Electron Capture by Protons Passing through Hydrogen*

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A formal treatment of the capture problem is presented and a suitable approximation scheme valid for fast collisions is developed. The approximation consists of: (1) using a suitable perturbed initial wave function instead of the unperturbed initial wave function used in the Born approximation, (2) neglecting the contribution of what we call two-step capture processes, and (3) in an impulse approximation fashion, neglecting the effect of the binding of the electron in the atom in the initial state "during" the collision. All the above three approximations result from an attempt to express the transition matrix for capture in terms of two-body operators. The improved wave function is orthogonal to the final wave function in the limit of infinitely heavy incident ion, unlike the Born approximation wave function. Consequently the (incident ion)-(nucleus) interaction has zero matrix element for transition from the initial state to the final state. Only the (incident ion)-(electron) interaction contributes to the capture cross section in this approximation. Good agreement with experiment is obtained in the particular case of protons picking up electrons from hydrogen gas for proton energies above 25 kev.

1. INTRODUCTION

1a. Review of Previous Theoretical Work

THEORETICAL work done so far on capture of electrons by ions passing through gases has been confined to the Born approximation[1–4] and other equivalent first-order approximations[5] for fast collisions. For slow collisions the method of "perturbed stationary states"[6] has been used. Oppenheimer[1] calculated the capture cross section for fast alpha particles passing through hydrogen gas using the Born approximation. The interaction Hamiltonian to be used in the Born approximation has two terms: (1) the Coulomb interaction between the alpha particle and the electron in the hydrogen atom, and (2) the Coulomb interaction between the alpha particle and the hydrogen nucleus. Oppenheimer neglected the contribution of the (alpha particle)-(hydrogen nucleus) interaction to the capture cross section. Such neglect is perfectly justified for inelastic collisions because the initial and final wave functions are orthogonal. In rearrangement collisions, such as the capture problem, however, this is not the case. Oppenheimer showed that the scalar product of the initial and final wave functions is small for fast collisions so that they can be considered approximately orthogonal. Following Oppenheimer, Brinkman and Kramers[2] (referred to hereinafter as BK) calculated the capture cross section for protons in hydrogen using Born approximation and neglecting the proton-proton interaction. They found for the cross section four times the experimental result for a proton energy of 100 kev and still larger value for lower energies. Jackson and Schiff[3] (referred to hereinafter as JS) and also Bates and Dalgarno,[4] on the other hand, have calculated the capture cross section using the complete interaction Hamiltonian in the Born approximation. Their results agree with experiment for proton energies above 25 kev ($e^2/\hbar v \leqslant 1$). Wick,[7] however, has pointed out that if one were to make an exact semiclassical calculation using an impact parameter treatment, the proton-proton interaction will give a negligible contribution to the capture cross section (of the order of m/M where m = electron mass and M = proton mass). Wick also points out that by an appropriate canonical transformation the proton-proton interaction can be removed from the total Hamiltonian in the limit $M/m \to \infty$. In view of Wick's remarks, the agreement of JS results with experiment looks paradoxical and, if his remarks are correct, it is not easy to see why BK's results should not agree with experiment.

1b. Summary of Results and Outline of Paper

In the present work the capture problem is investigated by the formal methods of collision theory and an approximation scheme is developed. The approximate wave function for the initial perturbed state obtained in the present work is found to be orthogonal to the final wave function in the limit of infinitely heavy protons. Consequently the proton-proton interaction does not contribute to the capture cross-section in keeping with Wick's remarks. It is also easily seen why BK's results do not agree with the experiment. The results obtained with this improved initial wave function agree very well with the experiment for energies above 25 kev.

A brief outline of the work leading to the above con-

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[1] J. R. Oppenheimer, Phys. Rev. **31**, 349 (1928).

[2] H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).

[3] J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953).

[4] D. R. Bates and A. Dalgarno, Proc. Phys. Soc. (London) **A65**, 919 (1952).

[5] K. Takayangi, Science Repts. Saitama Univ. Ser. A, **2**, 33 (1955).

[6] A. Dalgarno and H. N. Yadav, Proc. Phys. Soc. (London) **A66**, 173 (1953).

[7] See "Note added in proof" to the paper quoted in reference 3.

clusions runs as follows: First, an exact expression for the transition matrix for capture is derived following the formal methods of collision theory given by Gell-Mann and Goldberger.[8] The Møller matrix of this three-body system is then expressed in terms of two-body Møller matrices by using an operator identity given by Chew and Goldberger[9] in connection with the impulse approximation. The transition matrix expressed in terms of two-body operators has several terms. Some of these terms are small enough to be neglected. The terms that remain are shown to correspond to what we call direct or one-step capture and two-step capture processes. It is shown that the proton-proton interaction has zero matrix elements for direct capture in the limit $M/m\rightarrow\infty$. It has, however, nonzero matrix elements for two-step capture. This two-step capture is somewhat analogous to "double scattering" discussed by Chew and Goldberger[9] in connection with the impulse approximation. Since the two-step capture amplitude is one order higher in $e^2/\hbar v$ than the direct capture amplitude, it is neglected for energies for which $e^2/\hbar v<1$. The only term that contributes to direct capture is the one containing the proton-electron interaction. This term is evaluated and is found to give good agreement with experiment. Identity of protons is ignored because the cross section is so much peaked in the forward direction that the protons are effectively distinguishable. Capture into excited states has not been treated. The cross section for capture into excited states is presumably very small compared to that into the ground state. The calculations of BK, which are probably over-estimates, show that the cross section for capture into an excited state n decreases as $1/n^3$. We shall ignore the fact that the target hydrogen is actually in the form of molecular hydrogen.

