known forces; in fact almost nothing is known concerning the limits of error of commonly employed approximations.

For the aforementioned reasons it may be hoped that dispersion relations can prove a useful tool in analysis of atomic scattering experiments. In the present work we first develop the dispersion relations appropriate to the elastic scattering of electrons by atomic hydrogen, and then use these relations to analyze two conflicting experiments in the (incident electron) energy range below 10 eV.

II. DISPERSION RELATIONS FOR POTENTIAL SCATTERING

The dispersion relations for nonrelativistic scattering of a particle by a fixed potential have been derived lucidly by Klein and Zemach.¹ Denote the incident wave by $\psi_i = \exp(i\mathbf{k}_i \cdot \mathbf{r})$, representing a free particle incident along $\mathbf{k}_i = k\mathbf{n}_i$ with energy $E = \hbar^2 k^2 / 2m$; define $\psi_f = \exp(i\mathbf{k}_f \cdot \mathbf{r})$, $\mathbf{k}_f = k\mathbf{n}_f$; and let $\Psi_i^{(+)}$ denote the solution to the complete Schrödinger equation

$$(H - E)\Psi \equiv [-\hbar^2/2m \nabla^2 + V - E]\Psi = 0, \quad (1)$$

with incident wave ψ_i and everywhere outgoing

scattered waves. It is known that

$$f(\theta, E) = -\frac{m}{2\pi\hbar^2} \int d\mathbf{r} \psi_f^* V(\mathbf{r}) \Psi_i^{(+)} \quad (2)$$

is the exact amplitude for scattering of the particle into the direction \mathbf{n}_f making an angle θ with \mathbf{n}_i . The (first) Born approximation to $f(\theta, E)$ is

$$f_{\text{Born}}(\theta, E) = -\frac{m}{2\pi\hbar^2} \int d\mathbf{r} \psi_f^* V(\mathbf{r}) \psi_i. \quad (3)$$

Then in effect Klein and Zemach show that with $\mathbf{n}_f = \mathbf{n}_i$, the function

$$Q(E) = f(0, E) - f_{\text{Born}}(0, E) \quad (4)$$

is an analytic function of E in the complex energy plane with the properties: (i) $Q(E)$ has poles at negative real energies corresponding to bound states of the particle in the force field $V(\mathbf{r})$; (ii) $Q(E)$ has a branch point at $E=0$; (iii) in the domain $0 \leq \arg E < 2\pi$, i.e., with a branch cut along the positive real E axis, $Q(E)$ is analytic except at the aforementioned poles and branch point, and vanishes at large complex E .

It follows that

$$\begin{aligned} Q(E) &= \frac{1}{2\pi i} \int_{C_1} \frac{Q(E') dE'}{E' - E} \\ &= \frac{1}{2\pi i} \int_{C_2} \frac{Q(E') dE'}{E' - E} - \sum_j R_j(E), \end{aligned} \quad (5)$$

where the contours C_1 , C_2 are given in Fig. 1, and R_j are the residues of $(E' - E)^{-1} Q(E')$ at the poles $E' = E_j$. The integrals above and below the cut do not cancel. Rather, from Eqs. (1)–(4), the relation^{2–4}

$$\Psi_i^{(+)} = \psi_i - \frac{1}{H - E - i\epsilon} V \psi_i, \quad (6)$$

and the definition of k in terms of E , it is inferred that

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¹ A. Klein and C. Zemach, *Ann. Phys.* **7**, 365 (1959).

² B. A. Lippman and J. Schwinger, *Phys. Rev.* **79**, 469 (1950).

³ M. Gell-Mann and M. L. Goldberger, *Phys. Rev.* **91**, 398 (1953).

⁴ E. Gerjuoy, *Ann. Phys.* **5**, 58 (1958).

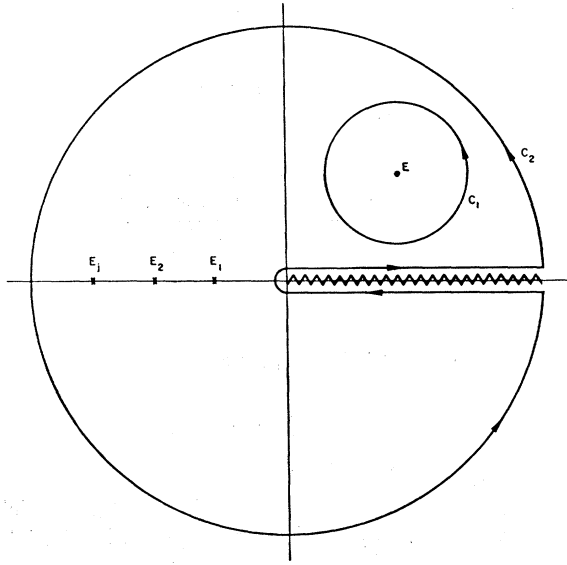


FIG. 1. Contours of integration in the complex energy plane; the function to be integrated has poles at E, E_1, E_2, \dots, E_j and has a branch point at the origin.

