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Distorted Wave Method for Electron Capture from Atomic Hydrogen*

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The distorted wave method, in which distorted waves replace plane waves in the matrix elements for the collision amplitude, is given a rigorous formulation for arbitrary rearrangement collisions. In atomic collisions involving electron rearrangement, the formulation enables removal of the unphysical internuclear Coulomb interaction from the "perturbation" Hamiltonian. The procedure is applied to the problem of electron capture by protons in atomic hydrogen, eliminating explicit dependence on the proton-proton interaction. Numerical results of a first order calculation are in good agreement with experiments from 35 to 200 kev. Despite this agreement and the agreement of previous calculations it is felt the charge transfer process is still not well understood.

1. INTRODUCTION

In our opinion the simplest charge transfer process

$$\mathrm{H}+\mathrm{H}^{+}\rightarrow\mathrm{H}^{+}+\mathrm{H}, \qquad (1\text{-}1)$$

which has been examined by many authors[1–6] does not yet have a satisfactory theory. Jackson and Schiff[3] (JS) and Bates and Dalgarno[4] (BD) have computed the cross section for Eq. (1-1) in first Born approximation. They find good agreement with experiment[7–12] at incident proton energies above about 40 kev, assuming that the charge transfer cross section per H atom in the molecular reaction

$$\mathrm{H}^{+}+\mathrm{H}_2\rightarrow\mathrm{H}+\mathrm{H}_2^{+} \qquad (1\text{-}2)$$

is the same as the cross section for the atomic reaction (1-1). This assumption is necessary because the cross section for (1-1) has been measured[13] only at energies less than 25 kev. Below 25 kev the incident proton velocity is less than the electron velocity in its first Bohr orbit (a_0), and Born approximation is not expected to hold. Unfortunately, there are grave theoretical objections to the assumption that for the purposes of charge transfer one H_2 molecule is equivalent to two isolated H atoms, but it is possible that this equivalence holds because of fortuitous cancellation of several opposing effects.[14] Granting the relevance of the experimental data with which the JS and BD calculation have been compared, there remain some theoretical difficulties connected with this calculation, which difficulties we proceed to describe.

In first Born approximation the differential cross section $d\sigma$ for (1-1) corresponding to capture with deflection of the incident proton into the direction $\mathbf{n}_f$ in the center-of-mass system is

$$(\mu/2\pi\hbar^2)^2|\langle\psi_f|V_i|\psi_i\rangle|^2. \qquad (1\text{-}3)$$

In Eq. (1-3), $\mu=M(M+m)/(2M+m)$ is the reduced mass; $V_i=V_{1e}+V_{12}$ is the prior "perturbation," proton 1 being incident along $\mathbf{n}_i$; $V_{1e}=-e^2/r_{1e}$; $V_{12}=e^2/R_{12}$; and ψ_i and ψ_f, the incident and final wave functions, respectively, are

$$\begin{aligned}\psi_i&=u(r_{2e})\exp[iK\mathbf{n}_i\cdot\mathbf{R}],\\ \psi_f&=u(r_{1e})\exp[-iK\mathbf{n}_f\cdot\mathbf{R}'].\end{aligned} \qquad (1\text{-}4)$$

Subscripts e, 1, 2 refer, respectively, to the electron and to protons 1 and 2; u is the ground-state wave function of the hydrogen atom; and $\hbar K=\mu v$, with v the incident proton velocity. The coordinates are as shown in Fig. 1; $[\mathbf{R}=\mathbf{R}_1-(m+M)^{-1}(m\mathbf{r}_e+M\mathbf{r}_2)$, $\mathbf{R}'=r_2-(m+M)^{-1}(m\mathbf{r}_e+M\mathbf{r}_1)$, $\mathbf{r}_{1e}=\mathbf{r}_e-\mathbf{r}_1$, etc.]. With the post interaction, V_i in (1-3) is replaced by $V_f=V_{2e}+V_{12}$. In general $\langle\psi_f|V_i|\psi_i\rangle=\langle\psi_f|V_f|\psi_i\rangle$; for the special case of capture into the ground state of the atom formed by e and 2, the only case we consider in this paper, the reaction (1-1) is so symmetric that the post and prior matrix elements are formally identical, not merely numerically equal.

As JS and BD have shown, the matrix element $\langle\psi_f|V_{12}|\psi_i\rangle$ of the proton-proton interaction is of the

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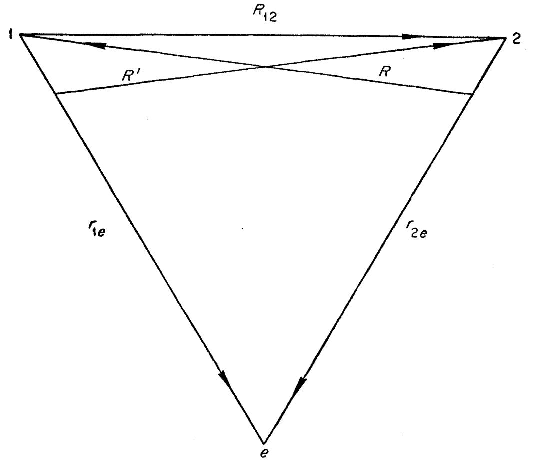

FIG. 1. Coordinate system. 1 refers to the incident proton, 2 to the nucleus, and e to the electron.