2. DERIVATION OF EXACT TRANSITION MATRIX

In this section we shall derive an exact expression for the transition matrix for capture. Let us assign numbers 1, 2, and 3, respectively to the hydrogen nucleus, incident proton and the electron. Figure 1(a) represents symbolically the situation before collision and Fig. 1(b) that after collision, i.e., after capture. We look for the probability of transition from the state described by Fig. 1(a) to the state described by Fig. 1(b). Let

$$H=K+U_{12}+U_{13}+U_{23},$$
$$H_a=K+U_{13},$$
$$H_b=K+U_{23},$$

where K is the kinetic energy operator for the system of three particles and the U's are interaction potentials between the different particles denoted by the suffixes.

The transition probability is given by

$$\omega_{ba}(t)=|\langle\Phi_b(t)|\Psi_a(t)\rangle|^2/\langle\Psi_a(t)|\Psi_a(t)\rangle, \quad (1)$$

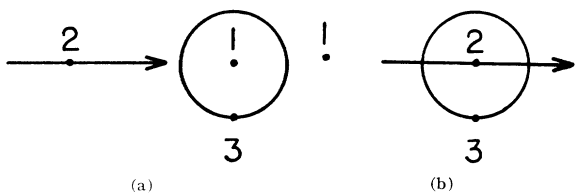

FIG. 1. (a) Situation before collision. (b) Situation after collision.

where $\Phi_b(t)$ and $\Psi_a(t)$ are state vectors defined by

$$H\Psi_a(t)=i\partial\Psi_a(t)/\partial t, \quad (2)$$
$$H_b\Phi_b(t)=i\partial\Phi_b(t)/\partial t. \quad (3)$$

(We use units such that $\hbar=1$.) We also need a state vector defined by

$$H_aU_a(t)=i\partial U_a(t)/\partial t. \quad (4)$$

The solutions of Eqs. (3) and (4) can be written as

$$\Phi_b(t)=\phi_be^{-iE_bt}, \quad (5)$$
$$U_a(t)=u_ae^{-iE_at}. \quad (6)$$

Following the methods of Gell-Mann and Goldberger,[8] we find for the transition probability per unit time (in the limit of infinite quantization volume)

$$\dot{\omega}_{ba}(0)=\lim_{\epsilon\rightarrow0^+}[-i\langle\phi_b|U_{12}+U_{13}|\Psi_a^\epsilon(0)\rangle \times\langle\phi_b|\Psi_a^\epsilon(0)\rangle^*+\text{c.c.}], \quad (7)$$

where

$$\Psi_a^\epsilon(0)=u_a+\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})u_a, \quad (8)$$

or

$$\Psi_a^\epsilon(0)=u_a+\frac{1}{E_a-K-U_{13}+i\epsilon}(U_{12}+U_{23})\Psi_a^\epsilon(0). \quad (9)$$

Equation (8) is the formal solution of Eq. (9). The latter is the integral equation for $\Psi_a^\epsilon(0)$. The introduction of the parameter ϵ is discussed in detail in reference 8. In the evaluation of cross section, ϵ is allowed to approach 0^+.

Our next step is to express $\langle\phi_b|\Psi_a^\epsilon(0)\rangle$ in terms of interaction potentials in a suitable form. For this we shall make use of Eq. (8). We then get

$$\langle\phi_b|\Psi_a^\epsilon(0)\rangle=\langle\phi_b|u_a\rangle+\left\langle\phi_b\left|\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})u_a\right.\right\rangle$$
$$=\langle\phi_b|u_a\rangle+\left\langle\phi_b\left|\frac{1}{E_a-H_b+i\epsilon}(U_{12}+U_{23})u_a\right.\right\rangle$$
$$+\left\langle\phi_b\left|\frac{1}{E_a-H_b+i\epsilon}(H-H_b)\right.\right.$$
$$\left.\left.\times\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})u_a\right.\right\rangle. \quad (10)$$

[8] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953). Also see: B. A. Lippmann, Phys. Rev. **102**, 264 (1956).
[9] G. F. Chew and M. L. Goldberger, Phys. Rev. **87**, 778 (1952).