$Q(E_+)$ is the complex conjugate of $Q(E_-)$ where E_+, E_- denote corresponding points immediately above and below the cut. Thus, since $Q(E)$ vanishes at infinity

$$\frac{1}{2\pi i} \int_{c_2} \frac{Q(E')dE'}{E'-E} = \frac{1}{2\pi i} \int_0^\infty \frac{dE'}{E'-E} \frac{Q(E_+)}{E'-E} - \frac{1}{2\pi i} \int_0^\infty \frac{dE'}{E'-E} \frac{Q(E_-)}{E'-E} = \frac{1}{\pi} \int_0^\infty \frac{dE'}{E'-E} \frac{\text{Im}Q(E')}{E'-E}. \quad (7)$$

Taking the real part of Eq. (5), employing Eq. (7), noting that $f_{\text{Born}}(0, E)$ is real, and remarking that (as will be shown later) the residues R_j are purely real, we have

$$\text{Re}f(0, E) = f_{\text{Born}}(0, E)$$

$$+\frac{1}{\pi} \int_0^\infty \frac{dE'}{E'-E} \frac{\text{Im}f(0, E')}{E'-E} - \sum_j R_j(E), \quad (8)$$

which is the desired dispersion relation. The integral is evaluated from the experimental data with the aid of the optical theorem for cross sections

$$\text{Im}f(0, E) = (k/4\pi)\sigma(E), \quad (9)$$

where σ is the total scattering cross section for incident particles of energy E and f is the elastic forward scattering amplitude.

III. DISPERSION RELATIONS FOR e - H SCATTERING

The above derivation of the dispersion relation for potential scattering has the virtue that it is conveniently applicable to many-particle collisions involving re-

arrangement. When electrons are incident on atomic hydrogen, the differential cross section for elastic scattering along \mathbf{n}_f is⁵

$$(d\sigma_{\text{el}}/d\Omega)_\theta = \frac{3}{4}|f-g|^2 + \frac{1}{4}|f+g|^2, \quad (10)$$

where the ordinary amplitude f and exchange amplitude g are given by

$$f(\theta, E) = -\frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{f_0}^* V_i(\mathbf{r}_1, \mathbf{r}_2) \Psi_i^{(+)}, \quad (11)$$

$$g(\theta, E) = -\frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{f_0}^* V_f(\mathbf{r}_1, \mathbf{r}_2) \Psi_i^{(+)}.$$

In Eqs. (11)

$$\psi_i = \exp(i\mathbf{k}\mathbf{n}_i \cdot \mathbf{r}_1) u_0(r_2),$$

$$\psi_{f_0} = \exp(i\mathbf{k}\mathbf{n}_f \cdot \mathbf{r}_1) u_0(r_2),$$

$$\psi_{f_0}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{f_0}(\mathbf{r}_2, \mathbf{r}_1) = \exp(i\mathbf{k}\mathbf{n}_f \cdot \mathbf{r}_2) u_0(r_1), \quad (12)$$

$$V_i = -(\epsilon^2/r_1) + \epsilon^2/|\mathbf{r}_1 - \mathbf{r}_2|,$$

$$V_f = -(\epsilon^2/r_2) + \epsilon^2/|\mathbf{r}_1 - \mathbf{r}_2|,$$

$$\Psi_i^{(+)} = \psi_i - \frac{1}{H - E + 13.6 - i\epsilon} V_i \psi_i, \quad (13)$$

and $u_0(r)$ is the wave function of atomic hydrogen in its ground state. The energy E is the total energy of the system measured relative to the binding energy of atomic hydrogen in its ground state, so that

$$k = (2m/\hbar^2)^{1/2} E^{1/2}, \quad (14)$$

when (as in the present case) an electron is incident on a ground-state hydrogen atom.

The dispersion relations for e - H scattering now are readily obtainable provided one assumes that the Green's function of the complete (spin-independent) Hamiltonian $(H - E + 13.6 - i\epsilon)^{-1}$: (i) has poles at negative real energies corresponding to bound states of the total Hamiltonian, i.e., to bound states of H^- ; (ii) has branch points at every energy E_i corresponding to the threshold of a new reaction channel, e.g., at incoming electron energy $E=0$, at $E=(\frac{3}{4})13.6$ (excitation of first excited state), etc.; (iii) is single-valued and analytic except at the aforementioned poles and branch points if a branch cut, starting at $E=0$ is drawn in the positive direction along the real axis, with the specification that $0 \leq \arg(E - E_i) < 2\pi$ for every threshold energy E_i ; (iv) has the (coordinate space) representation $(E_j - E)^{-1} w_j(\mathbf{r}) w_j^*(\mathbf{r}')$ in the vicinity of each pole E_j , where $w_j(\mathbf{r})$ is the space-dependent part of the eigenfunction corresponding to energy E_j . These assumptions have not been proved, but are consistent: with what is known about the behavior of the Green's function for one-particle potential scattering; with the belief that H is self-

⁵ N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1952), p. 215.

adjoint; and with the known asymptotic behavior of $(H-E+13.6-i\epsilon)^{-1}$, which in any reaction channel is $\sim r^{-1} \exp(ik_f r)$ at large r , where $k_f = [(2m/\hbar^2)(E-E_t)]^{1/2}$. The same assumptions lead directly⁶ to well-known and accepted formulas for many-particle scattering, e.g., Eqs. (12)–(14).