same order of magnitude, and has the same energy dependence at high energies, as the matrix element of V_{1e}. On the other hand Brinkman and Kramers (BK) have argued, with Oppenheimer,[15] that V_{12} should be negligible in the high-energy range where Born approximation is supposedly valid. Their argument is appealing; seemingly the only effect of V_{12} is a slight deflection of the fast incident proton, which deflection should hardly affect the probability of electron capture. Moreover, the protons are so heavy compared with the electron that it appears legitimate[16] to replace the protons by classical centers of force, reducing the original three-body reaction to a one-body problem in the fashion of Mott.[17] With this replacement, it can be proved rigorously[18] that the electron capture cross section is independent of the proton-proton interaction. The BK conjecture that V_{12} can be neglected receives added support from Drisko, who in the high energy limit $v\rightarrow\infty$ finds that the first Born approximation V_{12} contribution is canceled by proton-proton contributions in second Born approximation.

Attempting to resolve this difficulty, Pradhan[5] has considered an impulse approximation in which, to first order, the proton-proton matrix element vanishes. This theory also provides a good fit to the experimental data. However, Pradhan makes an approximation which casts some doubt on the validity of his calculation. He derives a matrix element which involves the final interaction $V_{12}+V_{2e}$. To expedite the integration, this interaction is replaced by the initial interaction $V_{12}+V_{1e}$. The physical processes represented by the two matrix elements are quite different. As Pradhan notes, the wave function in the initial channel appearing in his matrix element represents scattering of the electron by the incident proton. With the final interaction the matrix element describes a double scattering of the electron by the two protons. With the initial interaction the process is changed to a situation in which the electron first scattered by the incident proton re-interacts with the same proton. The two matrix elements should lead to different cross sections. The error involved is difficult to assess. Estimates of Drisko indicate that the error is serious in the high-energy limit.

In atomic collisions of the type

$$a+b\rightarrow c+d, \tag{1-5}$$

wherein electron rearrangement takes place, the so-called "distorted wave method" provides a convenient means of removing the unphysical internuclear Coulomb interaction from the "perturbation" whose matrix element yields the cross section. The requisite formulas for an arbitrary rearrangement (1-5) are obtained in Sec. 2, and applied to the electron capture problem (1-1) in Sec. 3. Therewith V_{12} is removed from the perturbation; in fact, in a first-order Born-like approximation, all dependence on V_{12} is removed. Section 4 is devoted to examining the numerical predictions of this first-order approximation. In Sec. 5 we make a semiclassical impact parameter calculation based on our first order distorted wave approximation and compare the results with the results of similar calculations by BK who use only the electron-proton interaction V_{1e}, and with Schiff[19] who considers the complete interaction V_i. Finally, in Sec. 6, we compare our predictions with the results of previous theories and measurements.

2. FORMULATION OF SCATTERING AMPLITUDE

In reactions such as (1-5) the total Hamiltonian H can be written in either the initial or final system; that is

$$H=H_i+V_i=H_f+V_f. \tag{2-1}$$

Here H_i describes the motion of the aggregates a and b in the absence of their mutual interaction V_i. H_f and V_f provide a similar description of the final system (c,d).

The matrix elements[20–22] $\langle\Psi_f^{(-)}|V_i|\psi_i\rangle=\langle\psi_f|V_f|\Psi_i^{(+)}\rangle$ yield the cross section for the reaction (2-1), where

$$\Psi_i^{(+)}=(1-GV_i)\psi_i\equiv\left(1-\frac{1}{H-E'-i\epsilon}V_i\right)\psi_i \tag{2-2}$$

is the unique[23,24] solution to $(H-E')\Psi=0$ with incident wave ψ_i in the initial channel and outgoing scattered

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[16] It must be remembered however, see Tuan and Gerjuoy, reference 14, that the effective wavelength in the capture process is not the wavelength of the incident proton, but the 2000 times greater wavelength of an electron moving with the incident proton velocity.

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parts, and

$$\Psi_f^{(-)}=\left(1-\frac{1}{H-E'+i\epsilon}V_f\right)\psi_f \tag{2-3}$$

is the unique solution to $(H-E')\Psi=0$ with incident wave ψ_f and incoming scattered parts. Of course $(H_i-E')\psi_i=(H_f-E')\psi_f=0$. Moreover, writing $V_i=U_i+V_i-U_i$, and employing either Eq. (4.9) of Gell-Mann and Goldberger[21] or Eq. (2.25b) of Gerjuoy,[22]

$$\Psi_i^{(+)}=\chi_i^{(+)}-G(V_i-U_i)\chi_i^{(+)}\equiv\chi_i^{(+)}+\phi, \tag{2-4}$$

where

$$\chi_i^{(+)}=(1-g_iU_i)\psi_i\equiv\left(1-\frac{1}{H_i+U_i-E'-i\epsilon}U_i\right)\psi_i, \tag{2-5}$$

is the unique solution to $(H_i+U_i-E')\chi=0$ with incident wave ψ_i and outgoing scattered parts.

