approach zero, but in this region the Hartree-Fock value has its greatest departure from the other three. The reason for this is that $F(K)$ approaches N, while the first part of the expression for $NS(K)$ approaches $N+N(N-1)$ because ψ_0 is normalized. Thus the result in this region is obtained as the difference between two nearly equal numbers and can be expected to be quite sensitive to the particular wave function used.

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Electron Detachment of H^- by e^- Collision

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An impact-parameter method using Coulomb trajectories has been used to calculate cross sections for the following two electron-detachment collision processes: (i) $e^- + H^- \rightarrow H(1S) + 2e^-$; (ii) $e^- + H^- \rightarrow H(2S) + 2e^-$. The cross section for process (ii) is found to be approximately two orders of magnitude smaller than that for (i). The results of process (i) are compared with the available experimental data. The plane- and Coulomb-wave cross sections in dipole approximations are calculated both at high and low energies and are compared with the semiclassical results. The asymptotic behavior of the cross sections at high energies is investigated in detail. Energy distributions of ejected electrons at three different incident energies are also calculated.

I. INTRODUCTION

Besides its being of intrinsic interest in the theory of atomic collision, the detachment of electrons from H^- by e^- impact is of importance in certain branches of astrophysics. Consequently, it has been studied both experimentally and theoretically by several authors in the past. In spite of this a number of divergencies prevail both among the theoretical calculations and the experimental observations. Experiments were done independently by Dance *et al.*,[1] by Tisone and Branscomb,[2] and, recently, by Peart *et al.*[3] A discrepancy is seen to exist between the measurements of the first two groups, at higher energies (where the errors are expected to be smaller). At around 10 eV (the region of lowest energy in all the measurements) the last two measurements differ significantly from that of the first group.[1]

Theoretical calculations were done by several authors[4–8] over the past ten years and the results in general differ widely between one another. Moreover, apart from the works of Mcdowell and Williamson[5] and Bely and Schwartz[7] these calculations are widely different from all the experiments. The calculation of Mcdowell and Williamson,[5] however, uses the plane-wave approximation for the incident electron and applies an *ad hoc* correction for the Coulomb effect, first introduced by Geltman,[4] which brings their result relatively closer to the experiments above 20 eV. At lower energies their theoretical approximations have little justifications and the departure from the experiment is large (with or without the *ad hoc* Coulomb correction). On the other hand, the calculation of Bely and Schwartz[7] uses the correct Coulomb waves for the colliding electron but are obliged to use partial-wave analysis. This, according to the authors, limits their numerical calculations up to 60 eV, above which too many partial waves, to be treated numerically, become important. In their investigations Bely and Schwartz use four different

approximations for the ejected-electron's wave function and conclude that the partial waves should be properly orthogonalized in order to obtain reasonable agreement with measurements.

Besides the absolute values of the detachment cross sections at lower energies, there is much theoretical interest[7,8] associated with the behavior of cross sections in the limit of high energies. The high-energy behavior in the present process is dominated by the dipole interaction which leads to the well-known Bethe result[8]:

$$\sigma = (2\pi a_0^2/E_i)(A + B \ln E_i) .$$

In an elegant calculation using the dipole sum rules to estimate the dipole matrix element Inokuti and Kim[8] have found a value of $B = 7.484$. The basic assumption of their calculation, however, is that the incident electron is described by a plane wave. The question naturally arises whether the plane-wave approximation is appropriate at high energies when there is a Coulomb force present between the incident electron and the ionic target H^-. We shall discuss this point in Sec. III.

In the present paper we have adopted an impact parameter method (much used in nuclear physics in connection with Coulomb excitations of nuclei[9] and, in atomic physics, for excitation of neutral atoms,[9,10] which overcomes the difficulty of adding contributions from numerous partial waves by an integration over the impact parameters. The dominant Coulomb repulsion of the incoming electron by the negatively charged ion is incorporated systematically by describing the motion of the colliding electron by a repulsive hyperbolic trajectory. The validity of such a replacement of Coulomb waves propagating at low energies by a Rutherford trajectory depends on the peculiar property of the Coulomb field. It is well known that in scattering by a Coulomb field the classical description depends on the size of the so-called Sommerfeld parameter η which is defined as $\eta = z_1 z_2 / v_i$, where v_i is the incident velocity and z_1 and z_2 are the effective charges on the ion and the electron, respectively. Thus it is easily seen that the smaller the velocity of incidence the greater is η. For any inelastic process, such as the present one, a second condition need also to be satisfied in order that the trajectory description should be valid. The condition required is that the difference between the initial and the final velocities should be small compared with the initial velocity itself. In our case, the binding energy of H^- being small, the incident velocity could be lowered considerably without violating the condition. Nevertheless, in the end we shall apply a symmetrizing procedure to account for the change in velocity, by invoking the principle of detailed balance.