The first three assumptions above imply that the ordinary function $Q_o(E)$, defined as in Eq. (4), and the corresponding exchange function

$$Q_e(E) = g(0, E) - g_{\text{Born}}(0, E), \quad (15)$$

have the properties (i), (ii), (iii) used previously. Proceeding as in the case of potential scattering, one obtains

$$\begin{aligned} \text{Ref}(0, E) &= f_{\text{Born}}(0, E) \\ &+ \frac{1}{\pi} \int_0^\infty dE' \frac{\text{Im}f(0, E')}{E' - E} - \sum_i R_{oj}(E), \quad (16a) \end{aligned}$$

$$\begin{aligned} \text{Reg}(0, E) &= g_{\text{Born}}(0, E) \\ &+ \frac{1}{\pi} \int_0^\infty dE' \frac{\text{Im}g(0, E')}{E' - E} - \sum_i R_{ej}(E). \quad (16b) \end{aligned}$$

Substituting Eq. (13) in Eq. (11),

$$\begin{aligned} Q_o(E) &= \frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{f\sigma}^* V_i \frac{1}{H-E+13.6-i\epsilon} V_i \psi_i, \\ Q_e(E) &= \frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{f\sigma}^* V_f \frac{1}{H-E+13.6-i\epsilon} V_i \psi_i, \end{aligned} \quad (17)$$

so that, making use of the assumption (iv) above,

$$\begin{aligned} R_{oj}(E) &= \frac{1}{E-E_j} \frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \\ &\times \exp(-\alpha_j \mathbf{n}_j \cdot \mathbf{r}_1) u_0(r_2) V_i(\mathbf{r}_1, \mathbf{r}_2) w_j(\mathbf{r}_1, \mathbf{r}_2) \\ &\times \int d\mathbf{r}_1' d\mathbf{r}_2' w_j^*(\mathbf{r}_1', \mathbf{r}_2') V_i(\mathbf{r}_1', \mathbf{r}_2') \\ &\times \exp(-\alpha_j \mathbf{n}_i \cdot \mathbf{r}_1') u_0(r_2'). \quad (18) \end{aligned}$$

In Eq. (18)

$$\alpha_j = (2m/\hbar^2) |E_j|^{1/2}, \quad (19)$$

where $|E_j|$ is the electron affinity of the j th H^- state, equal to 0.7 eV for the known ground singlet $1s^2$ state. The appearance of the exponential factors $\exp(-\alpha_j \mathbf{n}_j \cdot \mathbf{r}_1)$ and $\exp(-\alpha_j \mathbf{n}_i \cdot \mathbf{r}_1')$ in Eq. (18) is a consequence of the above assumption (iii), which implies $\arg E_j$ is π . In other words, when the expressions (17) are analytically continued to the negative energy E_j , $\arg k$ of Eq. (14) becomes $\frac{1}{2}\pi$, meaning k becomes

positive imaginary. Similarly

$$\begin{aligned} R_{ej}(E) &= \frac{1}{E-E_j} \frac{m}{2\pi\hbar^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \\ &\times \exp(-\alpha_j \mathbf{n}_j \cdot \mathbf{r}_2) u_0(r_1) V_f(\mathbf{r}_1, \mathbf{r}_2) w_j(\mathbf{r}_1, \mathbf{r}_2) \\ &\times \int d\mathbf{r}_1' d\mathbf{r}_2' w_j^*(\mathbf{r}_1', \mathbf{r}_2') V_i(\mathbf{r}_1', \mathbf{r}_2') \\ &\times \exp(-\alpha_j \mathbf{n}_i \cdot \mathbf{r}_1') u_0(r_2'). \quad (20) \end{aligned}$$

With $\mathbf{n}_f = \mathbf{n}_i$, the residue for the ordinary amplitude is

$$\begin{aligned} R_{oj}(E) &= \frac{1}{E-E_j} \frac{m}{2\pi\hbar^2} \left| \int d\mathbf{r}_1 d\mathbf{r}_2 \right. \\ &\times \exp(-\alpha_j \mathbf{n}_i \cdot \mathbf{r}_1) u_0(r_2) V_i(\mathbf{r}_1, \mathbf{r}_2) w_j(\mathbf{r}_1, \mathbf{r}_2) \left. \right|^2, \quad (21) \end{aligned}$$

which is real, as stated previously. Moreover, for singlet states of H^- , $w_j(\mathbf{r}_1, \mathbf{r}_2)$ is symmetric in the coordinates $\mathbf{r}_1, \mathbf{r}_2$; for triplet states w_j is antisymmetric. Thus

$$R_{ej}(E) = \pm R_{oj}(E) \equiv \pm R_j(E), \quad (22)$$

the upper and lower signs referring to singlet and triplet, respectively. Adding and subtracting Eqs. (16),

$$\begin{aligned} \text{Re}(f \pm g) &= (f \pm g)_{\text{Born}} + \frac{1}{\pi} \int_0^\infty dE' \frac{\text{Im}(f \pm g)}{E' - E} dE' \\ &- \sum_{j^s} (R_j \pm R_j) - \sum_{j^t} (R_j \mp R_j), \quad (23) \end{aligned}$$

where s, t indicate sums over singlet and triplet bound states, respectively, and it is understood that f, g refer to the forward direction $\theta = 0$. Equation (23) agrees with the expectation that the triplet amplitude $f-g$ has poles corresponding to triplet bound states of H^- but not to singlet bound states, and similarly for the singlet amplitude $f+g$.