Here we have made use of the operator relation

$$\frac{1}{P-Q}-\frac{1}{P}=\frac{1}{P-Q}Q\frac{1}{P}. \tag{11}$$

Now we have from Eqs. (3) and (5),

$$H_b\phi_b=E_b\phi_b, \tag{12}$$

and from Eq. (8),

$$\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})u_a=\Psi_a^{\epsilon}(0)-u_a. \tag{13}$$

Making use of Eqs. (12) and (13) in Eq. (10), we obtain

$$\langle\phi_b|\Psi_a^{\epsilon}(0)\rangle = \langle\phi_b|u_a\rangle+\frac{1}{E_a-E_b+i\epsilon}[\langle\phi_b|U_{12}+U_{13}|\Psi_a^{\epsilon}(0)\rangle - \langle\phi_b|K+U_{13}|u_a\rangle+\langle\phi_b|K+U_{23}|u_a\rangle],$$

and since

$$(K+U_{23})\phi_b=E_b\phi_b, \quad (K+U_{13})u_a=E_au_a,$$

we have

$$\langle\phi_b|\Psi_a^{\epsilon}(0)\rangle=(1+E_b-E_a)\langle\phi_b|u_a\rangle + \frac{1}{E_a-E_b+i\epsilon}\langle\phi_b|U_{12}+U_{13}|\Psi_a^{\epsilon}(0)\rangle. \tag{14}$$

Since $\langle\phi_b|u_a\rangle$ is real, we get, by substituting Eq. (14) into Eq. (7),

$$\dot{\omega}_{ba}(0)=\lim_{\epsilon\to 0^+}\left[|\langle\phi_b|U_{12}+U_{13}|\Psi_a^{\epsilon}(0)\rangle|^2\frac{2\epsilon}{(E_a-E_b)^2+\epsilon^2}\right], \tag{15}$$

or

$$\dot{\omega}_{ba}(0)=2\pi|\langle\phi_b|U_{12}+U_{13}|\Psi_a^{(+)}\rangle|^2\delta(E_a-E_b) =2\pi|R_{ba}^{(+)}|^2\delta(E_a-E_b), \tag{16}$$

where

$$R_{ba}^{(+)}=\langle\phi_b|U_{12}+U_{13}|\Psi_a^{(+)}\rangle, \quad \Psi_a^{(+)}=\lim_{\epsilon\to 0^+}\Psi_a^{\epsilon}(0). \tag{17}$$

$R_{ba}^{(+)}$ is the transition matrix or, as we shall call it, the capture amplitude. The interaction U_{23} is, of course, concealed in the integral Eq. (9) for $\Psi_a^{(+)}$.

One can derive an alternative expression for R_{ba} where U_{23} appears more explicitly. For this we define the incoming wave state vector $\Psi_b^{(-)}$:

$$\Psi_b^{(-)}=\phi_b+\frac{1}{E_b-K-U_{23}-i\epsilon}(U_{13}+U_{12})\Psi_b^{(-)}, \tag{18}$$

which has the formal solution

$$\Psi_b^{(-)}=\phi_b+\frac{1}{E_b-H-i\epsilon}(U_{12}+U_{13})\phi_b. \tag{19}$$

From Eqs. (17) and (8), we have, since $E_a=E_b$,

$$\begin{aligned}R_{ba}&=\langle\phi_b|U_{12}+U_{13}|u_a\rangle \\ &\quad+\left\langle\phi_b|U_{12}+U_{13}|\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})u_a\right\rangle \\ &=\langle\phi_b|U_{12}+U_{13}|u_a\rangle \\ &\quad+\left\langle\frac{1}{E_a-H-i\epsilon}(U_{12}+U_{13})\phi_b|U_{12}+U_{23}|U_a\right\rangle \\ &=\langle\phi_b|U_{12}+U_{13}|u_a\rangle+\langle(\Psi_b^{(-)}-\phi_b)|U_{12}+U_{23}|u_a\rangle \\ &=\langle\Psi_b^{(-)}|U_{12}+U_{23}|u_a\rangle+\langle\phi_b|U_{13}-U_{23}|u_a\rangle \\ &=\langle\Psi_b^{(-)}|U_{12}+U_{23}|u_a\rangle \\ &\quad+\langle\phi_b|K+U_{13}|u_a\rangle-\langle\phi_b|K+U_{23}|u_a\rangle \\ &=\langle\Psi_b^{(-)}|U_{12}+U_{23}|u_a\rangle+(E_a-E_b)\langle\phi_b|u_a\rangle,\end{aligned}$$

or

$$R_{ba}^{(-)}=\langle\Psi_b^{(-)}|U_{12}+U_{23}|u_a\rangle. \tag{20}$$

In this expression for the capture amplitude, U_{23} appears explicitly. It is to be noted that expressions (17) and (20) are equivalent. We shall use the form given by Eq. (17). The Born approximation is obtained if $\Psi_a^{(+)}$ and $\Psi_b^{(-)}$ in Eqs. (17) and (20) are replaced by u_a and ϕ_b respectively. Since Eqs. (17) and (20) equivalent, it then follows that

