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A PREFACE TO THE NONADIABATIC THEORY OF ELECTRON—HYDROGEN IONIZATION

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A PREFACE TO THE NONADIABATIC THEORY OF ELECTRON-HYDROGEN IONIZATION

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Some preliminary considerations of the nonadiabatic theory of e-H ionization are given. The zeroth order problem is shown to give rise to an $E^{\frac{3}{2}}$ threshold law. The stationary phase result for the asymptotic form of the zeroth order problem is shown to lead to a complete suppression of S-wave ionization events in which the energies of the scattered and ejected electron are equal. Extending the stationary phase results to our conjectured asymptotic form for the complete S-wave problem leads to an even greater suppression in the neighborhood of equal energy events. The combination of such an S-wave cross section together with reasonable higher partial wave cross sections yields a qualitative understanding of experimental ionization energy loss measurements in helium.

I INTRODUCTION

In this report, we continue to examine the very difficult problem of electron-hydrogen ionization from the point of view of the nonadiabatic theory[1]. In a previous note some preliminary results and observations were stated[2] (which were at variance with previous analyses of this problem[3]), which we shall attempt to quantify and amplify here. We shall continue to deal with total S-wave scattering.

Section II deals with the explicit demonstration of the $E^{\frac{3}{2}}$ threshold law for the zeroth order problem[2]. In section III we derive some of the salient physical consequences of the stationary phase integration for the closed form of the zeroth order ionization part of the wave function and extend the analysis to our conjectured asymptotic form for the complete S-wave problem.

The final section discusses these results and how they may elucidate experimental results of the energy spectrum of electrons emerging from electron-helium ionization. Additional arguments are given for expecting a nonlinear threshold in the electron-atom ionization yield curve.

For purposes of convenience, the main formulae of the nonadiabatic theory[1] are given here.

$$\left[\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}} + \frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}} + E\right]$$

$$\Psi(r_1, r_2, \theta_{12}) = 0 , \qquad (1.1)$$

$$\Psi = \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} \; \Phi_\ell \,(r_1, r_2)\, P_\ell\, (\cos \Theta_{12}) \;, \tag{1.2}$$

$$\left[\frac{\partial^2}{\partial r_1{}^2} + \frac{\partial^2}{\partial r_2{}^2} - \ell(\ell+1)\left(\frac{1}{r_1{}^2} + \frac{1}{r_2{}^2}\right) + \frac{2}{r_1} + \frac{2}{r_2} - M_{\ell\ell}\right] \Phi_\ell = \sum_{m=0}^{\infty} M_{\ell m}\, \Phi_m \;, \tag{1.3}$$

$$M_{\ell m} = \sqrt{(2\ell+1)(2m+1)} \sum_{n=0}^{\ell+m} \frac{r_<^n}{r_>^{n+1}} \; A_{\ell mn} \;, \tag{1.4}$$

$$A_{\ell mn} = \int_0^\pi P_\ell \, P_m \, P_n \, \sin\theta_{12} \, d\theta_{12} = \frac{2}{(2n+1)} \, (\ell moo/no)^2 \quad . \tag{1.5}$$

Ψ is $r_1 \, r_2$ times the S-wave function. Eq. (1.1) is the S-wave equation (energies in rydbergs, lengths in Bohr radii); Eq. (1.2) defines the basic expansion; Eqs. (1.3) are the coupled set of equations corresponding to (1.1). Eqs. (1.4) and (1.5) define the quantities occurring in (1.3). The symbol $(\ell moo/no)$ is a Clebsch-Gordan coefficient.

II THE ZEROTH ORDER PROBLEM

This problem is defined by neglecting the terms on the rhs of (1.3) for $\ell = 0$. In the region $r_1 \geq r_2$, this becomes:

$$\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r^2} + E\right) \Phi_o^{(o)} (r_1, r_2) = 0 \tag{2.1}$$

Expanding the solution in exact separable solutions, assuming $E \leq 0$, yields

$$\Phi_o^{(o)} = \frac{A \sin k_1 r_1}{k_1} R_{1s} (r_2) + \sum_{n=1}^{n_{max}} C_n e^{ik_n r_1} R_{ns} (r_2)$$

$$+ \sum_{n_{max}}^{\infty} C_n e^{-\kappa_n r_1} R_{ns}(r_2) + \int_0^{\infty} C(\kappa_2) e^{-\kappa_2 r_1} F_{\kappa_1}(r_2) d\kappa_2 , \tag{2.2}$$

where

$$E = -\frac{1}{n_<^2} + k_n^2 = -\frac{1}{n_>^2} - \varkappa_n^2 = \varkappa_2^2 - \varkappa_1^2 \tag{2.3}$$