The forward triplet and singlet amplitudes obey the cross-section theorem

$$\text{Im}(f \pm g)_{\theta=0} = (k/4\pi) \sigma_{\pm}(E), \quad (24)$$

with $\sigma_{\pm}(E)$ representing the total cross section, elastic plus inelastic, integrated over all angles, for incident electrons in singlet (+) or triplet (-) spin states relative to the H atom in its ground state. Equation (24), like Eq. (6), merely expresses conservation of total particle current, and can be proved by procedures similar to those employed to demonstrate the cross section theorem for colliding systems of many spinless particles.⁴ The measured total cross section σ_t is given by the usual combination of triplet and singlet contributions, i.e.,

$$\sigma_t = \frac{3}{4} \sigma_- + \frac{1}{4} \sigma_+ \quad (25)$$

⁶ E. Gerjuoy, Phys. Rev. **109**, 1806 (1958).

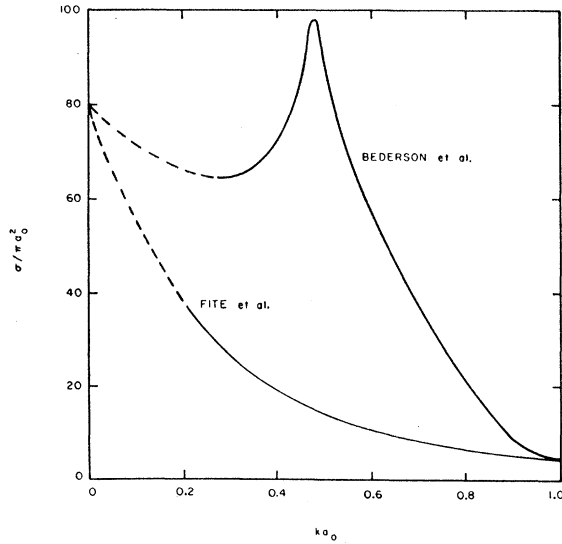


FIG. 2. Elastic scattering cross sections for electrons incident on hydrogen atoms, as measured by Bederson et al. (reference 7) and Fite et al. (reference 8); $ka_0=1$ corresponds to an energy of 13.6 eV. Broken lines show cross sections extrapolated to zero energy.

implying

$$\text{Im}(f - \frac{1}{2}g) = (k/4\pi)\sigma_t(E). \quad (26)$$

Subtracting half of (16b) from (16a) we obtain finally a dispersion relation which is useful for comparison with experimental $e-H$ scattering observations, namely

$$\text{Re}(f - \frac{1}{2}g) = (f - \frac{1}{2}g)_{\text{Born}} + \frac{1}{4\pi^2} \int_0^\infty dE' \frac{k'\sigma_t(E')}{E' - E} - \frac{1}{2}R. \quad (27)$$

In Eq. (27) we have explicitly included only the residue $R \equiv R_{01}$ corresponding to the singlet ground ($j=1$) state of H^- . Remarks concerning the possible existence of other bound states, and the effects on our conclusions of neglect of such states, are deferred until later.

IV. APPLICATION

The primary utility of Eq. (27) is as a consistency check on a given experimental measurement of σ_t ; the particular fashion in which Eq. (27) is employed depends on the kind of information about f and g which is available. For instance, taking E large enough so that the exchange amplitude g is small, we have

$$\frac{\text{Re}f - f_{\text{Born}}}{f_{\text{Born}}} = \left[\frac{1}{4\pi^2} \int_0^\infty \frac{k'\sigma_t(E')dE'}{E' - E} - \frac{1}{2}R \right] \frac{1}{f_{\text{Born}}}, \quad (28)$$

which gives the error in Born approximation at energy E as a function of the total cross section at other energies. If theory or measurement gives a reliable independent prediction of this error, then Eq. (28) provides a test of the accuracy with which σ_t is known. More realistically, it may be possible to use angular

distribution measurements as a check on the reliability of the often more difficult total cross section measurements. From the measured elastic scattering angular distribution one can compute the "directivity" $\langle \Delta\Omega \rangle$, defined in terms of the total elastic cross section σ_{el} and the differential cross section in the forward direction by the relation

$$\sigma_{el} = \int d\Omega \frac{d\sigma_{el}}{d\Omega} \Big|_{\theta} = \frac{d\sigma_{el}}{d\Omega} \Big|_{\theta=0} \langle \Delta\Omega \rangle. \quad (29)$$