In the foregoing equations E' is the center-of-mass energy and U_i is arbitrary, provided only that $\lim r_{ab}U_i=0$ as $r_{ab}\rightarrow\infty$, with r_{ab} the distance between the centers of mass of a and b. When U_i depends on $\mathbf{r}_{ab}$ only, $\chi_i^{(+)}$ contains only elastically scattered parts, so that $\phi=-G(V_i-U_i)\chi_i^{(+)}$ contains the description of all other possible reactions, i.e., excitation of a, b and rearrangements. Thus when $U_i\equiv U_i(\mathbf{r}_{ab})$, using

$$G=G_f-G_fV_fG, \tag{2-6}$$

where $G_f=(H_f-E'-i\epsilon)^{-1}$, one finds[21,22] the differential cross section for the reaction (1-5) is

$$\begin{aligned}d\sigma&\equiv|A(i\rightarrow f)|^2\\&=(\mu_f/2\pi\hbar^2)^2|\langle\Psi_f^{(-)}|V_i-U_i|\chi_i^{(+)}\rangle|^2,\end{aligned} \tag{2-7}$$

with μ_f the reduced mass of aggregates c, d. In Eq. (2-7) $\Psi_f^{(-)}$ is given by Eq. (2-3) or by the analogs of Eqs. (2-4) and (2-5), namely

$$\Psi_f^{(-)}=\left[1-\frac{1}{H-E'+i\epsilon}(V_f-U_f)\right]\chi_f^{(-)}, \tag{2-8}$$

$$\chi_f^{(-)}=\left(1-\frac{1}{H_f+U_f-E'+i\epsilon}U_f\right)\psi_f. \tag{2-9}$$

The distorted wave method[25] is characterized by the choice

$$U_i\equiv U_i(\mathbf{r}_{ab})=\langle u_a(\mathbf{s}_a)u_b(\mathbf{s}_b)|V_i|u_a(\mathbf{s}_a)u_b(\mathbf{s}_b)\rangle, \tag{2-10}$$

with u_a, u_b the initial bound states of the aggregates a, b. The matrix element in (2-10) is integrated over all values of the internal coordinates $\mathbf{s}_a$, $\mathbf{s}_b$ of a, b, holding $\mathbf{r}_{ab}$ constant. In other words $U_i(\mathbf{r}_{ab})$ is the average (over internal motions) static interaction between the initial aggregates a, b, and $\chi_i^{(+)}$ of Eq. (2-5) represents the elastic scattering of a, b by this static interaction.[25] Similarly the distorted wave $\chi_f^{(-)}$ in the final system represents elastic scattering of c, d in the static interaction

$$U_f\equiv U_f(\mathbf{r}_{cd})=\langle u_c(\mathbf{s}_c)u_d(\mathbf{s}_d)|V_f|u_c(\mathbf{s}_c)u_d(\mathbf{s}_d)\rangle. \tag{2-11}$$

When U_i is defined by Eq. (2-11), any term in V_i depending on $\mathbf{r}_{ab}$ only, $V_{12}(\mathbf{r}_{ab})$ say, will not appear in the interaction V_i-U_i of Eq. (2-7), because $\langle u_au_b|V_{12}(\mathbf{r}_{ab})u_au_b\rangle=V_{12}(\mathbf{r}_{ab})$. Since the atomic center of mass very nearly coincides with the position of the atomic nucleus, it now is apparent that in atomic collisions involving electronic rearrangement, the internuclear Coulomb interaction very nearly disappears from the distorted wave interaction V_i-U_i. Except in special circumstances when the remaining interactions in V_i-U_i yield unexpectedly small transition probabilities, the error made in altogether dropping the internuclear interaction from V_i-U_i will be of the order of m/M.

3. APPLICATION TO CHARGE TRANSFER

As an example of the utility of the method, we shall investigate the capture of electrons from atomic hydrogen by fast protons. For the reaction (1-1), H_i and V_i of Eq. (2-1) are, in the notation of Sec. 1,

$$H_i=-\frac{\hbar^2}{2\mu}\nabla_R^2-\frac{\hbar^2}{2\mu'}\nabla^2-\frac{e^2}{r_{2e}}, \tag{3-1}$$

$$V_i\equiv V_{12}+V_{1e}=\frac{e^2}{R_{12}}-\frac{e^2}{r_{1e}}, \tag{3-2}$$

where $\mu'=mM(M+m)^{-1}$, and ∇_2^2 represents the Laplacian with respect to $\mathbf{r}_{2e}$. U_i of Eq. (2-10) is

$$U_i(\mathbf{R})=\left\langle u(r_{2e})\left|\frac{e^2}{R_{12}}-\frac{e^2}{r_{1e}}\right|u(r_{2e})\right\rangle, \tag{3-3}$$

integrated over $\mathbf{r}_{2e}$ holding $\mathbf{R}$ constant. Since $u(r_{2e})$ is spherically symmetric, U_i is independent of the orientation of $\mathbf{R}$. $-\mathbf{R}_{12}=\mathbf{R}+m(M+m)^{-1}\mathbf{r}_{2e}$, and one finds

$$\begin{aligned}&\left\langle u(r_{2e})\left|\frac{1}{R_{12}}\right|u(r_{2e})\right\rangle\\&\qquad=\frac{1}{R}\left[\frac{1}{R}+\frac{M}{ma_o}\right]\exp\left(-\frac{2M}{m}\frac{R}{a_o}\right)\end{aligned} \tag{3-4}$$

with $a_o=\hbar^2/me^2$. Equation (3-4) shows $V_{12}-\langle u|V_{12}|u\rangle$ is indeed negligible at all significant values of $\mathbf{r}_{1e}$, $\mathbf{R}$ in the matrix element (2-7); the error made in dropping the proton-proton interaction from V_i-U_i is of the order m/M as stated. Similarly $\mathbf{r}_{1e}=M(m+M)^{-1}\mathbf{r}_{2e}-\mathbf{R}$, and

$$\left\langle u(r_{2e})\left|\frac{1}{r_{1e}}\right|u(r_{2e})\right\rangle=\frac{1}{R}\left[\frac{1}{R}+\frac{1}{a_o}\right]\exp\left(-\frac{2R}{a_o}\right), \tag{3-5}$$