II. MATHEMATICAL FORMULATION

We shall briefly sketch the mathematical formulation of electron-detachment problem, closely paralleling the method of Coulomb excitation in nuclear physics.[9] We shall use atomic units throughout this paper.

According to the time-dependent scattering theory of Dirac[11] the transition amplitude between a state $|i\rangle$ and a state $|f\rangle$ is given by

$$T_{if} = -i \int_{-\infty}^{\infty} dt\, e^{i\Delta E_{if} t} \langle f | V_{eff}(t) | i \rangle , \tag{1}$$

where $\Delta E_{if} = E_i - E_f$ is the difference between the initial and final energies and $V_{eff}(t)$ is the effective interaction. For the present problem

$$V_{eff}(t) = -\frac{1}{r(t)} + \frac{1}{|\vec{r}(t) - \vec{r}_1|} + \frac{1}{|\vec{r}(t) - \vec{r}_2|} - \frac{1}{r(t)} , \tag{2}$$

where $\vec{r}(t)$ is the position vector of the incident electron and $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the two target electrons, all measured from the nucleus (see Fig. 1). We note that a term $1/r(t)$ of the total Hamiltonian of the system is utilized in obtaining the Coulomb trajectory, and hence is subtracted in the effective interaction (2). In the present calculation we have chosen to represent the inital state of the H^- by a variational wave function involving 20-correlated Hylleraas-type terms:

$$\psi_i(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[e^{-\gamma r_1 - \delta r_2} \sum_{lmn} C_{lmn} r_1^l r_2^m r_{12}^n + 1 \leftrightarrow 2 \right] . \tag{3}$$

This produces for the electron affinity w_0

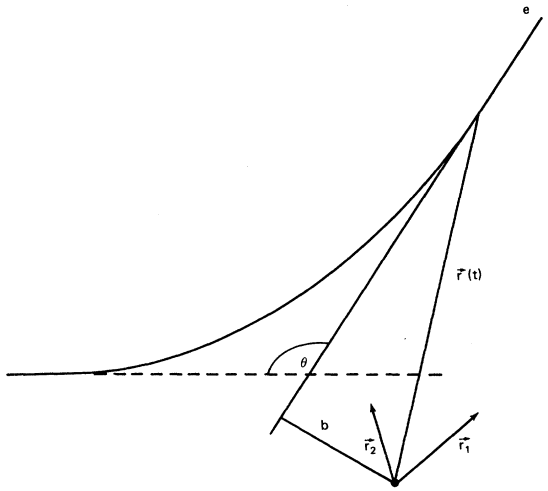

FIG. 1. Collision diagram. $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the target electrons. $\vec{r}(t)$ is the trajectory of the incident electron with impact parameter b and deflection angle θ.

$= -0.026\,386$ a.u. which is comparable to the 444-term calculation of Pekeris,[14] $w_0 = -0.026\,387$ a.u. The reason for this choice is to leave no uncertainty in the target wave function so that the entire burden of approximation is borne by the rest of the theory. We approximate the final target state by a residual hydrogen atom and an outgoing free plane wave for the ejected electron:

$$\psi_f(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_0(\vec{r}_1) e^{i\vec{k}\cdot\vec{r}_2} + \phi_0(\vec{r}_2)\, e^{i\vec{k}\cdot\vec{r}_1}\right] . \quad (4)$$

We now make the most vulnerable of our approximations by replacing the interaction (2) by its expansion in the outer region $r(t) > r_1, r_2$. We have

$$V_{eff}(t) = \sum_{\lambda=1}^{\infty} \left(\frac{r_1^{\lambda} P_\lambda(\hat{r}_1 \cdot \hat{r}(t))}{r^{\lambda+1}(t)} + \frac{r_2^{\lambda} P_\lambda(\hat{r}_2 \cdot \hat{r}(t))}{r^{\lambda+1}(t)} \right) , \quad (5)$$

where P_λ's are Legendre polynomials of order λ. In this approximation the transition integrals T_{if} can be factored out into matrix elements between the target states and a time integral over the projectile trajectory. We get

$$T_{if} = -i \sum \frac{4\pi}{(2\lambda+1)} \langle f | r_1^{\lambda} Y_{\lambda\mu}^*(\hat{r}_1) + r_2^{\lambda} Y_{\lambda\mu}^*(\hat{r}_2) | i \rangle J_{\lambda\mu} , \quad (6)$$

where

$$J_{\lambda\mu} = \int_{-\infty}^{\infty} e^{i\Delta E_{if} t} \frac{Y_{\lambda\mu}(\hat{r}(t))}{r^{\lambda+1}(t)}\, dt . \quad (7)$$