The quantity $\langle \Delta\Omega \rangle$ is interpretable as the solid angle within which the elastic scattering remains about as large as it is in the forward direction, assuming the elastic angular distribution is peaked (as usual) in the forward direction. Employing Eq. (10) for $(d\sigma_{el}/d\Omega)$ at $\theta=0$, noting that

$$\frac{3}{4}|f-g|^2 + \frac{1}{4}|f+g|^2 = [\text{Re}(f - \frac{1}{2}g)]^2 + [\text{Im}(f - \frac{1}{2}g)]^2 + \frac{3}{4}|g|^2, \quad (30)$$

and using Eq. (26),

$$\sigma_{el} = \{ [\text{Re}(f - \frac{1}{2}g)]^2 + [k\sigma_t/4\pi]^2 + \frac{3}{4}|g|^2 \} \langle \Delta\Omega \rangle, \quad (31)$$

wherein all quantities are evaluated at the same energy E . Consequently

$$\langle \Delta\Omega \rangle \leq \sigma_{el} \{ [\text{Re}(f - \frac{1}{2}g)]^2 + [k\sigma_t/4\pi]^2 \}^{-1}. \quad (32)$$

Through Eq. (27) the right side of Eq. (32) is known in terms of measured cross sections, whose accuracies are tested by experimental determination of $\langle \Delta\Omega \rangle$. For example, if at some energy the elastic angular distribution is isotropic meaning $\langle \Delta\Omega \rangle = 4\pi$, the measured total cross sections cannot be accurate unless the right side of Eq. (32) turns out to exceed 4π .

Eqs. (28) and (32) have been applied to the analysis of two conflicting experiments,^{7,8} both intended to yield the total cross section for electron scattering from atomic hydrogen at energies below 10 eV. The results of their measurements are indicated in Fig. 2. Our calculations are summarized in Table I, which for Bederson's data (B) and Fite's (F) lists, as a function of incident electron energy E , the values of: $(f - \frac{1}{2}g)_{\text{Born}}$; $\text{Im}(f - \frac{1}{2}g)$, from the total cross sections; $\text{Re}(f - \frac{1}{2}g)$, computed from Eq. (27); and $\langle \theta \rangle$, computed from the right side of Eq. (32) via the definition $\sin^2 \frac{1}{2} \langle \theta \rangle = (4\pi)^{-1} \langle \Delta\Omega \rangle$. The wave number k is in units of $1/a_0 = (\hbar^2/me^2)^{-1}$, f and g are in units of a_0 ; f_{Born} equals a_0 at all energies. The definition equates $\langle \theta \rangle$ to the half angle of a cone subtending the solid angle $\langle \Delta\Omega \rangle$. We tabulate $\langle \theta \rangle$ rather than $\langle \Delta\Omega \rangle$ because it is more easily approximately estimated from a glance at a given angular distribution; if the angular distribution peaks in the forward direction, $\langle \theta \rangle$ is the polar angle outside of which the differential cross section should be small.

⁷ B. Bedersen, J. M. Hammer, and H. Malamud, New York University College of Engineering Research Division Technical Report No. 2, Electron Scattering Project, 1958 (unpublished).

⁸ R. Brackmann, W. Fite, and R. Neynaber, Phys. Rev. **112**, 1157 (1958).

TABLE I. Scattering amplitudes and maximum widths in the angular distribution for various values of incoming electron momentum $\hbar k$. Subscripts B and F refer to use of experimental cross sections due to Bederson and Fite (Fig. 2) below 13 ev. Cross sections used above 13 ev are indicated in Fig. 3 by the solid line.

ka_0	0.1	0.5	0.7	0.8	0.9	1.0	1.5	2	3	6
$E(\text{ev})$	0.14	3.4	6.7	8.7	11	13.6	30.6	54	120	500
$(f-\frac{1}{2}g)_{\text{Born}}$	-2	0	0.6	0.75	0.83	0.9	1	1	1	1
$\text{Im}(f-\frac{1}{2}g)_{\text{B}}$	0.6	3.5	2.0	1.2	0.8	0.4	0.35	0.5	0.5	0.3
$\text{Re}(f-\frac{1}{2}g)_{\text{B}}$	3.7	2.4	-0.8	-1.1	...	1.0	2.2	2.2	1.8	1.2
$\text{Im}(f-\frac{1}{2}g)_{\text{F}}$	0.44	0.52	0.42	0.4	0.4	0.4	0.35	0.5	0.5	0.3
$\text{Re}(f-\frac{1}{2}g)_{\text{F}}$	-1.5	1.2	2.5	2.8	2.8	2.8	2.8	2.5	1.97	1.2
$\langle\theta\rangle_{\text{B}}$	80°	80°	102°	100°	180+°	72°	26°			
$\langle\theta\rangle_{\text{F}}$	180+°	110°	35°	30°	28°	26°	20°			