As $E \to o$ from below this reduces to

$$\lim_{E \to o^-} \Phi_o^{(o)} = A \sin r_1 + \sum_{n=1}^{\infty} C_n e^{\frac{1}{n} r_1} R_{ns}(r_2)$$

$$+ \int_o^{\infty} C(\varkappa) e^{-\varkappa r_1} F_\varkappa(r_2) \, d\varkappa \, . \tag{2.4}$$

Consider the triplet case; the boundary condition for $\Phi_o^{(o)}$ is

$$\Phi_o^{(o)}(r_1, r_2) \Big|_{r_1 = r_2 \equiv r} = 0 \tag{2.5}$$

Inserting Eq. (2.4) into (2.5) gives

$$- A \sin r \, R_{1s}(r) = \sum_{n=1}^{\infty} C_n \, e^{\frac{i}{n} r} R_{ns}(r)$$

$$+ \int_0^{\infty} C(q) e^{-qr} F_q(r) \, dq \tag{2.6}$$

The normalized radial functions are given by

$$R_{ns}(r) = \frac{2r}{n^{\frac{3}{2}}} e^{-r/n} F\left(1-n;\ 2;\ \frac{2r}{n}\right) , \tag{2.7a}$$

$$F_q(r) = 2rq^{\frac{3}{2}} e^{-iqr} F\left(1 + \frac{i}{q}\ ;\ 2;\ 2iqr\right) , \tag{2.7b}$$

where F(a, b, c) is the confluent hypergeometric function. Expanding both sides of (2.6) as a power series in r and demanding that the equation be an identity in r, we find that the first two terms give rise to the equations

$$\sum_{n=1}^{\infty} \frac{C_n}{n^{\frac{3}{2}}} = - \int_0^{\infty} C(q)\, q^{\frac{3}{2}}\, dq \qquad (2.8a)$$

$$A = - i \sum \frac{C_n}{n^{\frac{5}{2}}} + \int_0^{\infty} C\,(q)\, q^{\frac{5}{2}}\, dq \quad , \qquad (2.9)$$

where (2.8) has been used to simplify (2.9). Let us now invoke the conservation of current (in the limit $k_n \to \frac{i}{n}$) :

$$\mathcal{I}\,(A^*C_1) = \sum_{n=1}^{\infty} \frac{1}{n} |C_n|^2 \qquad (2.10)$$

Substituting (2.9) into (2.10) we arrive at

$$\mathcal{R}(C_1)\sum_{n=1}^{\infty}\frac{\mathcal{R}(C_n)}{n^{\frac{5}{2}}}+\mathcal{I}(C_1)\sum_{n=1}^{\infty}\frac{\mathcal{I}(C_n)}{n^{\frac{5}{2}}}$$

$$=\sum_{n=1}^{\infty}\frac{1}{n}|C_n|^2+\mathcal{R}(C_1)\int\mathcal{I}\;(C(q))\;q^{\frac{5}{2}}\,dq-\mathcal{I}(C_1)\int\mathcal{R}\;(C(q))q^{\frac{5}{2}}dq \quad (2.11)$$

If we assume that C_n is of the form

$$C_n = C_1/n^{\mu}\ , \qquad (2.12)$$

then (2.11) reduces to an identity when

$$\tfrac{5}{2}+\mu=2\mu+1\ (\Rightarrow\mu=\tfrac{3}{2})$$

providing

$$\mathcal{R}(C_1)\int\mathcal{I}\;(C(q))\;q^{\frac{5}{2}}\,dq=\mathcal{I}(C_1)\int\mathcal{R}\;(C(q))\;q^{\frac{5}{2}}\,dq \qquad (2.13)$$

Thus

$$C_n = \frac{C_1}{n^{\frac{3}{2}}} \tag{2.14}$$

satisfies the boundary condition to second order and is consistent with the conservation of current.