$$\langle\phi_b|U_{13}|u_a\rangle=\langle\phi_b|U_{23}|u_a\rangle.$$

3. APPROXIMATE REDUCTION TO TWO-BODY OPERATORS

We now begin to express the exact capture amplitude in terms of two-body operators in so far as possible. As mentioned in the previous section, we shall use Eq. (17) for our reduction. It is convenient to introduce the Møller wave function matrix $\Omega^{(+)}$, defined by

$$\Psi_a^{(+)}=\Omega^{(+)}u_a.$$

It then follows from the integral equation for $\Psi_a^{(+)}$, that

$$\Omega^{(+)}=1+\frac{1}{E_a-K-U_{13}+i\epsilon}(U_{12}+U_{23})\Omega^{(+)}.$$

The formal solution of this integral equation is given by

$$\Omega^{(+)}=1+\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23}). \tag{21}$$

When expressed in terms of $\Omega^{(+)}$, Eq. (17) becomes

$$R_{ba}^{(+)}=\langle\phi_b|U_{12}+U_{13}|\Omega^{(+)}u_a\rangle. \tag{22}$$

We now define two-body Møller matrices and two-body

state vectors by the following integral equations:

$$\omega_{23}^{(+)}=1+\frac{1}{E_m-K-U_{23}+i\epsilon}U_{23}, \tag{23a}$$

$$\omega_{13}^{(-)}=1+U_{13}\frac{1}{E_n-K-U_{13}+i\epsilon}, \tag{23b}$$

$$\psi_m^{(+)}(23)=\chi_m+\frac{1}{E_m-K+i\epsilon}U_{23}\psi_m^{(+)}(23), \tag{24a}$$

$$\psi_n^{(-)}(13)=\chi_n+\frac{1}{E_n-K-i\epsilon}U_{13}\psi_n^{(-)}(13). \tag{24b}$$

The χ's are the wave functions for the system of three particles when there is no interaction between them. $\psi_m^{(+)}(23)$ is the wave function of the system of three particles when there is interaction between particles 2 and 3 only. Similarly, $\psi_n^{(-)}(13)$ is the wave function of the system when there is interaction between particles 1 and 3 only. The superscript $(+)$ stands for outgoing waves and superscript $(-)$ stands for incoming waves. This is clearly seen from the structure of the integral equations. The differential equations for χ's and ψ's are

$$K\chi_n=E_n\chi_n,$$
$$(K+U_{23})\psi_m^{(+)}(23)=E_m\psi_m^{(+)}(23),$$
$$(K+U_{13})\psi_n^{(-)}(13)=E_n\psi_n^{(-)}(13),$$

where the appropriate boundary conditions are imposed on the ψ's. It is now obvious that the ψ's are products of Coulomb wave functions and plane waves. It follows from Eqs. (23) and (24) that

$$\omega_{23}^{(+)}\chi_m=\psi_m^{(+)}(23), \quad \omega_{13}^{(-)}\chi_n=\psi_n^{(-)}(13).$$

With these definitions and preliminaries, we are now in a position to express the transition matrix given by Eq. (22) in terms of two-body Møller matrices. For this we make use of an identity used by Chew and Goldberger.[9] According to this, if

$$B^{(+)}=\frac{1}{E_a-K-U_{13}-V_a+i\epsilon}A,$$

and

$$b_{2k}^{(+)}=\frac{1}{E_a-K-U_{2k}+i\epsilon}A,$$

where $V_a=U_{12}+U_{23}$, and A is an arbitrary operator, then

$$B^{(+)}=b_{2k}^{(+)}+\frac{1}{E_a-K-U_{13}-V_a+i\epsilon}\times\{[U_{13},b_{2k}^{(+)}]+(V_a-U_{2k})b_{2k}^{(+)}\}.$$

Using this identity, we get

$$\frac{1}{E_a-H+i\epsilon}(U_{12}+U_{23})=(\omega_{23}^{(+)}-1)+\frac{1}{E_a-H+i\epsilon}[U_{13},\omega_{23}^{(+)}]+\frac{1}{E_a-H+i\epsilon}U_{12}\omega_{23}^{(+)},$$

so that

$$\Omega^{(+)}=1+\frac{1}{E_0-H+i\epsilon}(U_{12}+U_{23})=\omega_{23}^{(+)}+\frac{1}{E_a-H+i\epsilon}U_{12}\omega_{23}^{(+)}+\frac{1}{E_a-H+i\epsilon}[U_{13},\omega_{23}^{(+)}], \tag{25}$$

and consequently the expression for transition matrix expressed in terms of $\omega_{23}^{(+)}$ becomes

$$R_{ba}^{(+)}=\langle\phi_b|\,U_{12}+U_{13}\,|\omega_{23}^{(+)}u_a\rangle+\left\langle\phi_b|\,U_{12}+U_{13}\,|\frac{1}{E_a-H+i\epsilon}U_{12}\omega_{23}^{(+)}u_a\right\rangle+\left\langle\phi_b|\,U_{12}+U_{13}\,|\frac{1}{E_a-H+i\epsilon}[U_{13},\omega_{23}^{(+)}]u_a\right\rangle. \tag{26}$$