Equation (28) is useful only at energies E where f_{Born} is expected to be a good approximation, at which energies a deviation of $(f-f_{\text{Born}})/f_{\text{Born}}$ from unity would be meaningful. Table I shows that at energies above 50 volts there is no significant difference between $\text{Re}(f-\frac{1}{2}g)_{\text{B}}$ and $\text{Re}(f-\frac{1}{2}g)_{\text{F}}$; both these amplitudes rapidly approach the Born value of unity as the energy is increased. Since the differences between the measured σ_{F} and σ_{B} are very large, it appears that Eq. (28) is not useful for evaluating low-energy data, although it may be able to check measurements at higher energies. The computed values of $\langle\theta\rangle$ do have some interesting features. In particular $\langle\Delta\Omega\rangle_{\text{B}}$ becomes very large ($>4\pi$) at an energy near 13.6 ev, and then rapidly decreases to a value corresponding to $\langle\theta\rangle_{\text{B}}\cong 26^\circ$ at $E=30$ ev; on the other hand $\langle\theta\rangle_{\text{F}}$ decreases smoothly as the energy increases. Now Eq. (32) is an inequality instead of an equality only because $\frac{3}{4}|g|^2$ was neglected, and $|g|_{\text{Born}^2}$ is quite negligible at $k=1$ (as can be inferred from $(f-\frac{1}{2}g)_{\text{Born}}$ in Table I). We infer: if experiment F is correct the elastic scattering angular distribution should change smoothly with energy; if experiment B is correct the angular distribution must be very broad and may even peak sideways in a narrow range of energies near 13.6 ev.

It is important to note that these distinctly different predicted features of the angular distributions consistent with experiments F and B are not altered by small changes in σ_{F} and σ_{B} . Instead very severe changes are required; so angular distribution measurements really can confirm or contradict the qualitative correctness, within reasonable experimental error, or experiments F or B. As can be seen from Table I and Eq. (32), the larger $\langle\Delta\Omega\rangle_{\text{B}}$ in the range $k=0.5$ to 1.0, and especially the feature that the angular distribution is a rapid function of energy in a narrow energy band, occur mainly because in the range $0.5\leq k\leq 1.0$ $\text{Re}(f-\frac{1}{2}g)_{\text{B}}$ changes sign and is smaller in absolute magnitude than $\text{Re}(f-\frac{1}{2}g)_{\text{F}}$. In turn these negative values of $\text{Re}(f-\frac{1}{2}g)_{\text{B}}$ occur because σ_{B} has a so much larger negative slope than σ_{F} in $0.5\leq k\leq 1.0$; without drastic reduction in the magnitude of the slope, these negative $\text{Re}(f-\frac{1}{2}g)_{\text{B}}$ cannot be eliminated. For instance, if Bederson's curve in Fig. 2 is retained for $k\geq 0.62$, but is reduced to the constant value $\sigma=50\pi a_0^2$ for

$0\leq k\leq 0.62$, then at $k=0.8$ $\text{Re}(f-\frac{1}{2}g)_{\text{B}}$ in Table I is increased only to -0.5 . We also observe that $\langle\theta\rangle_{\text{F}}$ are rather smaller than one might expect in the energy range 7-13 ev, although sharp low-energy forward peaking, supposedly resulting from polarization of the atom by the incident electron, has been observed in electron scattering from He and other atoms.⁹ These small $\langle\theta\rangle_{\text{F}}$ would be increased by increasing σ_{F} , as comparison of $\langle\theta\rangle_{\text{F}}$ and $\langle\theta\rangle_{\text{B}}$ shows. In this connection it is of interest that experiment F measured the scattering into a cone of restricted angle centered at polar angle $\theta=90^\circ$. The total cross section inferred from this experiment depends therefore on assumptions concerning the angular distribution, as Fite et al.⁸ themselves point out; the distributions they assume are considerably broader than those deduced here. If they had assumed somewhat sharper angular distributions they would have inferred larger total cross sections than they did, though certainly not as large as Bedersen's.

In computing Table I certain approximations have been made, whose effects must be discussed. These approximations are: (i) extrapolation of the measured cross sections to zero energy and to higher energies, so as to make possible computation of the integral; (ii) the use of approximate H^- wave functions in computing the residue; (iii) the neglect of all H^- bound states other than the ground state. The low-energy end point $80\pi a_0^2$ employed to compute Table I was chosen because it seemed consistent with the low-energy trends of the measurements and with theoretical estimates of this end point.^{10,11} Changing this end point from $80\pi a_0^2$ to $60\pi a_0^2$ changes the tabulated values of Table I by at most a few percent.¹² The total cross sections σ_t above ten volts were extrapolated so as to join smoothly with Born approximation calculations¹³

⁹ H. S. W. Massey and E. H. S. Burhop, *Electronic and Ionic Impact Phenomena* (Clarendon Press, Oxford, 1956), Chap. III.

¹⁰ S. Borowitz and H. Greenberg, *Phys. Rev.* **108**, 716 (1957).

¹¹ M. J. Seaton, *Proc. Roy. Soc. (London)* **A241**, 522 (1957).

¹² Note added in proof. L. Rosenberg, L. Spruch, and T. F. O'Malley, *Phys. Rev.* **118**, 184 (1960), obtained an upper bound on the end point even lower than $60\pi a_0^2$, but using this lower value of the zero energy σ would not modify our conclusions in any significant way. The dispersion integral at intermediate energies is quite insensitive to the values of σ near zero energy.