The additional requirement (2.8a) provides no obstacle to C_n being continuously extendable to $C(q)$. If, for example, we assume

$$C(q) = - C_1 \, e^{-\gamma q} \, q^{\frac{3}{2}} \quad , \tag{2.15a}$$

then (2.8) is satisfied by a reasonable choice of γ:

$$\gamma = [6/\xi(3)]^{\frac{1}{4}} \quad ,$$

where $\xi(3) = 1.202057$ is the Riemann zeta function. We have also examined the effect of satisfying the boundary condition to the next higher power in r. It turns out that all the previous equations can still be maintained and that one has one additional requirement to satisfy:

$$\sum_{n=1}^{\infty} \frac{C_n}{n^{\frac{7}{2}}} = \int q^{\frac{7}{2}} C_{(q)} \, dq \tag{2.8b}$$

Thus (2.12) still provides a consistent solution, but (2.15a) must be generalized to a two parameter extension in order that both (2.8a) and (2.8b) be satisfied. For instance the form

$$C(q) = -C_1 \, e^{-\gamma_1 q} \left(q^{\frac{3}{2}} + b \, q^{\frac{7}{2}} \right) \tag{2.15b}$$

can fulfill both equations.

The fact that we have demonstrated that (2.14) provides a consistent solution is not a proof that it is correct. Eq. (2.11) could be satisfied by not requiring the sum and integral parts be separately equal. We suspect, in fact, that the true solution is of this latter variety. The present demonstration is really intended to show that one can confidently expect (2.14) to be the first term of an asymptotic series in inverse powers of n, and this is all that is needed to complete the derivation of the $E^{\frac{3}{2}}$ threshold law.

The derivation of the singlet result is closely analogous to the above. The boundary condition is

$$\left.\frac{\partial \Phi_o^{(o)}}{\partial n}\right|_{r_1 = r_2 \equiv r} = 0 , \tag{2.16}$$

and the first two boundary condition equations are (2.8a) plus

$$A = \sum_{n=1}^{\infty} C_n \left(- \frac{i}{n^{\frac{5}{2}}} + \frac{1}{n^{\frac{7}{2}}} \right) + \int_0^{\infty} C(q)(q^{\frac{5}{2}} - q^{\frac{7}{2}})\, dq . \tag{2.17}$$

Substituting this into the conservation of current now yields

$$\sum_{n=1}\left[\left(\frac{\mathcal{R}(c_n)}{n^{\frac{5}{2}}}-\frac{\mathcal{I}(c_n)}{n^{\frac{7}{2}}}\right)\mathcal{R}(c_1)+\left(\frac{\mathcal{I}(c_n)}{n^{\frac{5}{2}}}+\frac{\mathcal{R}(c_n)}{n^{\frac{7}{2}}}\right)\mathcal{I}(c_1)\right]$$

$$+\int_0^\infty\left[\mathcal{R}(c(q))\mathcal{I}(c_1)-\mathcal{I}(c(q))\mathcal{R}(c_1)\right](q^{\frac{5}{2}}-q^{\frac{7}{2}})\,dq$$

$$=\sum_{n=1}^{\infty}\frac{1}{n}|c_n|^2 \qquad (2.18)$$

Again this will be satisfied by (2.14) with the auxiliary condition that the q integral in (2.18) be zero.

To show that (2.14) implies an $E^{\frac{3}{2}}$ threshold law we are indebted to K. Omidvar for a simple demonstration.[4] Assume that one is considering excitation to a group of neighboring discrete (s) states for high n. The total cross section is given by

$$Q(E)=\sum_{n=n_1}^{n_2}K_n|c_n|^2 \qquad (2.19)$$

The energies of these states are given by

$$\epsilon_n = -\frac{1}{n^2} \tag{2.20}$$

from which it follows that there are $2n^3 d\epsilon_n$ (s) states in an energy range $d\epsilon_n$. Converting (2.19) to an integral

$$Q(E) \propto \int k_n \left|C_n\right|^2 n^3 d\epsilon_n , \tag{2.21}$$

continuing n into the continuum whereby

$$k_n = \sqrt{E-\epsilon_n} , \tag{2.22}$$

and using (2.14) for C_n, we obtain

$$Q(E) \propto \int_0^E \sqrt{E-\epsilon_n}\ d\epsilon_n \propto E^{\frac{3}{2}} . \tag{2.23}$$

III STATIONARY PHASE RESULTS AND THEIR PHYSICAL IMPLICATIONS

Contrary to what was stated in Ref. 2, the stationary phase result can be made to satisfy Kato's theorem, and therefore it may represent the correct asymptotic form of the zeroth order problem[5]. Explicitly for $E > 0$ the separable solutions of (2.1) which do not vanish in the ionization region are $(q_1{}^2 + q_2{}^2 = E)$:

$$\lim_{r_1 > r_2 \to \infty} \Phi_0{}^{(o)} = \int_0^{\sqrt{E}} C(q_2)\, e^{iq_1 r_1}\, F_{q_2}(r_2)\, dq_2 \tag{3.1}$$