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[25] H. S. W. Massey, Revs. Modern Phys. 28, 199 (1956); H. S. W. Massey, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36, p. 285.

so that, replacing R by R_{12} which simplifies the integration of (2-7) and again makes an error of order m/M,

$$V_i - U_i = e^2\left[\frac{1}{R_{12}} - \frac{1}{r_{1e}} - \left(\frac{1}{R_{12}} + \frac{1}{a_o}\right)\exp\left(-\frac{2R_{12}}{a_o}\right)\right]. \quad (3\text{-}6)$$

The reappearance of the term e^2/R_{12} in $V_i - U_i$ after its cancellation in $V_{12} - \langle u | V_{12} | u \rangle$, is a noteworthy consequence of the fact that in (3-5) we are evaluating the average value of $1/r_{1e}$ which, since the electron is centered at 2, naturally has a leading term proportional to $1/R_{12}$. If the electron interaction were anything but the inverse first power of r_{1e}, its average would not contain terms so similar to the proton-proton interaction; it is evident from (3-5) that $V_i - U_i$ will contain e^2/R_{12}, but not Ze^2/R_{12}, when the proton is incident on a hydrogenic atom with nuclear charge Ze.

4. FIRST-ORDER CROSS SECTION

We take as a first-order approximation to the amplitude $A(i \rightarrow f)$ of Eq. (2-7) a Born-like approximation in which, recollecting Eqs. (2-3) and (2-5), $\Psi_f^{(-)}$ and $\chi_i^{(+)}$ are replaced by the corresponding plane waves ψ_f and ψ_i of Eq. (1-4). The reaction (1-1) is so symmetric that, as in the usual Born approximation, no post-prior discrepancy is produced by our plane wave approximation to the exact $A(i \rightarrow f)$, i.e., $\langle \psi_f | V_i - U_i | \psi_i \rangle = \langle \psi_f | V_f - U_f | \psi_i \rangle$. Higher order approximations will be considered in a forthcoming paper. Then

$$\begin{aligned} I(i \rightarrow f) &\equiv (2\pi\hbar^2/\mu) A(i \rightarrow f) = \langle \psi_f | V_i - U_i | \psi_i \rangle \\ &= \int d\mathbf{r}_{2e} d\mathbf{R}\, u^*(r_{1e}) \exp[iK\mathbf{n}_f \cdot \mathbf{R}'] \\ &\qquad \times (V_i - U_i) u(r_{2e}) \exp[iK\mathbf{n}_i \cdot \mathbf{R}] \\ &= \int d\mathbf{r}_{2e} d\mathbf{r}_{1e}\, u^*(r_{1e}) \exp[-i\mathbf{A} \cdot \mathbf{r}_{1e}] \\ &\qquad \times (V_i - U_i) u(r_{2e}) \exp[i\mathbf{B} \cdot \mathbf{r}_{2e}]. \end{aligned} \quad (4\text{-}1)$$

In (4-1) we have used the quantities

$$\mathbf{A} = K\left(\mathbf{n}_i - \frac{M}{m+M}\mathbf{n}_f\right), \qquad \mathbf{B} = K\left(\frac{M}{m+M}\mathbf{n}_i - \mathbf{n}_f\right). \quad (4\text{-}2)$$

The plane waves (1-4) are so defined that $\mathbf{n}_f = \mathbf{n}_i$ when the incident proton 1 is undeflected. To lowest order in m/M

$$|\mathbf{A}| = |\mathbf{B}| = a_o^{-1} E^{\frac{1}{2}} (1+\lambda)^{\frac{1}{2}}, \quad (4\text{-}3)$$

where

$$\lambda = [(2M/m) \sin(\theta/2)]^2,$$

θ is the center-of-mass scattering angle, and $E = (\hbar v/2e^2)^2$ is the energy of the incoming proton in units of $2(137)^{-2}Mc^2 = 100$ kev. We shall also have need of the quantity $|\mathbf{A}-\mathbf{B}|$ which, to the same order in m/M, is

$$|\mathbf{A}-\mathbf{B}| = (\hbar v/e^2) a_o^{-1} = 2a_o^{-1}E^{\frac{1}{2}}.$$

Inserting (3-6), $I(i \rightarrow f)$ can be written in the form

$$I(i \rightarrow f) = I_{\mathrm{BK}} + I_{\mathrm{JS}} + I_{\mathrm{BG}}.$$

The first term

$$I_{\mathrm{BK}} = -e^2 \int d\mathbf{r}_{1e} d\mathbf{r}_{2e}\, u^*(r_{1e}) \exp[-i\mathbf{A} \cdot \mathbf{r}_{1e}] \times (1/r_{1e}) u(r_{2e}) \exp[i\mathbf{B} \cdot \mathbf{r}_{2e}], \quad (4\text{-}4)$$

is the matrix element considered by BK and evaluated by a number of authors.[1,26] We quote the results:

$$I_{\mathrm{BK}} = -32\pi e^2 a_o^2 [E(1+\lambda)+1]^{-3}. \quad (4\text{-}5)$$

The second term

$$I_{\mathrm{JS}} = e^2 \int d\mathbf{r}_{1e} d\mathbf{r}_{2e}\, u(r_{1e}) \exp[-i\mathbf{A} \cdot \mathbf{r}_{1e}] \frac{1}{R_{12}} \times u(r_{2e}) \exp[i\mathbf{B} \cdot \mathbf{r}_{2e}], \quad (4\text{-}6)$$

is the JS and BD matrix element. It has been exactly evaluated by JS, but is a special case of our third term and will be rewritten in our formalism. This third term, which in the present first-order distorted wave treatment represents a correction to the JS and BD results, is

$$\begin{aligned} I_{\mathrm{BG}} &= -e^2 \int d\mathbf{r}_{1e} d\mathbf{r}_{2e}\, u(r_{1e}) \exp[-i\mathbf{A} \cdot \mathbf{r}_{1e}] \\ &\qquad \times \left(\frac{1}{R_{12}} + \frac{1}{a_o}\right) \exp(-2R_{12}/a_o) \\ &\qquad \times u(r_{2e}) \exp[i\mathbf{B} \cdot \mathbf{r}_{2e}] \\ &= -e^2\left(1 - \frac{1}{a_o}\frac{\partial}{\partial y}\right) \int d\mathbf{r}_{1e} d\mathbf{r}_{2e}\, u(r_{1e}) \exp[-i\mathbf{A} \cdot \mathbf{r}_{1e}] \\ &\qquad \times \frac{1}{R_{12}} \exp(-yR_{12}) u(r_{2e}) \exp(i\mathbf{B} \cdot \mathbf{r}_{2e}) \\ y &= 2/a_o. \end{aligned} \quad (4\text{-}7)$$

This term is most readily evaluated in momentum space. We find, after making the appropriate transformations,

$$I_{\mathrm{BG}} = -\frac{32e^2}{\pi a_o^5}\left(1 - \frac{1}{a_o}\frac{\partial}{\partial y}\right) \int d\mathbf{p} \left[(\mathbf{p}+\mathbf{A})^2 + \frac{1}{a_o^2}\right]^{-2} \times (p^2+y^2)^{-1} [(\mathbf{p}+\mathbf{B})^2 + 1/a_o^2]^{-2} \quad (4\text{-}8)$$

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[26] M. N. Sahu and D. Basu, Indian J. Phys. **19**, 121 (1945).

$$y=2/a_o$$

$$=-\frac{8e^2}{\pi aba_o^5}\frac{\partial^2}{\partial a\partial b}\left(1-\frac{1}{a_o}\frac{\partial}{\partial y}\right)\int d\mathbf{p}\,[(\mathbf{p}+\mathbf{A})^2+a^2]^{-1}$$
$$\times(p^2+y^2)^{-1}[(\mathbf{p}+\mathbf{B})^2+b^2]^{-1}$$
$$y=2a=2b=2/a_o. \tag{4-9}$$

The integral

$$I'=\int d\mathbf{p}\,[(\mathbf{p}+\mathbf{A})^2+a^2]^{-1}(\mathbf{p}^2+y^2)^{-1}[(\mathbf{p}+\mathbf{B})^2+b^2]^{-1},$$

has been evaluated by Lewis,[27] with the result (adopting his notation)

$$I'=2\pi^2(\alpha\gamma-\beta^2)^{-\frac{1}{2}}\tan^{-1}\left[\frac{(\alpha\gamma-\beta^2)^{\frac{1}{2}}}{\beta}\right], \tag{4-10}$$

where

$$\alpha\gamma=[(\mathbf{A}-\mathbf{B})^2+(a+b)^2][A^2+(a+y)^2][B^2+(b+y)^2],$$

and

$$\beta=y[(\mathbf{A}-\mathbf{B})^2+(a+b)^2]+b(A^2+a^2+y^2)$$
$$+a(B^2+b^2+y^2).$$

Examining Eqs. (4-6)–(4-9), evidently

$$I_{\mathrm{JS}}=\frac{8e^2}{\pi aba_o^5}\frac{\partial^2}{\partial a\partial b}\int d\mathbf{p}\,[(\mathbf{p}+\mathbf{A})^2+a^2]^{-1}$$
$$\times p^{-2}[(\mathbf{p}+\mathbf{B})^2+b^2]^{-2}$$
$$a=b=a_o^{-1},$$

yielding

$$I_{\mathrm{JS}}=8\pi e^2a_o^2\left(\frac{(2+\lambda)\tan^{-1}E^{\frac{1}{2}}}{E^{\frac{1}{2}}[(1+\lambda)E+1]^3}+\frac{1}{2(1+E)^2[(1+\lambda)E+1]}-\frac{\lambda}{(1+E)[(1+\lambda)E+1]^3}\right), \tag{4-11}$$

I_{BG} is quite lengthy. In the limit $v\longrightarrow\infty$

$$I_{\mathrm{BG}}\sim-\frac{4\pi e^2a_o^2}{(1+E)^2[(1+\lambda)E+1]}. \tag{4-12}$$

Thus in the high-energy limit I_{BG} cancels the JS-BD I_{JS} term, so that the total amplitude I is given by I_{BK}, i.e., by the matrix element of the proton-electron interaction, as BK expected.