The orbit integrals $J_{\lambda\mu}$ are exactly the same as appear in the case of Coulomb excitation of nuclei and are extensively studied in the literature.[9] We shall merely quote the results[9]:

$$J_{\lambda\mu} = Y_{\lambda\mu}(\tfrac{1}{2}\pi, 0) \frac{1}{v_i a^{\lambda}} I_{\lambda\mu}(\xi, \theta), \quad (8)$$

where the constants

$$Y_{\lambda\mu}(\tfrac{1}{2}\pi, 0) = \left(\frac{2\lambda+1}{4\pi}\right)^{1/2} \frac{[(\lambda-\mu)!\,(\lambda+\mu)!]^{1/2}}{(\lambda+\mu)!!\,(\lambda-\mu)!!} \times (-1)^{(\lambda+\mu)/2}, \quad \lambda+\mu \text{ even}$$

$$= 0, \quad \lambda+\mu \text{ odd} \quad (8a)$$

$$a = z_1 z_2 / m_0 v_i^2 , \quad (9)$$

$$\xi = a \Delta E_{if} / v_i . \quad (10)$$

In the above, v_i is the initial velocity, m_0 is the reduced mass, and z_1 and z_2 are the effective charges on the target and the projectile, respectively.

Using the wave functions (3) and (4) and performing all angular momentum algebra, the target matrix element can be written as

$$\langle \psi_f(\vec{r}_1, \vec{r}_2) | r_1^{\lambda} Y_{\lambda\mu}^*(\hat{r}_1) + r_2^{\lambda} Y_{\lambda\mu}^*(\hat{r}_2) | \psi_i(\vec{r}_1, \vec{r}_2) \rangle = B_\lambda(k) Y_{\lambda\mu}^*(\hat{k}) , \quad (11)$$

where $B_\lambda(k)$ is a function of the wave number k of the ejected electron only. The photoionization cross sections of H^- obtained by using the present $B_1(k)$ compare well with the cross sections calculated by Bell and Kingston[12] (see Table I).

The transition can now be written as

$$T_{if} = -i \sum \left(\frac{4\pi}{2\lambda+1}\right) a^{-\lambda} v_i^{-1} Y_{\lambda\mu}(\tfrac{1}{2}\pi, 0) \times I_{\lambda\mu}(\xi, \theta) B_\lambda(k) Y_{\lambda\mu}^*(\hat{k}) . \quad (12)$$

Defining the ejection angle integrated transition probability by

$$P_{if}(k | E_i) = \int | T_{if} |^2 d\hat{k}$$

and noting that the differential cross section

$$d\sigma(k | E_i) = P_{if}(k | E_i) \, | 2\pi b db | ,$$

where $b = a \cot \frac{1}{2}\theta$ is the impact parameter and θ is the angle of scattering, we find

$$d\sigma(k | E_i) = \sum_{\lambda=1}^{\infty} (2\lambda+1) | B_\lambda(k) |^2 a^{-2\lambda+2} v_i^{-2}\, df_\lambda(\xi, \theta) \quad (13)$$

and the total cross section

$$\sigma(k | E_i) = \sum_{\lambda=1}^{\infty} (2\lambda+1) | B_\lambda(k) |^2 a^{-2\lambda+2} v_i^{-2} f_\lambda(\xi) , \quad (14)$$

where

$$df_\lambda(\xi, \theta) = \frac{4\pi^2}{(2\lambda+1)^3} \times \sum_{\mu} \left| Y_{\lambda\mu}\left(\frac{\pi}{2}, 0\right) I_{\lambda\mu}(\xi, \theta) \right|^2 \frac{1}{\sin^4 \frac{1}{2}\theta}\, d\Omega \quad (15)$$

and

$$f_\lambda(\xi) = \int \frac{df_\lambda(\xi, \theta)}{d\Omega} d\Omega = \frac{32\pi^3}{(2\lambda+1)^3} \sum_{\mu} | Y_{\lambda\mu}(\tfrac{1}{2}\pi, 0) |^2 \times \int_1^{\infty} | I_{\lambda\mu}(\xi, \epsilon) |^2 \epsilon\, d\epsilon , \quad (16)$$

with ϵ related to the scattering angle, and hence

TABLE I. Photoionization cross sections of H^-.

Incident energy (a.u.)	Cross sections (10^{-17} cm^2)	
	Present	Bell and Kingston
0.005	0.804	0.737
0.020	3.116	3.227
0.045	3.348	3.933
0.080	2.178	2.762
0.125	1.326	1.662
0.180	0.876	1.067
0.320	0.429	0.542

the impact parameter, by the relation $\epsilon = [1+(b/a)^2]^{1/2}$.