Stationary phase now gives for this integral

$$\lim_{r_1 > r_2 \to \infty} \Phi_0{}^{(o)} = \frac{f_0(\alpha)}{\rho^{\frac{1}{2}}}\, e^{\,i\{\sqrt{E}\,\rho + \frac{W_0(\alpha)}{\sqrt{E}} \ln (2\sqrt{E}\,\rho)\}}, \tag{3.2}$$

where

$$W_0(\alpha) = \begin{cases} 1/\sin\alpha & r_1 > r_2 \\ 1/\cos\alpha & r_1 < r_2 . \end{cases}$$

The requirement of Kato's theorem (which is this case reduces to the continuity of $\Phi_0{}^{(o)}$ and its first derivative at $\alpha = \pi/4$) is

$$f_0(\alpha)\Big|_{\alpha=\frac{\pi}{4}} = \frac{\partial f_0(\alpha)}{\partial\alpha}\Big|_{\alpha=\frac{\pi}{4}} = 0 \tag{3.3}$$

Higher derivatives may have cusps. Likewise the assumption made for the asymptotic form of the complete S-wave function[2] leads under stationary phase to

$$\lim_{r_1,r_2\to\infty} \Psi = \frac{f(\alpha,\theta_{12})}{\rho^{\frac{5}{2}}} e^{i\left\{\sqrt{E}\,\rho + \frac{W_0(\alpha)}{\sqrt{E}} \ln(2\sqrt{E}\,\rho)\right\}} \tag{3.4}$$

In the full S-wave case the validity of this result is very uncertain, because it requires a factorization of the exponential part through an infinite sum of relative partial wave terms. However, if the expansion is not suitably convergent in relative partial waves or if the regions in which the asymptotic forms for the relative partial waves become valid differ sufficiently among themselves, it may be that such a factorization is not justified. Assuming it to be alright, then since $W_0(\alpha)$ has a cusp at $\alpha = \frac{\pi}{4}$ for any value of θ_{12}, whereas the true potential is completely continuous at $\alpha = \frac{\pi}{4}$ $(\theta_{12} \neq 0)$, it follows that the $f(\alpha, \theta_{12})$ and all its derivatives (with respect to α) must be zero at $\alpha = \frac{\pi}{4}$. Nonzero functions of this kind can be constructed. For example,

$$f(\alpha, \theta_{12}) = g(\theta_{12}) \exp\left[- c/(1 - \gamma)\right] \tag{3.5}$$

where

$$\gamma = \frac{r_<}{r_>} = \begin{cases} \tan \alpha & \alpha < \frac{\pi}{4} \\ \cot \alpha & \alpha > \frac{\pi}{4} \end{cases} \tag{3.6a}$$

The analyticity at $\alpha = \frac{\pi}{4}$ puts severe restrictions on the velocity distribution of the ionized particles. In the ionization cross section the quantity γ is replaced by

$$\gamma \to \frac{k_<}{k_>} \tag{3.6b}$$

where $k_<$ and $k_>$ are the lesser and greater of k_1 and k_2. It is convenient in exploring the physical consequences of (3.6) to work in terms $\sigma(\epsilon)$, the cross section for one of the electrons to appear with energy ϵ. Such a curve for a fixed available energy E must clearly be symmetric about $\frac{E}{2}$, thus

$$Q = \int_0^E \sigma(\epsilon)\, d\epsilon = 2 \int_0^{\frac{E}{2}} \sigma(\epsilon)\, d\epsilon \tag{3.7}$$

The quantity $\sigma(\epsilon)$ is related to f by

$$\sigma(\epsilon) = |f|^2 \begin{cases} \sqrt{E-\epsilon} & \epsilon < \frac{E}{2} \\ \sqrt{E} & \epsilon > \frac{E}{2} \end{cases} \tag{3.8}$$

In this way both $\sigma(\epsilon)$ and f are symmetric about $\frac{E}{2}$ (and as long as f depends on γ and not E this gives rise to an $E^{\frac{3}{2}}$ threshold law). Although the square root factor in (3.8) is essential to the threshold law, it has no important effect on the shape of σ as a function of ϵ. In Fig. 1 we have suppressed the square root factor and have plotted $(\epsilon \leq \frac{E}{2})$

$$\sigma_S(\epsilon) = e^{-c/(1-\frac{2\epsilon}{E})} \tag{3.9}$$

for various choices of c. The normalization of $\sigma_S(\epsilon)$ is chosen so that $\sigma_S(0) = 1$.