This expression still contains the three-body operator $1/(E_a-H+i\epsilon)$, and so we try to reduce it further into two-body operators $\omega_{13}^{(-)}$. This is done by making use of the relation

$$B^{(-)}=b_{1k}^{(-)}+\{[b_{1k},U_{23}]+b_{1k}^{(-)}(V_b-U_{1k})\}\times\frac{1}{E_b-K-U_{23}-V_b+i\epsilon},$$

where

$$B^{(-)}=A\frac{1}{E_b-K-U_{23}-V_b+i\epsilon},$$

$$b_{1k}^{(-)}=A\frac{1}{E_b-K-U_{1k}+i\epsilon}, \quad V_b=U_{13}+U_{12}.$$

Using this relation we have

$$(U_{12}+U_{13})\frac{1}{E_a-H+i\epsilon}=(\omega_{13}^{(-)}-1)+\{[\omega_{13}^{(-)},U_{23}]+\omega_{13}^{(-)}U_{12}\}\frac{1}{E_a-H+i\epsilon}. \tag{27}$$

We now make use of Eq. (27) in the second and third terms of Eq. (26) as a second step of an iteration procedure. It is then enough to keep only the first term in Eq. (27). We thus get the following approximate expression for the transition matrix:

$$R_{ba}^{(+)}=\langle\phi_b|\,U_{12}+U_{13}|\,\omega_{23}^{(+)}u_a\rangle +\langle\phi_b|\,(\omega_{13}^{(-)}-1)U_{12}|\,\omega_{23}^{(+)}u_a\rangle +\langle\phi_b|\,(\omega_{13}^{(-)}-1)([U_{13},\omega_{23}^{(+)}])|\,u_a\rangle. \quad (28)$$

The third term in Eq. (28) contains the commutator $[U_{13},\omega_{23}^{(+)}]$. U_{13} does not commute with $\omega_{23}^{(+)}$, because $\omega_{23}^{(+)}$ contains the operator K. The assumption that the third term is small is precisely what is called the impulse approximation. Chew and Wick[10] have given as a rough criterion for its validity, the relation:

$$\langle\tau[U_{13},\omega_{23}^{(+)}]\rangle_{Av}\ll 1, \quad (29)$$

where τ is the "collision time" and is equal to the inverse of the extent to which conservation of energy is violated during collision. The left-hand side of Eq. (29) is certainly less than $e^2/\hbar v$, and in keeping with our approximations we shall consequently drop the third term in Eq. (28).

Let us now examine the second term in Eq. (28). We shall designate the capture process represented by this term as a two-step capture process and the capture process represented by the first term as a direct or one-step capture process. The justification for this designation will be clear from the following discussion. The first term is the sum of matrix elements of U_{13} and U_{12} between the state $\omega_{23}^{(+)}u_a$ and the state ϕ_b. It will be shown later that $\omega_{23}^{(+)}u_a$ is proportional to the continuum wave function of the hydrogen atom formed by particles 2 and 3. The term $\langle\phi_b|\,U_{12}|\,\omega_{23}^{(+)}u_a\rangle$ and $\langle\phi_b|\,U_{13}|\,\omega_{23}^{(+)}u_a\rangle$ in Eq. (28) represent direct capture from the continuum states of the hydrogen atom 23 to the ground state of the same hydrogen atom through the interactions U_{12} and U_{13}, respectively. The term

$$\langle\phi_b|\,(\omega_{13}^{(-)}-1)U_{12}|\,\omega_{23}^{(+)}u_a\rangle$$

also represents a capture from the continuum state $\omega_{23}^{(+)}u_a$ to the ground state ϕ_b of the hydrogen atom 23, but not directly. It takes place through two successive interactions, U_{21} and U_{13}, and hence we designate this as a two-step capture. Such processes are less likely than the direct capture process by a factor of $e^2/\hbar v$ as is evident from Eq. (28) and so we can neglect the second term in Eq. (28) for fast collisions.

It is worthwhile to mention that the third term in Eq. (28) vanishes more rapidly with proton energy than the second term. This is seen as follows: In the high-energy limit $\omega_{23}^{(+)}\to 1$. When this limit is approached, the third term approaches zero while the second term remains finite.

It is now clear that we obtain a fairly good approximation by retaining only the first term in Eq. (28):

$$R_{ba}^{(+)}\simeq\langle\phi_b|\,U_{12}+U_{13}|\,\omega_{23}^{(+)}u_a\rangle. \quad (30)$$

[10] G. F. Chew and G. C. Wick, Phys. Rev. **85**, 636 (1952).