In Fig. 2 is shown (labeled BG) a representative plot of the differential cross section

$$\frac{d\sigma}{d\Omega}=\left(\frac{\mu}{2\pi\hbar^2}\right)^2|I_{\mathrm{BK}}+I_{\mathrm{JS}}+I_{\mathrm{BG}}|^2. \tag{4-13}$$

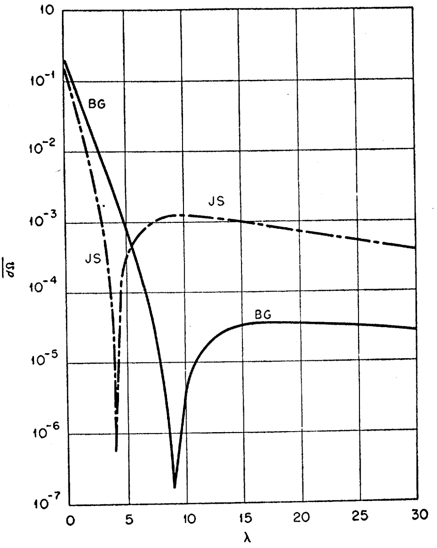

FIG. 2. Comparison of BG and JS angular distributions at proton energy of 25 kev. The angular distributions are in arbitrary units.

In the same graph is shown (labeled JS) the angular distribution predicted by JS-BD who use $I_{\mathrm{BK}}+I_{\mathrm{JS}}$, the matrix element of V_i. Both theories predict that the main contribution to the total capture cross section comes from small λ. However, the peaking in the present calculation is much more enhanced than in the corresponding JS cross section. A nonnegligible portion of their cross section comes from a "large" angle tail which has its origin in the deflection by the nuclear proton. Our correction term (I_{BG}) cancels this tail and restricts the significant region of λ to a single narrow lobe (which is somewhat broader however than the JS central lobe). We shall return to this point in the discussion of the impact parameter calculation where the effect is more striking.

The total cross section

$$\sigma=\pi\left(\frac{m}{M}\right)^2\left(\frac{\mu}{2\pi\hbar^2}\right)^2\int^\infty d\lambda\,|I_{\mathrm{BK}}+I_{\mathrm{BG}}+I_{\mathrm{JS}}|^2 \tag{4-14}$$

does not admit of analytic evaluation but must be integrated numerically. The results are shown in Figs. 7 and 8, Sec. 6.

5. IMPACT PARAMETER CALCULATION

Schiff[19] and Drisko[6] have shown that the probability amplitude $C_l(q)$ for electron capture by a proton whose impact parameter is q is given by

$$C_l(q)=\frac{m^2K}{2M^2}\frac{\mu}{2\pi\hbar^2}\int_0^\infty d\lambda\,J_0(E^{\frac{1}{2}}\lambda^{\frac{1}{2}}q/a_o)I(\lambda,E), \tag{5-1}$$

where $I(\lambda,E)$ is the capture amplitude.

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[27] R. R. Lewis, Phys. Rev. 102, 537 (1956).

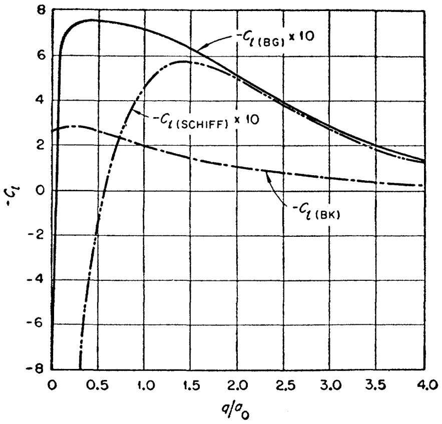

FIG. 3. The negative of the probability amplitude (C_l) at an energy of 25 kev as a function of impact parameter.

The cross section is then

$$\sigma = 2\pi\int_0^\infty qdq\,|C_l|^2, \qquad (5\text{-}2)$$

which can be shown to be the same as (4-14).

We have evaluated (5-1) with our first-order matrix element I of (4-1), over a range of impact parameters q at energies of 25 and 100 kev. The results are shown in Figs. 3 and 4, along with the comparable results of BK who consider only the electron-proton interaction V_{1e}, and those of Schiff who employs the matrix element $I_{\mathrm{BK}}+I_{\mathrm{JS}}$ of the total interaction V_i.

The BK results for 25 kev show transition probabilities greater than unity for small impact parameters. Those of Schiff, for the same energy, are more reasonable except for an unphysical region near zero impact parameter. There the transition probability is logarithmically infinite, a result of the wide-angle tail, $\sim\lambda^{-1}$ as $\lambda\rightarrow\infty$, in the JS-BD term (4-11). The addition of our correction term gives transition probabilities that are less than unity for all impact parameters at this energy. For 100 kev, the present theory and BK give physically allowable transition probabilities for all q, while those of Schiff diverge for very small q.

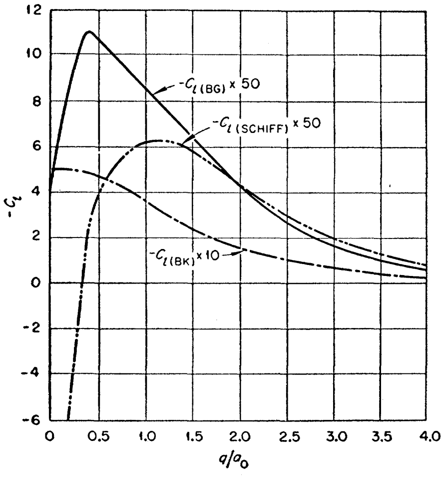

FIG. 4. The negative of the probability amplitude (C_l) at an energy of 100 kev as a function of the impact parameter.