IV DISCUSSION

The primary observation to be made from Fig. 1 is that the region of momentum space in which the two outgoing particles have equal speeds is highly suppressed. This is an obvious consequence of the zeroth order problem in which any correlations which could be otherwise taken up in Θ_{12} are eliminated in the definition of the model (thus all correlations are necessarily in relative energies only). It is an interesting consequence of the full S-wave problem with the asymptotic form of Eq. (3.4) that this suppression is enhanced! Such an unexpected consequence might in fact be used to argue against Eq. (3.4) (and we do not think that (3.4) can rigourously be correct) and possibly against the asymptotic form (15) of Ref. 2. However, in the absence of a definitive analysis, it is worthwhile to be guided as much as much as possible by experiment.

Before doing this, let us note that distributions of Fig. 1 are directly opposite to what one would expect from phase space. For phase space is proportional to $[\epsilon(E-\epsilon)]^{\frac{1}{2}}$ which has its maximum at $\epsilon = \frac{E}{2}$ and is zero at the end points.

In Fig. 2 we have plotted the energy loss cross section, $\sigma(\epsilon)$, for S-wave together with assumed P and D waves cross sections. The experiment that is envisioned here is one in which one of the emerging particles in the ionization process is observed with energy ϵ in the forward direction relative to an incoming beam of energy $k^2 = E + I_H$; I_H being the binding energy of ejected electrons in the atom. The energy of the second particle is therefore $E - \epsilon$, and the experiment automatically averages over the directions of the second particle relative to the first (Θ_{12}). The S-wave is independent of the angle of observation relative to the direction of the incoming beam, therefore it is necessarily symmetric in ϵ about $\frac{E}{2}$ for any angle of observation. This is not so for higher partial waves in which cases only the integrated cross sections over all angles of observation is symmetric in ϵ. Appendix I contains a brief analysis of the P wave. For zero angle of observation the higher partial cross sections are drawn as increasing function of ϵ corresponding to the simple physical expectation that the more energetic the collision products, the more in the forward direction they should emerge. In the Appendix it is shown why the P wave, however, must decrease for ϵ near its maximum value of E. The curve representing the sum of these partial cross sections is in qualitative accord with preliminary experimental results of Heideman[7], for the case of electron-helium ionization.

The above experiment is not at low enough energies, as compared with that of McGowan et al.[8], to establish the form of the threshold energy dependence of the ionization cross section. Rather it serves to illustrate the primary correlation of the two outgoing particles as an anticorrelation in the available energy. However, this correlation itself can be quite significant in determining the form of the threshold law. To illustrate this point, let us note that when we say that in elastic scattering the scattered electron is completely shielded from the nucleus we do not mean

$$\lim_{r_1 \to \infty} \Psi = \sin (kr_1 + \delta) R_{1s} (r_2) \tag{4.1}$$

<u>for all values of r_2</u>. In particular it is probably incorrect as $r_2 \to r_1$, but that makes no difference, since the wave function itself vanishes in the joint limit. In the case of ionization, the region $r_1 \cong r_2 \to \infty$ is not energetically disallowed, however, it may be dynamically unfavored to the extent of providing complete shielding for the outer particle. That is what, in effect, we have been arguing happens.

In addition to the dynamical effects that we have already discussed, there are additional effects which we believe should strengthen the cogency of the concept of shielding. It has been customary in dealing with this problem to divide the asymptotic region into a reaction zone and an emerging zone or zones[9]. This implies that the phenomenon or ionization takes place fairly close to the nucleus and that as the particles emerge their "orbits" change relatively slowly as a result of the asymptotic interactions. However, at any distance from the nucleus there are bound orbits, and it always is possible that the inner particle, in particular, as it emerges can get caught in a bound state. If such transitions can occur into high bound states, they can also occur to states of lower continuum energy also. Thus the combination of possibilities can only serve to separate further the energies of the emergent particles, and to lower the absolute ionization cross section as a function of energy relative to elastic and inelastic events. Near threshold this is an additional argument for a nonlinear (concave up) dependence.

APPENDIX

We give here a brief outline of the analysis of P-wave ionization. Let Θ_B, Φ_B be the spherical angles of an observed electron in an ionization event relative to a fixed coordinate system whose z-axis in the direction of the incoming electron. The P-wave function can be written[10]

$$\Psi_P = \cos\Theta_{12}\,[f_P + \cos\Theta_{12}\,\tilde{f}_P]$$

$$+ \sin\Theta_B \cos\Psi_B \sin\Theta_{12}\,\tilde{f}_P\ , \tag{A1}$$

where for purposes of computing the ionization amplitude

$$\begin{aligned} f_P &= f_P\,(k_1,\,k_2,\,\Theta_{12}) \\ \tilde{f}_P &= f_P\,(k_2,\,k_1,\,\Theta_{12})\,. \end{aligned} \tag{A2}$$

Ψ_B is angle between k_1-k_2 plane and the z-axis.