The results (13) and (14) do not take into account the change in the projectile velocity before and after the collision. This may be incorporated by symmetrizing the cross-sectional expressions with respect to the initial and final velocities as required by the principle of detailed balance. This is most readily achieved by replacing Eqs. (9) and (10) by the symmetrized expressions

$$a \to z_1 z_2/m_0 v_i v_f\,, \quad \xi \to z_1 z_2\,(1/v_f - 1/v_i)$$

and substituting them in Eqs. (13) and (14). To obtain the total cross section of electron detachment for a given initial velocity and all ejection energies we must integrate over the energy of the ejected electron. Thus,

$$\sigma_{\rm tot}(E_i) = \int_0^{k_{\rm max}} dk\, k^2\, \sigma(k|E_i)\,, \tag{17}$$

where $k_{\rm max}$ is the maximum available momentum of ejection k, for a given energy of incidence E_i. By using Eq. (14) in Eq. (17) we are making a nonexchange approximation of the exact $\sigma(k|E_i)$ by the semiclassical expression (14), which does not include any exchange probability. In the event the probability of exchange is small, the approximation should be good. For numerical calculations we have retained the leading term $\lambda = 1$ which corresponds to a dipole approximation of the interaction. Thus we need to evaluate the quantity $f_1(\xi)$ from Eq. (16). Although $f_1(\xi)$ remains finite when integrated over all scattering angles (i.e., over all impact parameters), the multipole expansion of the potential necessitates a finite cutoff at some nonzero minimum impact parameter b_0.[10] We therefore redefine the quantity $f_1(\xi)$ by the modified expression

$$\tilde{f}_1(\xi) = \frac{32\pi^3}{27} \sum_\mu |Y_{1\mu}(\tfrac{1}{2}\pi, 0)|^2 \int_{\epsilon_0}^{\infty} |I_{1\mu}(\xi,\theta)|^2 \epsilon\, d\epsilon\,, \tag{18}$$

where

$$\epsilon_0 = [1+(b_0/a)^2]^{1/2}\,.$$

We can perform the above integral over ϵ analytically and obtain

$$f_1(\xi) = -\tfrac{32}{9}\pi^2 e^{-\pi\xi}\,(\xi\epsilon_0)\,K_{i\xi}(\xi\epsilon_0) K'_{i\xi}(\xi\epsilon_0). \tag{19}$$

We note that for $b_0 = 0$, $\tilde{f}_1(\xi)$ coincides with the usual result quoted in Ref. 9.

The choice of a minimum impact parameter in the present theory is necessitated by our use of the dipole approximation for the interaction potential. There is however no unique method of choice for such a parameter. In the present problem we have a natural minimum cutoff, provided by the distance of closest approach. This corresponds to $b_0 = 2a$. An alternative choice of the cutoff parameter is $b_0 = r_0$, where r_0 is a measure (radius) of the size of the target. We have calculated cross sections using both of them and found that the choice $b_0 = r_0$ is consistent with the quantum-mechanical Coulomb-Bethe approximation. One reason for the breakdown of the choice $b_0 = 2a$ is that at higher energies it violates the condition required for the validity of dipole expansion itself.

It is interesting to note that unlike for the case of straight-line trajectories[10] the present integration in Eq. (18) over the impact parameters converges even with $b_0 = 0$; this result is due to the strong curvature of the Coulomb trajectory near the origin.

III. TOTAL CROSS SECTIONS AND HIGH-ENERGY BEHAVIOR

Using Eqs. (14) and (17) we obtain for the total cross section in dipole approximation ($\lambda = 1$),

$$\sigma_{\rm tot}(E_i) = \frac{3a_0^2}{2E_i} \int_0^{[2(E_i - w_0)]^{1/2}} dk\, k^2 |B_1(k)|^2 \tilde{f}_1(\xi), \tag{20}$$

where $\tilde{f}_1(\xi)$ is given by Eq. (19).

Formal expressions similar to Eqs. (13) and (20) can also be written using the quantum-mechanical dipole approximation and the total cross section can again be given by Eq. (20), provided $\tilde{f}_1(\xi)$ is replaced by the corresponding quantum-mechanical expression

$$f_1(\eta_i, \xi) = \tfrac{4}{27} k_i k_f \int d\Omega \sum_{\mu=-1}^{1} |\langle \vec{k}_f | r^{-2} Y_{1\mu}(\hat{r}) | k_i \rangle|^2\,, \tag{21}$$

where $|\vec{k}_i\rangle$ and $|\vec{k}_f\rangle$ are the incident and the scattered waves, respectively.

In this section we compare the asymptotic behavior of total cross sections obtained from the semiclassical and quantum-mechanical equations (19) and (21) when used along with Eq. (20).

From Eq. (21) using plane waves for $|\vec{k}_i\rangle$ and $|\vec{k}_f\rangle$ it is easy to show that the dipole-Born expression for f_1 is

$$f_1^{\rm DB} = \tfrac{32}{9}\pi^2 \int_{q_{\rm min}}^{q_{\rm max}} dq/q\,, \tag{22}$$

where we have defined $\vec{q} = \vec{k}_i - \vec{k}_f$ and hence $d\Omega = (2\pi/k_i k_f)\, q\, dq$. If $|\vec{k}_i\rangle$ and $|\vec{k}_f\rangle$ are chosen to be Coulomb waves the integration is no longer simple but has been evaluated by Mullin and Guth[9,13] in terms of Gauss hypergeometric functions and may be written as