4. COMPUTATION OF THE CROSS SECTION

We shall now compute the cross section for capture using the approximate transition matrix given by Eq. (30). The differential cross section for capture is given by

$$\frac{d\sigma_{ba}}{d\Omega}=\left(\frac{\mu}{2\pi\hbar^2}\right)^2|\,R_{ba}^{(+)}|^2\frac{v_b}{v_a}, \quad (31)$$

where v_a and v_b are relative velocities before and after collision, respectively, and are related by the following equation by energy conservation:

$$\tfrac{1}{2}\mu v_a^2-\epsilon_a=\tfrac{1}{2}\mu b_b^2-\epsilon_b,$$

where $\mu=[(M+m)M]/(2M+m)$ is the reduced mass of the system, ϵ_a and ϵ_b are binding energies of the hydrogen atom before and after collision, respectively. For capture into the ground state, $\epsilon_a=\epsilon_b$ and $v_a=v_b$.

In order to compute $d\sigma/d\Omega$ we have to evaluate the transition matrix $R_{ba}^{(+)}$ given by Eq. (30). It will be shown in the Appendix A that

$$\langle\phi_b|\,U_{12}|\,\omega_{23}^{(+)}u_a\rangle=0 \quad (32)$$

in the limit $M/m\to\infty$, so that we have

$$R_{ba}=\langle\phi_b|\,U_{13}|\,\omega_{23}u_a\rangle. \quad (33)$$

We shall drop the superscript (+) hereafter. The integral given by Eq. (33) is difficult to evaluate. Fortunately, there exists an approximate identity between this integral and that obtained by replacing U_{13} by U_{23} in Eq. (33), i.e.

$$\langle\phi_b|\,U_{13}|\,\omega_{23}u_a\rangle\simeq\langle\phi_b|\,U_{23}|\,\omega_{23}u_a\rangle. \quad (34)$$

The validity of this approximation will be discussed in the Appendix B. Thus our working formula for R_{ba} now becomes

$$R_{ba}=\langle\phi_b|\,U_{23}|\,\omega_{23}u_a\rangle. \quad (35)$$

The coordinate system to be used for the computation is described below. Figure 2 gives the geometry of the

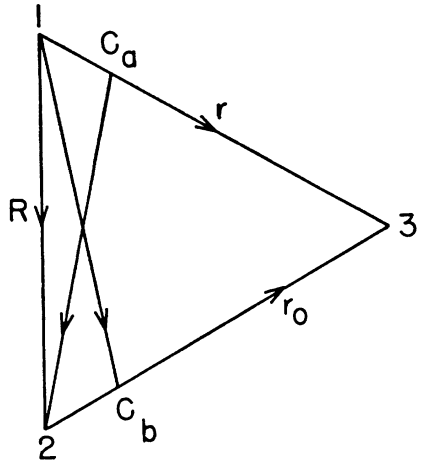

FIG. 2. Relative coordinates used for the computation of transition matrix.

relative coordinates. C_a and C_b are the centers of mass of particles 1 and 3 and of particles 2 and 3 respectively. Relative coordinate vector between 1 and 2 is $\mathbf{R}$, between 2 and 3 is $\mathbf{r}_0$, and between 1 and 3 is $\mathbf{r}$. It is clear from the geometry that the relative coordinate vector $\mathbf{R}_{13,2}$ between C_a and 2 is $(\mathbf{r}-a\mathbf{r}_0)$ and the relative coordinate vector $\mathbf{R}_{23,1}$ between C_b and 1 is $(a\mathbf{r}-\mathbf{r}_0)$, where $a=M/(M+m)$. Let the momentum vectors conjugate to the coordinate vectors $\mathbf{r}_0$, $\mathbf{R}_{23,1}$ and $\mathbf{R}_{13,2}$ be $\mathbf{K}$, $\mathbf{K}_{23,1}$ and $\mathbf{K}_{13,2}$, respectively. Our next task is to write down expressions for u_a, ϕ_b, χ_l and $\psi_l(23)$ in terms of the above coordinates and momenta. We have

$$u_a=\frac{1}{(2\pi)^{\frac{3}{2}}}\exp[i\mathbf{k}_0\cdot(a\mathbf{r}-\mathbf{r}_0)]\varphi_{1s}(\mathbf{r}), \tag{36a}$$

$$\phi_b=\frac{1}{(2\pi)^{\frac{3}{2}}}\exp[i\mathbf{k}_s\cdot(\mathbf{r}-a\mathbf{r}_0)]\varphi_{1s}(\mathbf{r}_0), \tag{36b}$$

where φ_{1s} is the hydrogen atom ground state wave function.

$$\chi_l=\frac{1}{(2\pi)^{\frac{3}{2}}}\exp[i(\mathbf{K}+a\mathbf{K}_{23,1})\cdot\mathbf{r}_0-i\mathbf{K}_{23,1}\cdot\mathbf{r}], \tag{36c}$$

and

$$\psi_l(23)=N(K)\chi_l F(isa/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0), \tag{36d}$$

where

$$N(K)=e^{+\frac{1}{2}\pi\alpha}\Gamma(1-i\alpha),\quad \alpha=as/K,\quad s=1/a_0,$$

a_0 being the Bohr radius. F stands for the confluent hypergeometric function. The arguments of this function are properly chosen so as to correspond to outgoing waves.