Actually the f_P should be multiplied by a function of r_1 and r_2 which gives outoing current for two particles in the directions $\hat{k}_1$, $\hat{k}_2$ respectively. Although there is some discussion as to what this function should be, we shall assume that <u>for higher partial waves</u>, it is not such as to exclude events in which $k_1 = k_2$.

The probability for a given event characterised by the two vectors $\underset{\sim}{k_1}$ and $\underset{\sim}{k_2}$ is the absolute square of Ψ_P. For one electron to be observed in the direction θ_B and the second to be anywhere, we have

$$\sigma_P(\theta_B) = \frac{1}{4\pi} \int \left| \Psi_P(k_1 \; k_2 \; \theta_B \; \Psi_B \theta_{12}) \right|^2 \sin \theta_{12} \, d\,\theta_{12} \, d\Psi_B \; .$$

Special cases:

$$\theta_B = 0$$

$$\sigma_P(0) = \frac{1}{2} \int_0^{\pi} \left(|f_P|^2 + |\tilde{f}_P|^2 \cos^2 \theta_{12} \right) \sin \theta_{12} \, d\theta_{12}$$

$$+ \int_0^{\pi} \mathcal{R} \, [f_P \tilde{f}_P^*] \sin \theta_{12} \, d\theta_{12}$$

$$\theta_B = \frac{\pi}{2}$$

$$\sigma_P\left(\frac{\pi}{2}\right) = \frac{1}{4} \int_0^{\pi} |\tilde{f}_P|^2 \sin^3 \theta_{12} \, d\theta_{12}$$

Note also that $\sigma_P(0) = \sigma_P(\pi)$. Thus if it is unlikely to find a high ϵ (P-wave) particle in the backward direction, then it must also be unlikely to find one in the forward direction. This is the justification for having the P-wave descend rapidly for the higher ϵ as pictured in Fig. 2.

Although the various $\sigma_P(\theta_B)$ cross sections for a given θ_B are not symmetric about $\epsilon = \frac{E}{2}$, we show below that the integrated cross section over all θ_B is symmetric, as it must be, since each ionization event which gives rise to an electron of energy ϵ must also give rise to one of energy $E-\epsilon$ somewhere on the scattering sphere.

Integrating over the whole sphere, we find

$$\int |\Psi_P|^2 \sin\Theta_B \, d\Theta_B \, d\Psi_B \sin\Theta_{12} \, d\Theta_{12}$$

$$\propto \int \left[|f_P|^2 + |\tilde{f}_P|^2 \right] \sin\Theta_{12} \, d\Theta_{12}$$

$$+ \int \mathcal{R} \, (f_P \tilde{f}_P^*) \sin 2\Theta_{12} \, d\Theta_{12}$$

The first integral is, recalling (A_2), obviously symmetric with respect to $k_1 \rightleftarrows k_2$. If one separates f_P and $\tilde{f}_P$ into real and imaginary parts and uses the symmetry under $k_1 \rightleftarrows k_2$ of each part separately, one can see that the second integral is also symmetric.

Finally for higher partial waves a similar analysis can be carried out by using symmetric Euler angles[11] and converting to the Hylleraas-Breit Euler angles (labelled by the subscript B above) via Eqs. (3.1) and (3.2) of Ref. 11.

1. A. Temkin, Phys. Rev. 126, 130 (1962).

2. A. Temkin, Phys. Rev. Letters 16, 835 (1966).

3. R. K. Peterkop, Izv, Akad. Nauk Latv. S.S.R., Riga 9 79 (1960).
M. Rudge and M. J. Seaton, Proc. Roy. Soc. (London), A 283, 262 (1965).

4. cf. however, R. McCarroll, Proc Phys. Soc. 70, 460 (1957).

5. Similarly, the PRS asymptotic (Ref. 3) form can be formally made to obey Kato's theorem at $r_{12} = 0$ by having the amplitude function of $f(\alpha,\theta_{12})$ [cf. Eq. (5) of Ref. 2] and all its derivatives with respect to θ_{12} vanish at $\alpha = \frac{\pi}{4}$, $\theta_{12} = 0$. However, there is another argument one can use to show that that function cannot be correct in the neighborhood of $r_{12} = 0$. For there one may expand the solution in terms of r_{12} and the center of mass coordinate of the two electrons. The dependence on r_{12} is essentially a repulsive Coulomb-wave which vanishes smoothly exponentially as $r_{12} \to 0$, whereas the PRS form would vanish oscillatingly at $r_{12} \to 0$.