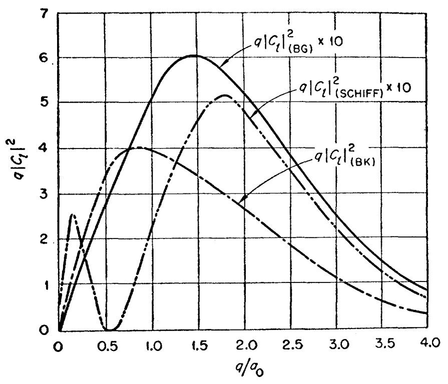

FIG. 5. The electron capture probability multiplied by q/a_0 for an energy of 25 kev. The areas under the curves are proportional to the respective cross sections.

In Figs. 5 and 6 the integrand of (5-2) is plotted as a function of q for the same energies. We see that the present theory and the theory of Schiff give roughly the same prediction for the important range of impact parameters contributing to the cross section. BK predict capture more probably taking place closer to the nucleus. The wide-angle I_{JS} tail here manifests itself in the unnatural vanishing of Schiff's integrand at impact parameters $\sim\frac{1}{2}a_0$.

6. CONCLUSIONS AND SUMMARY OF RESULTS

The scattering amplitude in the distorted wave formalism has been simply and rigorously derived. The method can be applied to rearrangements of, and excitation of, the incident aggregates. We think our expressions are simpler and easier to interpret than those given

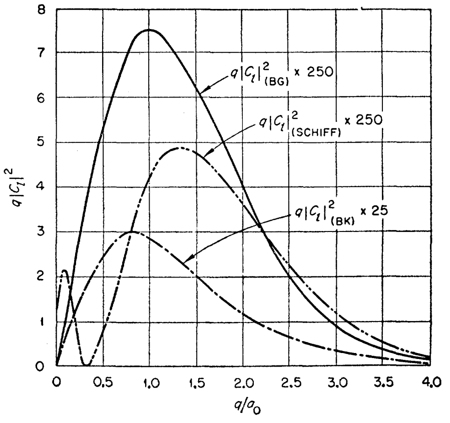

FIG. 6. The electron capture probability multiplied by q/a_0 for an energy of 100 kev. The areas under the curves are proportional to the respective cross section.

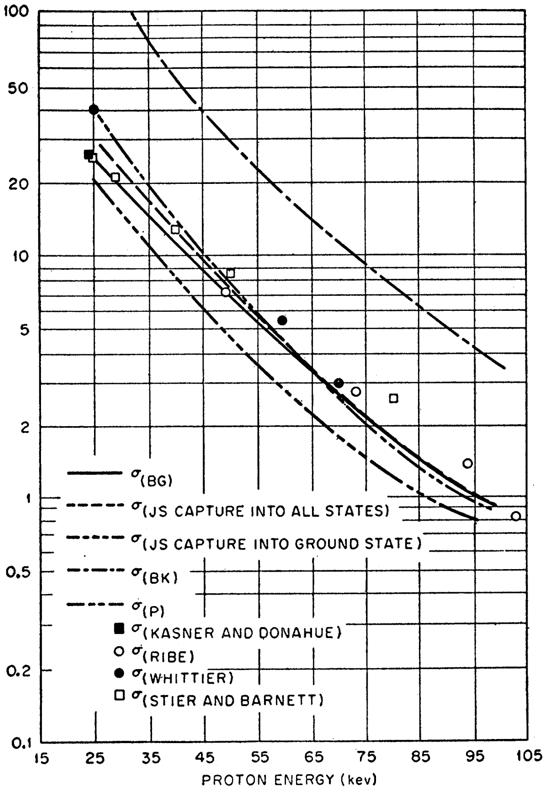

FIG. 7. Electron capture cross section. The theories (represented by curves) are for protons in atomic hydrogen. The experimental data (represented by single points) are in molecular hydrogen.

by Massey and co-workers,[28–30] especially when applied to rearrangement collisions.

The results of the application of our theory to the electron capture problem are displayed in Figs. 7 and 8. In Fig. 7 we have plotted the results of our calculations along with the results of JS,[31] BK, and Pradhan, and the properly normalized experimental data for energies less than 100 kev. In Fig. 8 we have compared our theory, the theory of Pradhan, and the JS cross section for capture into the ground state with the measurements of Barnett and Reynolds who have extended the energy range of the experiments. Our theory fits well to an energy of 200 kev. There our prediction diverges from the experimental points. We hold no brief for this apparent success or the success of the other theories. Our theory, and the JS-BD theory, neglects higher order matrix elements which should be of importance at these energies, and Pradhan has evaluated the wrong matrix element. Perhaps of more importance is the fact that these theories, perforce, have been compared with the experiments in molecular hydrogen. As Tuan and Gerjuoy[14] have pointed out, capture from molecular hydrogen is very different from capture in atomic hydrogen, and the agreement must be accidental. It is our opinion that judgment of the theories for atomic hydrogen should await the appropriate experiments.