$$f_1(\eta_i,\xi)=\frac{64\pi^4}{\xi^2 k_i k_f}\,\eta_i\eta_f\,\frac{e^{2\pi\eta_i}}{(e^{2\pi\eta_i}-1)(e^{2\pi\eta_f}-1)}\int_{q_{\min}}^{q_{\max}} dq\,q\,\frac{d}{dx}\left\{-x\,\frac{d}{dx}\,|F(-i\eta_i,-i\eta_f,1,\kappa)|^2\right\}, \tag{23}$$

where

$$x=x(q)=-\frac{\eta_i\eta_f}{\xi^2 k_i k_f}\,(q^2-q_{\min}^2).$$

In the high-energy limit the above expression (23) simplifies considerably,[13] yielding

$$f_1(E_i,\xi)\underset{E_i\to\infty}{=}\tfrac{32}{9}\pi^2\,G(k)\int_{q_{\min}}^{q_{\max}} dq/q, \tag{24}$$

where

$$G(k)=\frac{4\pi^2\eta_i\eta_f}{(e^{2\pi\eta_i}-1)(e^{2\pi\eta_f}-1)}\,g^2\ ,$$

with

$$g^2=1, \qquad k_i\neq k_f$$
$$=\frac{\sinh(\pi\eta_i)}{\pi\eta_i}, \quad k_i=k_f\ . \tag{25}$$

In the limit $V_i\to\infty$, $G(k)\to 1$, and comparing Eqs. (22) and (24), we find that only in this limit the Coulomb calculation approaches the plane-wave result.

If one integrates Eqs. (22) and (24) over the complete range of $q_{\min}=k_i-k_f$ to $q_{\max}=k_i+k_f$, one obtains in the dipole-Born case

$$f_i^{\mathrm{DB}}(E_i,\xi)=\tfrac{32}{9}\pi^2\ln\frac{\frac{1}{2}(v_i+v_f)}{\Delta E}^2. \tag{26}$$

In the dipole-Coulomb case likewise, one finds

$$f_i^{\mathrm{DC}}(E_i,\xi)=\tfrac{32}{9}\pi^2\,G(k)\ln\frac{\frac{1}{2}(v_i+v_f)^2}{\Delta E}. \tag{27}$$

TABLE II. Slope and $\beta(k)$ in different approximations.

Case	Approximation	$\beta(k)$	n	Slope
I	Dipole-Born (without cutoff)	$(1+v_f/v_i)^2$	2	$2I_B$
II	Dipole-Bethe (with cutoff)	$\frac{(1+v_f/v_i)}{\sqrt{2}\,r_0}$	1	I_B
III	Dipole-Coulomb (without cutoff)	$8(1+v_f/v_i)$	2	$2I_B$
IV	Dipole-Coulomb-Bethe (with cutoff)	$(1/\sqrt{2}\,r_0)(1+v_f/v_i)$	1	I_B
V	Semiclassical	$\frac{\sqrt{2}}{R_0}$	1	I_B

Various cutoffs:

(i) $b_0=0$, $\epsilon_0=1$,
(ii) $b_0=2a$, $\epsilon_0=\sqrt{5}$,
(iii) $b_0=r_0$, $\epsilon_0=[1+(r_0/a)^2]^{1/2}$

However, in order to use the dipole expansion consistently (following Bethe) if one restricts oneself to the condition $q_{\max}\,r_0\simeq 1$ (where r_0 is of the order of the radius of the target) one obtains

$$f_1^{\mathrm{DBB}}(E_i,\xi)=\tfrac{32}{9}\pi^2\ln\frac{\frac{1}{2}(v_i+v_f)}{R_0\Delta E} \tag{28}$$

and

$$f_i^{\mathrm{DCB}}(E_i,\xi)=\tfrac{32}{9}\pi^2\,G(k)\ln\frac{\frac{1}{2}(v_i+v_f)}{R_0\Delta E}. \tag{29}$$

In the semiclassical case we note that $\xi=z_1z_2\Delta E/v_i^3$ as $v_i\to\infty$ and Eq. (19) gives

$$\tilde{f}_1(\xi)=\tfrac{32}{9}\pi^2\ln\frac{1}{\xi\epsilon_0}=\tfrac{32}{9}\pi^2\ln\left(\frac{v_i^3}{z_1z_2\Delta E\epsilon_0}\right). \tag{30}$$

Using the different limiting forms of f_1 [Eqs. (26)–(30)] in Eq (20), the total cross section at high energy may be written as

$$\sigma_{\mathrm{tot}}(E_i)=\frac{2\pi a_0^2}{E_i}\,[I_A+nI_B\ln E_i]\ , \tag{31}$$

where

$$I_A(E_i)=\frac{8\pi}{3}\int_0^{[2(E_i-w_0)]^{1/2}} dk\,k^2\,|B_1(k)|^2\,G(k)\ln\frac{\beta}{\Delta E} \tag{32}$$

and

$$I_B(E_i)=\frac{4\pi}{3}\int_0^{[2(E_i-w_0)]^{1/2}} dk\,k^2\,|B_1(k)|^2\,G(k)\ . \tag{33}$$

Table III. Detachment cross sections for $e^-+H^-\to 2e^-+H(1S)$ at low energies.