¹³ Reference 9, p. 178.

TABLE II. Effect on the dispersion integral I , and the maximum angular width (θ) of changing extrapolated cross sections above 13 ev. Subscripts B and F refer to the use of cross sections below 13 ev due to Bederson and Fite. Subscripts σ_1 , σ_2 refer to cross sections above 13 ev in Fig. 3. For comparison, the residue $\frac{1}{2}R$ is also shown.

k	0.1	0.5	0.7	0.8	0.9	1.0	1.5
E	0.14	3.4	6.7	8.7	11	13.6	30.6
I_F	5.1	2.5	2.4	2.45	2.3	2.2	2.0
I_B	10.3	3.7	-0.9	-1.45	-0.48	0.4	1.4
$I(\sigma_1) - I(\sigma)$	0.5	0.5	0.4	0.3	0.5	0.7	0.4
$I(\sigma_2) - I(\sigma)$	-0.2	-0.2	-0.4	-0.4	-0.5	-0.8	-0.6
$\frac{1}{2}R$	4.6	1.3	0.5	0.4	0.35	0.3	0.2
$\langle\theta\rangle_B$ spread	90°-70°	80°-70°	95°-115°	80°-120°	180+°	180+°-35°	37°-20°
$\langle\theta\rangle_F$ spread	180+°	130°-70°	48°-31°	33°-29°	32°-25°	34°-21°	25°-17°

of the elastic, excitation, and ionization cross sections; the extrapolations employed are shown in Fig. 3 (solid line). Figure 3 also shows two reasonable alternative extrapolations (dashed lines), based on the assumption that Born approximation is accurate above 500 volts. Table II lists: the dispersion integral, namely the second term on the right side of Eq. (27), computed for σ_F and σ_B using the intermediate solid line extrapolation of Fig. 3; the changes (the same for F and B) in the integral produced by using the upper (1) or lower (2) extrapolations; $\frac{1}{2}R$ (the same for F and B); and the spread in the computed $\langle\theta\rangle$ which, for F and B, result from using extrapolated cross sections in the range between curves 1 and 2 of Fig. 3. The quantities $\frac{1}{2}R$ and the integral are in units of a_0 . Comparing Tables I and II, it appears that reasonable alternative extrapolations of the measured cross sections would not qualitatively modify the discussion of the previous paragraph. Table II suggests that once the total cross section at low energies is known accurately, the measured angular distributions at low energies can indicate whether the total cross sections at higher energies lie above or below the Born approximation. Sharper angular distributions would be consistent with larger high energy cross sections when

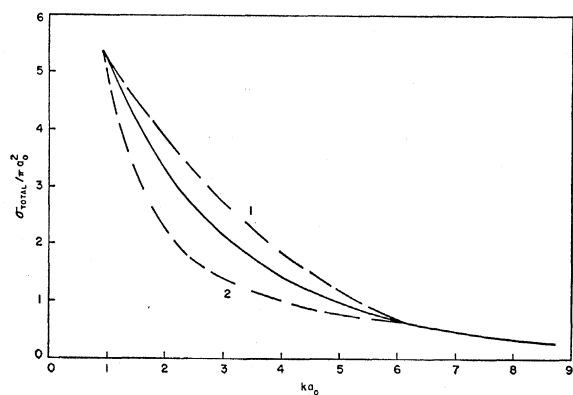


FIG. 3. Extrapolated cross sections for energies above 13 ev. The solid line indicates values used to compute Table I. The broken lines indicate alternate extrapolations. The effect of these changes is indicated in Table II. These values represent total (elastic and inelastic) cross sections for electrons on hydrogen.

(as is usually the case in Table I) $\text{Re}(f - \frac{1}{2}g)$ is computed to be positive.

The residue R was calculated analytically using H^- wave functions of the type discussed by Geltman.¹⁴ The residue could be changed as much as 20% by drastic alteration of the H^- wave function, e.g., by using an unsymmetrized product wave function of the form

$$w(r_1, r_2) = e^{-r_1/a_0} e^{-\alpha r_2}, \quad (33)$$

where α is defined by Eq. (19) for the ground state. Except at the very lowest energies, and except where $\text{Re}(f - \frac{1}{2}g)$ is close to zero, as in case B near $k=0.9$, this change in R makes only a few percent change in the values of Table I; near $k=0.9$ this change in R slightly shifts the energy where $\langle\Delta\Omega\rangle_B$ becomes larger than 4π , but does not otherwise qualitatively modify the energy dependence of θ_B and θ_F .

The question of the existence of other bound states of H^- is a knotty one. There is no experimental evidence for such states, but if additional positive electron affinity bound states ($E_j < 0$) occur, they make the computed $\text{Re}(f - \frac{1}{2}g)$ in Table I more negative. This is so because every R_{oj} is positive, Eq. (21), and because Eqs. (17) and (22) imply that singlet bound states j add $\frac{1}{2}R_{oj}$ to the $\frac{1}{2}R$ in Eq. (27), while triplet bound states add $\frac{3}{2}R_{oj}$. It follows that such additional bound states would not alter the qualitative feature that $\langle\Delta\Omega\rangle_B$ becomes very large and then small at same energy < 13.6 ev, but would tend to increase θ_F , i.e., would make Fite's cross sections consistent with broader angular distributions than indicated in Table I. Any large effect would require a large number of bound states.