We now proceed to evaluate the integral given in Eq. (35). For this we expand u_a in the complete set of eigenfunctions χ_l:

$$u_a=\sum_l \chi_l\langle\chi_l|u_a\rangle,$$

so that

$$\omega_{23}u_a=\sum_l \omega_{23}\chi_l\langle\chi_l|u_a\rangle=\sum_l\psi_l(23)\langle\chi_l|u_a\rangle. \tag{37}$$

Using expressions for χ_l and u_a given in Eq. (36), we get

$$\langle\chi_l|u_a\rangle=\frac{1}{(2\pi)^3}\int d\mathbf{r}\int d\mathbf{r}_0\varphi_{1s}(\mathbf{r})\times\exp[i(a\mathbf{k}_0+\mathbf{K}_{23,1})\cdot\mathbf{r}+i(\mathbf{k}_0+a\mathbf{K}_{23,1}+\mathbf{K})\cdot\mathbf{r}_0]=G_{1s}(a\mathbf{k}_0+\mathbf{K}_{23,1})\delta(\mathbf{k}_0+a\mathbf{K}_{23,1}+\mathbf{K}), \tag{38}$$

where

$$G_{1s}(\mathbf{K})=\int d\mathbf{r}e^{i\mathbf{K}\cdot\mathbf{r}}\varphi_{1s}(\mathbf{r})=\frac{8\pi^{\frac{1}{2}}s^{\frac{5}{2}}}{(s^2+K^2)^2}$$

is the Fourier transform of the hydrogen atom ground state wave function. Substituting Eq. (38) into Eq. (37) and using the expression (36d) for $\psi_l(23)$, we get, after integrating over $\mathbf{K}_{23,1}$ space by making use of the δ function,

$$\omega_{23}u_a=\frac{1}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{K}G_{1s}(\mathbf{K})\exp[i(1/a)(\mathbf{k}_0+\mathbf{K})\cdot\mathbf{r}-i\mathbf{k}_0\cdot\mathbf{r}_0]N(K)F(isa/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0). \tag{39}$$

Using this we get

$$\begin{aligned}R_{ba}&=\langle\phi_b|U_{23}|\omega_{23}u_a\rangle\\&=\frac{-e^2}{(2\pi)^3}\int d\mathbf{r}\int d\mathbf{r}_0\int d\mathbf{K}\frac{1}{r_0}\varphi_{1s}^*(\mathbf{r}_0)\\&\quad\times\exp[i\mathbf{p}\cdot\mathbf{r}_0+i(1/a)(\mathbf{K}-\mathbf{p})\cdot\mathbf{r}]\\&\quad\times G_{1s}(\mathbf{K})N(K)F(isa/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0)\\&=-e^2a\int d\mathbf{r}_0\int d\mathbf{K}(1/r_0)\delta(\mathbf{K}-\mathbf{p})\\&\quad\times\exp(i\mathbf{p}\cdot\mathbf{r}_0]\varphi_{1s}^*(\mathbf{r}_0)G_{1s}(\mathbf{K})N(K)\\&\quad\times F(isa/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0).\end{aligned} \tag{40a}$$

Performing the integration over $\mathbf{K}$ space we get

$$\langle\phi_b|U_{23}|\omega_{23}u_a\rangle=-e^2a\int d\mathbf{r}_0N(p)G_{1s}(\mathbf{p})\frac{e^{i\mathbf{p}\cdot\mathbf{r}_0}}{r_0}\varphi_{1s}^*(\mathbf{r}_0)\times F(isa/p,1,ipr_0-i\mathbf{p}\cdot\mathbf{r}_0). \tag{40b}$$

Here $\mathbf{p}=a\mathbf{k}_s-\mathbf{k}_0$, so that $p^2=(k_0^2/g^2)+4k_0^2\sin^2(\theta/2)$, where $k_0=|\mathbf{k}_0|=|\mathbf{k}_s|$, $g=M/m$, and θ is the angle between $\mathbf{k}_0$ and $\mathbf{k}_s$.

At this point it will be worthwhile to attempt to visualize as to what kind of process the transition matrix $R_{ba}=\langle\phi_b|U_{23}|\omega_{23}u_a\rangle$ represents physically and how is this illustrated in the structure of the integrands in Eqs. (40a) and (40b). To start with we have a state u_a which represents a proton approaching a neutral hydrogen atom in its ground state. This state is perturbed by the potential U_{23} when the proton comes close to the hydrogen atom giving a perturbed state $\omega_{23}u_a$. From Eqs. (37) and (39) it is clear that the state $\omega_{23}u_a$ represents the scattering of particle 2 by a wave packet of the particle 3 which has the same momentum distribution as that of the hydrogen atom ground state. In other words, $\omega_{23}u_a$ describes a continuum of states of particles 2 and 3 interacting through their Coulomb potential, but one of them has a momentum distribution restricted in a definite manner. Capture is the process of transition from this state $\omega_{23}u_a$ to the state ϕ_b through the interaction U_{23}. The δ function in the integrand of Eq. (40a) tells us further that only those states of the continuum states $\omega_{23}u_a$ which have a momentum $\mathbf{K}=\mathbf{p}$ can make transition to the state ϕ_b. Equation (40b) shows that the transition matrix $\langle\phi_b|U_{23}|\omega_{23}u_a\rangle$ is pro-