Incident energy (a.u.)	Cross sections (πa_0^2) $b_0=0$	$b_0=2a$	$b_0=3.42$	Coulomb wave Bethe	Plane wave Bethe
0.05	7.1×10^{-5}		7.0×10^{-5}	6.4×10^{-5}	82.9
0.06	0.006		0.006	0.005	109.5
0.07	0.065		0.061	0.054	127.2
0.08	0.317		0.291	0.25	133.3
0.09	0.954		0.859	0.76	135.7
0.10	2.13	0.58	1.89	1.67	135.6
0.15	16.47		13.33	12.02	121.2
0.20	36.82	18.8	27.31	25.29	106.8
0.25	54.63		37.63	35.68	95.4
0.30	68.01	41.5	43.90	42.39	86.4

TABLE IV. Detachment cross sections for $e^- + H^- \rightarrow e^- + e^- + H$ (1S).

Incident energy (a.u.)	Cross section (πa_0^2) $b_0 = 0$	$b_0 = 2a$	$b_0 = 3.42$	Coulomb wave (Bethe)	Plane wave (Bethe)
0.3	68.0	41.5	43.9	34.5	86.4
0.4	85.1	55.1	48.7	40.3	73.1
0.5	93.5	61.9	48.8	41.7	63.7
0.6	95.6	64.8	47.0	41.2	56.8
0.8	92.1	65.0	42.4	38.2	47.1
1.0	85.3	62.4	38.1	34.9	40.4
1.2	78.5	59.0	34.4	31.8	
1.4	72.4	55.7	31.3	29.2	
1.6	67.2	52.5	28.8	27.0	
1.8	62.6	49.7	26.6	25.1	
2.0	58.7	47.0	24.8	23.4	24.6
2.2	55.2	44.7	23.2	22.0	
2.4	52.2	42.6	21.8	20.7	
2.6	49.5	40.6	20.6	19.6	
2.8	47.0	38.9	19.5	18.6	
3.0	44.9	37.3	18.5	17.7	18.2
4.0	36.6	31.0	14.9	14.3	14.6
5.0	31.1	26.7	12.6	12.1	12.2
5.5	29.0		11.7	11.2	11.4
6.0	27.1	23.5	10.9	10.5	10.6
6.5	25.5		10.2	9.8	9.9
7.0	24.1	21.0	9.7	9.3	9.4
9.0	19.9	17.5	7.9	7.6	7.6
10.0	18.3	16.2	7.2	7.0	7.0
11.0	17.0	15.0	6.7	6.5	6.5
12.0	15.9	13.2	6.2	6.0	6.0
13.0	14.9		5.8	5.6	5.7
14.0	14.0		5.5	5.3	5.3
15.0	13.3	11.8	5.2	5.0	5.0
20.0	10.6		4.1	3.9	3.9
25.0	8.8	7.9	3.4	3.2	3.2
30.0	7.6	6.9	2.9	2.8	2.7
35.0	6.7	6.1	2.6	2.4	2.3
40.0	6.0		2.3	2.1	2.0
45.0	5.5	5.0	2.1	1.8	1.7
50.0	5.0		1.9	1.6	1.5
55.0	4.6	4.2	1.7	1.4	1.3

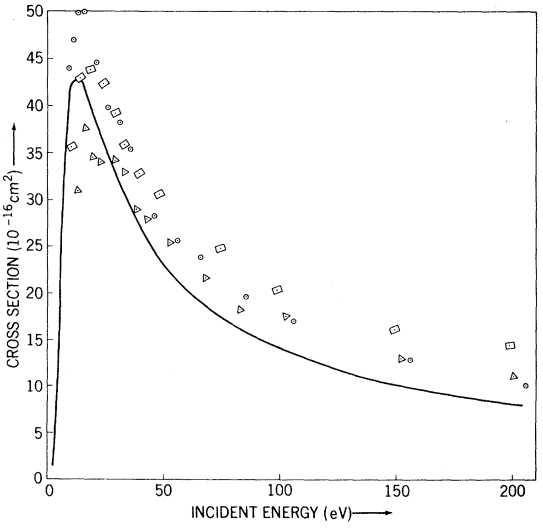

FIG. 2. Comparison of the calculated cross section for $e^- + H^- \rightarrow e^- + e^- + H(1S)$ with experiments. The solid curve is the present calculation. Circles, squares, and triangles are the experimental data of Refs. 1, 2, and 3, respectively.