There remains the possibility that there exist bound states of H^- with negative electron affinity ($E_j > 0$), which for some reason do not autoionize,¹⁵ as in the well-known $\text{He}^- \ ^4P_{\frac{1}{2}}$ state¹⁶; if the states autoionize they are not bound, do not correspond to real energies E_j , and therefore cannot have poles in the complex energy plane defined by the aforementioned assumptions (i) to (iv), wherein the Green's function is

¹⁴ S. Geltman, Phys. Rev. **104**, 346 (1956).

¹⁵ E. Holøien, J. Chem. Phys. **29**, 676 (1958).

¹⁶ E. Holøien, Proc. Phys. Soc. (London) **71**, 357 (1958).

presumed to be the inverse of a Hermitian (real eigenvalues) operator. Nonautoionizing states with $E_j > 0$ have poles on the branch cut and could modify the conclusions which have been drawn, since for such states the sign of $E - E_j$ appearing in Eq. (21) need not be positive. It can be proved however that for such states the integrals appearing in Eq. (20) necessarily vanish [note α_j is now imaginary, equals ik_j , where k_j is defined in terms of E_j by Eq. (14)]. Consequently such nonautoionizing states cannot contribute to the dispersion relations.

V. CONCLUSIONS

In the light of the foregoing discussion the following assertions seem justified. If experiment F is taken to be correct the angular distribution should change smoothly with energy, and must be considerably peaked at low energies. If experiment B is correct, the angular distribution must change rapidly from a very broad or even sideways peaked shape to a highly forward peaked distribution, in a narrow range of

energies near 13.6 ev. Dispersion relations are not able to rule out either experiment B or F, but do suggest the experiment which will distinguish between them, namely: angular distribution measurements at low energies. A closer distinction would be possible if there were more accurate measurements of the total cross sections at high energies, which would obviate the need for extrapolations and increase the reliability of the computed dispersion integral. Direct information on combinations of f and g other than $f - \frac{1}{2}g$, e.g., direct measurement of $|g|^2$ by polarized atomic beam techniques,¹⁷ also would be helpful.

ACKNOWLEDGMENTS

We are indebted to E. Sobolak and Dr. R. Drisko for pointing out an important error in a preprint of this paper. Correction of this error greatly modifies assertions made previously.¹⁸

¹⁷ K. Rubin, J. Perel, and B. Bederson, *Phys. Rev.* **117**, 151 (1960).

¹⁸ N. A. Krall and E. Gerjuoy, *Bull. Am. Phys. Soc. Ser. II*, **5**, 119 (1960).

Cross Section for Formation of Doubly-Ionized Helium by Electron Impact*

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The cross section for the formation of He^{++} by electron impact has been measured relative to that of He^+ for electron energies between 100 ev and 2400 ev. A relative minimum in the measured ratio of the yields of He^+ to He^{++} at an energy of about 600 ev is believed to be real. For incident energies above 1400 ev the results are consistent with a constant value of 145 for this ratio.

INTRODUCTION

THE cross section for ionization of helium by electron impact has been measured by Smith¹ for electron energies between the appearance potential and about 4000 ev. Since the quantity actually measured by Smith is the ratio of positive-ion current produced in the helium gas to the current of the penetrating electrons, it is necessary to know the fraction of the positive current associated with each type of ion, He^+ and He^{++} , in order to deduce the cross sections Q_i and Q_{ii} for single and double ionization, respectively. Apparently the only measurement of this ratio is that reported in 1936 by Bleakney and Smith.² These latter authors measured the relative yield of doubly-charged helium ions for a range of incident electron energies

from 100 ev to 500 ev. In order to relate these measurements to an absolute cross section, they measured the ratio of the yields of He^+ to He^{++} at an energy of 300 ev.

The only theoretical calculation pertaining to the process of double ionization in helium seems to be Ninti's³ estimate of an upper limit for the sum of oscillator strengths for simultaneous excitation or ionization involving both electrons. As pointed out by Miller,⁴ a value of the oscillator strength for double excitation of the order of magnitude of Ninti's estimate would indicate that double excitations play a considerable role in many processes, particularly those that depend sensitively on the energy transfer between initial and final states.

In this paper are described the results of measurements of the ratio of yields of He^+ and He^{++} for electron energies between 100 ev and 2400 ev. One problem considered for these measurements at higher energies

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¹ P. T. Smith, *Phys. Rev.* **36**, 1292 (1930). Experimental points determined by W. Hanle and D. Riede, *Z. Physik* **133**, 537 (1952) are included in Fig. 1.

² W. Bleakney and L. Smith, *Phys. Rev.* **49**, 402 (1936).

³ J. P. Ninti, *Phys. Rev.* **42**, 632 (1932).

⁴ William F. Miller, Ph.D. thesis, Purdue University, January, 1956 (unpublished).