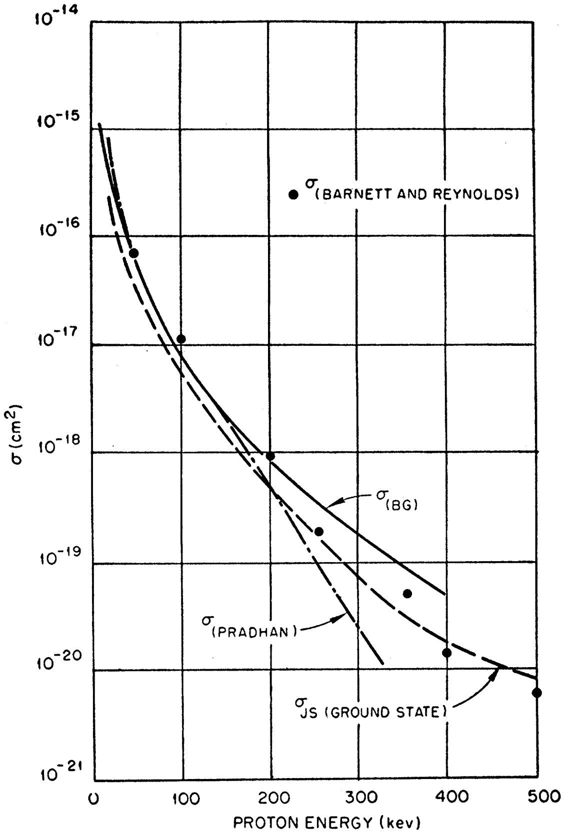

FIG. 8. Electron capture cross section (cm^2). The theories are for protons in atomic hydrogen; the experimental data are in molecular hydrogen.

We feel, however, that our first-order approximation shows important improvements over first Born approximation. In the high-energy limit our cross section reduces, as we have argued the correct first-order approximation to the exact cross section should do, to the BK cross section. The JS-BD Born approximation, in this limit, leads to a cross section with the same energy dependence as the BK cross section, but differing by a factor of 0.661. Also, the capture probabilities, predicted by an impact parameter calculation using the distorted wave amplitude, are physically reasonable at all impact parameters for energies greater than 25 kev. The corresponding probabilities for the JS-BD Born amplitude show an unphysical region for all energies.[19]

We believe the above comments, as well as a comparison of the angular distributions predicted by our

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[28] D. R. Bates *et al.*, Phil. Trans. Roy. Soc. (London) **A243**, 93 (1950–1951).

[29] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **A139**, 198 (1932).

[30] H. S. W. Massey and G. A. Erskine, Proc. Roy. Soc. (London) **A212**, 521 (1952).

[31] Two "Jackson and Schiff" curves are shown, one for capture only into the ground state, the second, taken from their paper, includes capture into all states. Multiplication of our ground state capture curve by the ratio of these two JS curves should yield a reasonable estimate of our (first-order distorted wave) predicted total capture cross section.

theory and the JS-BD theory, refute the argument of Bates[32] explaining the "success" of the conventional first Born approximation. Bates has derived a matrix element similar to ours but argues that for moderate or large inter-proton distances the interaction $(R_{12}^{-1}+a_o^{-1})\exp(-2R_{12}/a_o)$ is negligible compared with the interaction $R_{12}^{-1}-r_{1e}^{-1}$. But close encounters, as we have shown, are important in the capture process and the correction term cannot properly be dropped. Its inclusion changes the character of the interaction. In our opinion the "success" of either the JS-BD or our first-order theory in the intermediate energy range 35–200 kev still is not completely understood, because of the following (usually conveniently overlooked) difficulties: (i) In the classical limit the capture cross section should behave like v^{-11} at high velocities,[6] whereas the BK, JS-BD, and our cross sections all behave like v^{-12}. (ii) The impact parameter treatment of each of these theories shows that with increasing proton energy the cross section results from capture at smaller and smaller impact parameters, whereas physical expectation suggests capture should be possible for any proton passing through the electron cloud; in other words, although the total probability of capture decreases, there seems no reason why at high energies capture is possible only for those protons with vanishingly small impact parameters.

7. ACKNOWLEDGMENTS

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Charge Transfer in Molecular Hydrogen*

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The effects of the molecule on electron capture by protons in hydrogen gas have been investigated in first Born approximation with different types of electronic wave functions. It always has been supposed that if the incident proton velocity is large compared to electronic velocities molecular effects may be neglected, and that one may then assume one H_2 molecule is equivalent to two hydrogen atoms for purposes of charge transfer. Instead it appears that charge transfer in H_2 at high energies bears no simple relationship to charge transfer in atomic hydrogen. In particular, among other effects: (i) in the high-energy limit $\frac{1}{2}\sigma_M=1.2-1.4\sigma_A$; (ii) at lower energies there is important interference between the capture amplitudes from the two atoms in the molecule. It also is found that transitions to ungerade states of H_2^+, although unimportant in the energy range of present experiments, become appreciable at high energies.

1. INTRODUCTION

THE theoretical problem of the charge transfer reaction

$$p+H_1 \rightarrow H_1+p \qquad (1a)$$

has received considerable attention from a large number of investigators.[1–9] In the energy range from about 10^2 ev to 10^4 ev, the cross section σ_A for the above reaction has been measured by crossed beam techniques.[10] There are, however, no data available at energies well above 10 kev where the Born approxima-

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