6. Cf. the discussion in N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965), pp. 489 et seq.

7. H. G. M. Heideman, Bulletin of the American Phys. Soc. Series II, 10, 455 (1965). I am indebted to Dr. C. Kuyatt for discussions of this experiment. Cf. also M. Goodrich, Phys. Rev. 52, 259 (1937).

8. J. W. McGowan, M. A. Fineman, E. M. Clarke, H. P. Hanson (to be published).

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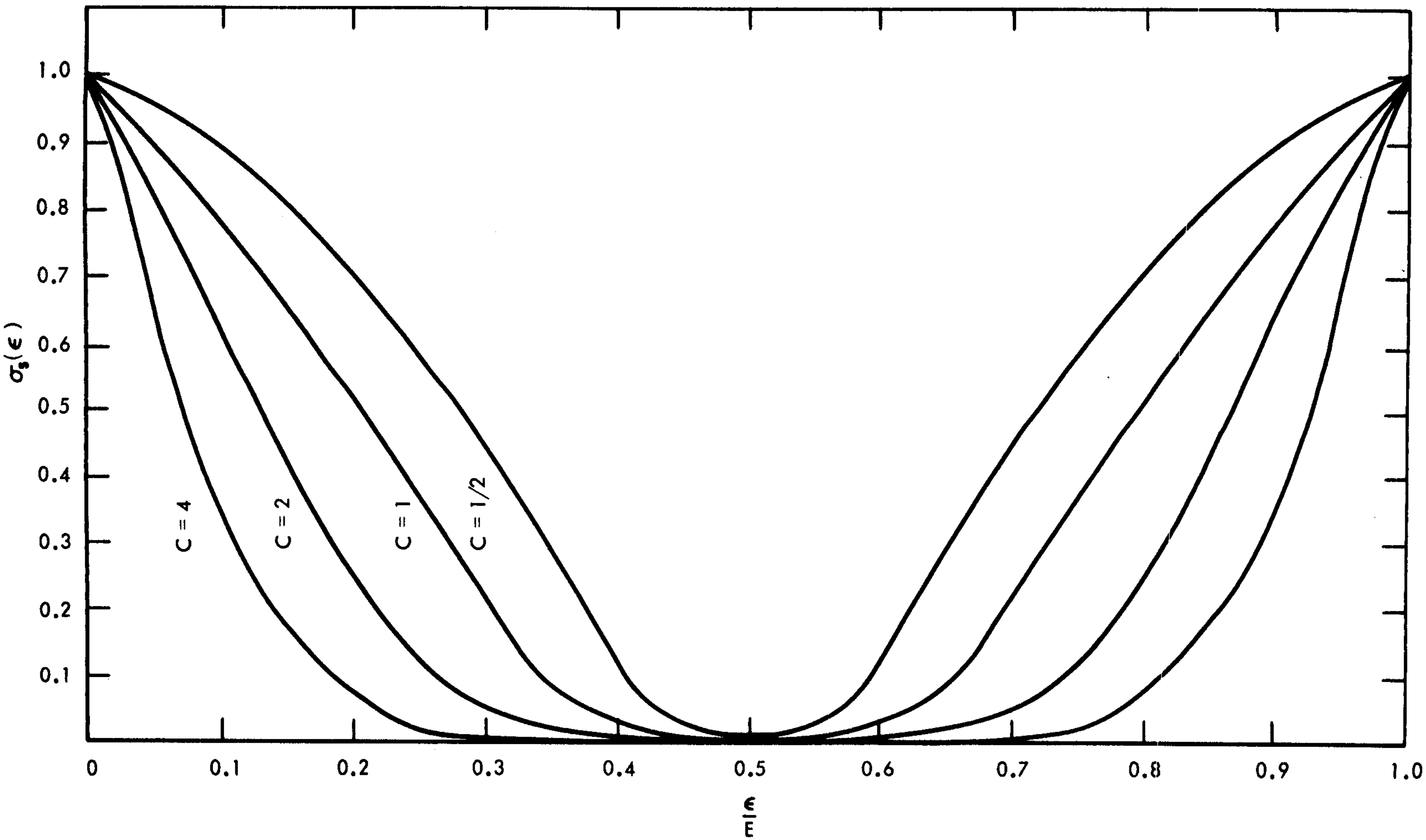
10. G. Briet, Phys. Rev. 35, 569 (1930).