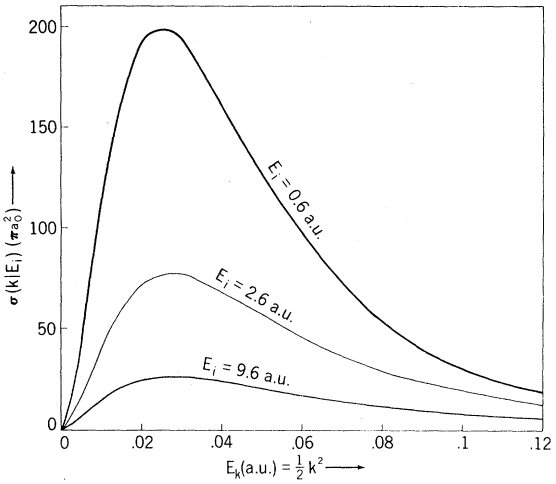

FIG. 3. Calculated energy distribution of the ejected electron. $\sigma(k|E_i)$ is the cross section at ejection energy $E_k = \frac{1}{2}k^2$ for a given incident energy E_i.

We note that $I_B(E_i)$ is not a completely independent function of E_i. The slope in the present plane-wave approximation for the continuum wave is thus found to be a slowly varying function of E_i at any finite incident energy. We find for example $I_B(E_i = 55$ a.u.$) = 8.7$ $(2\pi a_0^2)$, which is about 10% larger than $I_B(E_i = 45$ a.u.$) = 7.8$ $(2\pi a_0^2)$.

Finally, we note from Eq. (33) that the slopes I_B in the corresponding Bethe plots will be different according to the choice of different approximations.

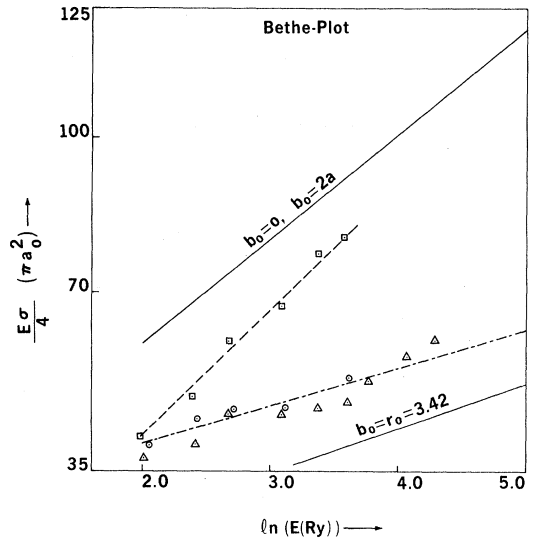

FIG. 4. The solid lines are the present calculations. The dash-dotted line is obtained from the asymptotic form of Inokuti and Kim. Circles, squares, and triangles are the experimental data of Refs. 1, 2, and 3, respectively. The dashed line represents the asymptotic result of Ref. 1.

TABLE V. Electron-detachment cross section for $e^- + H^- \rightarrow e^- + e^- + H(2S)$.

Incident energy (a.u.)	Cross section (πa_0^2)
0.1	1.6×10^{-4}
0.25	6.8×10^{-3}
0.50	5.7×10^{-2}
1.0	7.2×10^{-1}
1.5	1.4×10^{-1}
2.0	1.4×10^{-1}
2.5	1.3×10^{-1}
3.0	1.3×10^{-1}
3.5	1.2×10^{-1}
4.0	1.1×10^{-1}
4.5	1.1×10^{-1}
5.0	1.0×10^{-1}
5.5	9.9×10^{-2}
6.0	9.6×10^{-2}
6.5	9.2×10^{-2}
7.0	8.8×10^{-2}

We summarize the results in Table II.

IV. RESULTS

Within the approximations introduced in this paper we have calculated the primary detachment cross sections for the following two processes: (i) $e^- + H^- = H(1S) + 2e^-$; (ii) $e^- + H^- = H(2S) + 2e^-$. In Table III we present the low-energy cross sections for process (i) calculated within the semiclassical plane-wave and Coulomb-wave approximations. The low-energy Coulomb-wave results may be obtained from the limit $\eta_i \gg 1$ of expression (23).[13] This gives for

$$\sigma(E_i) \underset{v_i \to 0}{=} \frac{32\pi^3}{3\sqrt{3}}\,\eta_i^2 \int_0^{[2(E_i - w_0)]^{1/2}} dk\, k^2 \left| B_1(k) \right|^2 e^{-2\pi(\eta_i - \eta_f)}.$$

The table shows that the plane-wave result is completely unreliable in this region while the semiclassical approximations with various choices of cutoff parameters are compatible with the corresponding results of the Coulomb-Bethe approximation.

In Table IV, we present the cross sections at higher energies. This table shows clearly that the semiclassical calculation with minimum impact parameter $b_0 = r_0$ (which corresponds to Bethe's prescription $q_{\max} r_0 \approx 1$ in the corresponding quantum-mechanical dipole approximation) gives consistent results with the Coulomb-Bethe approximation. The other choices such as $b_0 = 0$ and $b_0 = 2a$ are seen to be quite inconsistent with the Coulomb-wave calculation and can be rejected on the ground that these cases violate the condition for the validity of dipole expansion of the potential itself.

In Fig. 2 we have plotted the cross sections obtained from our semiclassical calculation ($b_0 = r_0$) and compared the results with various experiments. In Fig. 3 we show typical energy distributions of ejected electrons for a few given incident energies. The Bethe plots in Fig. 4 shows the high-energy behavior of cross sections in various theoretical approximations and compares them with those obtained from experiments.

In Table V we present the cross sections (with $b_0 = r_0$) for reaction (ii). Comparison of this result with that in Table IV shows that the cross section for the residual atom to be in $H(2S)$ state is about two orders of magnitude smaller than to be in $H(1S)$ state.

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APPENDIX

In this Appendix we show the correspondence between the quantity I_B with the usual matrix element[8] $M^2_{\rm tot}$:

$$M^2_{\rm tot} = \frac{1}{3a_0^2} \langle \Psi_i | (\vec{r}_1 + \vec{r}_2)^2 | \Psi_i \rangle$$

$$= \frac{1}{3a_0^2} S \langle \Psi_i | \vec{r}_1 + \vec{r}_2 | \Psi_f \rangle \langle \Psi_f | \vec{r}_1 + \vec{r}_2 | \Psi_i \rangle,$$

where S stands for summation over all final discrete and continuum states of the system. Approximating Ψ_f by Eq. (4) and neglecting all other residual target states, we find

$$M^2_{\rm tot} = \frac{4\pi}{3a_0^2} \int d\vec{k}\, \left| \langle \Psi_i | r_1 Y_{10}(\hat{r}_1) + r_2 Y_{10}(\hat{r}_2) | \Psi_f \rangle \right|^2.$$

Using Eq (11), we have

$$M^2_{\rm tot} \simeq \frac{4\pi}{3a_0^2} \int_0^{[2(E_i - w_0)]^{1/2}} dk \left| B_1(k) \right|^2 = I_B(E_i)\ .$$

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Determination of the Scattering Amplitude from the Differential Cross Section for Scattering by an Arbitrary Noncentral Potential

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The unitarity relation of quantum-scattering theory is studied for the general case of scattering by an arbitrary noncentral force and it is shown how it can be utilized to determine the phase of the scattering amplitude from the measured differential cross section. It is found that the unitarity relation leads to a pair of nonlinear integral equations for the phase of the scattering amplitude if the cross section is known. It is shown that from these equations one can obtain, without introducing approximations, a system of linear algebraic equations for a certain set of scalars from the values of which one can readily calculate the phase. In general, the above system of linear equations may admit also redundant nonphysical solutions for the phase. However, when the magnitude of the cross-section data satisfies certain conditions the solution of the equations is unique and must equal the correct physical value of the phase. Unlike previous methods for phase determination, the present approach is based on a form of the unitarity equation which is not simplified by any of the assumptions of parity, rotational, or time-reversal invariance for the underlying scattering interaction. Therefore, it can be applied to the determination of the phase also in cases such as particle scattering by, or in the presence of, external fields which do not possess the above-mentioned symmetries. A generalization of this method to many-channel scattering is also provided. Similar results hold also for the determination of phases in the theory of electromagnetic-wave scattering by an obstacle of arbitrary shape.

I. INTRODUCTION

Considerable progress was made recently towards a complete solution of the problem of determining the scattering amplitude from the corresponding differential cross section.[1-3] One of the main motivations for interest in this question has been the theoretically proven possibility of constructing systematically the potential from the scattering amplitude at a fixed energy and for all the angles, in the case of elastic scattering by a central potential.[4] This result indicates that the determination of the scattering amplitude from the measured cross section is likely to be an essential preliminary step in any scheme of obtaining the potential from experimental data. That statement is bound to be valid also for the general case of scattering by noncentral forces, for which the problem of determining the interaction from the scattering amplitude has not been solved yet.

The question of determining the scattering amplitude from the differential cross section has been investigated mainly for central potentials, but the results obtained,[1-3] which will be reviewed briefly below, hold also for parity-invariant forces in general. Within this scope, at least a formal mathematical answer to the problem at hand was given. The tool suggested for the determination of the phase of the scattering amplitude (this is the only quantity which is unknown, the absolute value of the amplitude being, of course, the square root of the cross section) is the unitarity relation of quantum-scattering theory.[5] When the differential cross section for scattering by a central (or, more generally, parity-invariant) potential is known, the unitarity relation yields a certain integral equation for the phase of the scattering amplitude. Newton,[1] Martin,[2] and Gerber and Karplus[3] have all independently shown that, under a certain restriction on the magnitude of the given cross section, the phase of the scattering amplitude is determined *uniquely* by this equation, except for a certain, relatively trivial, twofold ambiguity. Also, the above authors have shown that the unitarity equations can be solved iteratively, and that the iterations converge uniformly in the scattering angle to the true value