11. A. K. Bhatia and A. Temkin, Rev. Mod. Phys. 36, 1050 (1964).

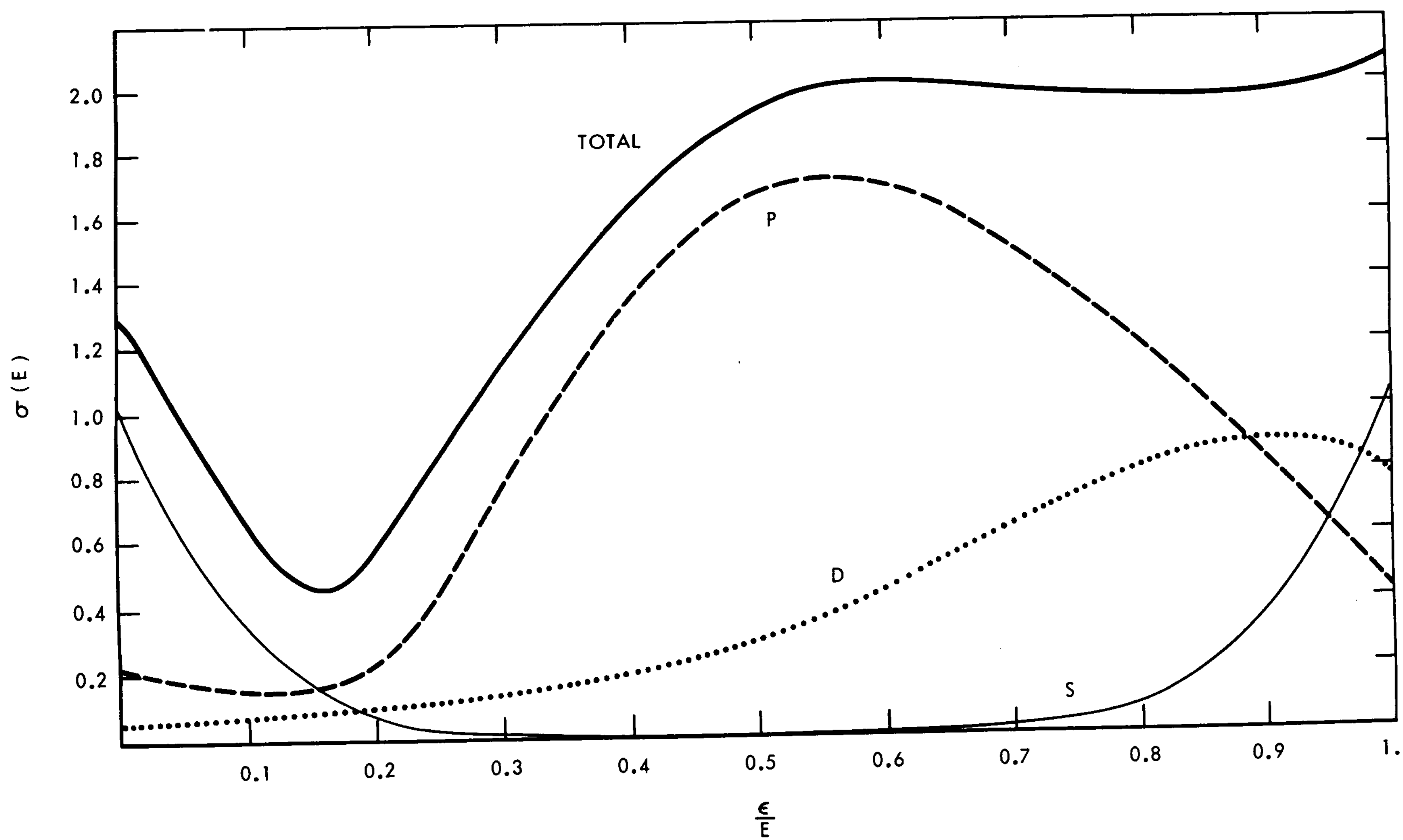
FIGURE CAPTIONS

Fig. 1 S-wave ionization cross sections vs. the residual energy ϵ for a fixed bombarding energy calculated on the basis of Eq. (3.9), for various values of c. The experiment of Heideman (Ref. 7) indicates a large value of c.

Fig. 2 S-wave cross section corresponding to $c = 2$ of Fig. 1. The higher partial waves are supposed to correspond to ionization events in which one of the emerging particles is observed in the forward direction.



$\sigma_s(\epsilon)$
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
C = 4
C = 2
C = 1
C = 1/2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$\frac{\epsilon}{E}$


σ (E)
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
TOTAL
P
D
S
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.
ε/E