portional to the matrix element of U_{23} between the continuum state, with momentum $\mathbf{p}$, of the hydrogen atom formed by 2 and 3 and the ground state of the same hydrogen atom, i.e.,

$$\langle\phi_b|U_{23}|\omega_{23}u_a\rangle=(2\pi)^{\frac{3}{2}}aG_{1s}(\mathbf{p})\langle\varphi_{1s}(\mathbf{r}_0)|U_{23}|\mathcal{U}_c(\mathbf{p},\mathbf{r}_0)\rangle$$
$$=-e^2aN(p)G_{1s}(\mathbf{p})(s^3/\pi)^{\frac{1}{2}}I, \tag{40c}$$

where

$$I=\int d\mathbf{r}e^{-r_0s}\frac{e^{i\mathbf{p}\cdot\mathbf{r}_0}}{r_0}F(isa/p,1,ipr_0-i\mathbf{p}\cdot\mathbf{r}_0), \tag{41}$$

and $\mathcal{U}_c$ is the hydrogen atom continuum wave function with momentum $\mathbf{p}$. It should be noted here that BK's result would follow if our perturbed initial wave function $\omega_{23}u_a$ is approximated by the unperturbed wave function u_a. This is equivalent to putting

$$N(p)F(isa/p,1,ipr_0-i\mathbf{p}\cdot\mathbf{r}_0)$$

equal to unity. This would be possible if $as/p\ll1$. One finds, however, that the transition matrix is large for small values of p, i.e., for small angles between $\mathbf{k}_0$ and $\mathbf{k}_s$. Thus for the most important scattering angles, $as/p>1$ and hence $\omega_{23}u_a$ cannot in general be approximated by u_a unless the energy of the incoming proton is very large.

The integral given in Eq. (41) is evaluated in Appendix C. The result is:

$$I=\frac{4\pi}{s^2+p^2}\exp\left[\frac{2s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right], \tag{42}$$

Substituting this in Eq. (40c), we obtain

$$R_{ba}=\frac{4\pi^{\frac{1}{2}}N(p)G_{1s}(p)s^{\frac{3}{2}}}{(s^2+p^2)}\exp\left[\frac{2s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right]; \tag{43}$$

and using this expression for R_{ba} in Eq. (31), we get the following expression for the differential cross section:

$$\frac{d\sigma}{d\Omega}=\frac{64g^2s^{10}}{(s^2+p^2)^6}\frac{\pi s/p}{\sinh(\pi s/p)}\exp\left[\frac{4s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right]$$
$$=\frac{d\sigma_{BK}}{d\Omega}\cdot\frac{\pi s/p}{\sinh(\pi s/p)}\exp\left[\frac{4s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right], \tag{44}$$

or

$$\frac{d\sigma}{d\Omega}=\frac{d\sigma_{BK}}{d\Omega}f(\theta),$$

where

$$f(\theta)=\frac{\pi s/p}{\sinh(\pi s/p)}\exp\left[\frac{4s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right].$$

For large θ, $d\sigma/d\Omega\to d\sigma_{BK}/d\Omega$ and for small values of θ, $d\sigma/d\Omega<d\sigma_{BK}/d\Omega$. The factor $f(\theta)$ reduces the BK cross section in the most important range of angles and approaches unity for angles where the cross section is so small that the contribution to the total cross section from these angles is practically zero. Integrating over all angles we get the total cross section:

$$\sigma=2\pi\int_0^\pi\frac{d\sigma}{d\Omega}\sin\theta d\theta=\frac{128\pi s^2g^2A}{k_0^2}(\pi a_0^2), \tag{45}$$

where

$$A=\int_{k_0/sg}^{2k_0/g}dx\frac{\exp[(4/x)\arctan(1/x)-(\pi/x)]}{(1+x^2)^6\sinh(\pi/x)}. \tag{46}$$

The integration variable $x=p/s$ is introduced for convenience in doing the numerical computation of A. It was not possible to evaluate the integral in Eq. (46) analytically.

5. COMPARISON WITH BORN APPROXIMATIONS OF BK AND JS

In this section we shall discuss the relation of the present work to the earlier work of BK and JS. Both of these sets of authors use Born approximation, the difference being that BK consider only the proton-proton forces. We shall see that both results may be obtained as further approximations to our result. Furthermore we shall see that the paradoxical situation noted by Wick may also be understood quite readily.

Our final expression for the transition matrix has been written as

$$R_{ba}=\langle\phi_b|U_{12}+U_{13}|\omega_{23}u_a\rangle.$$

The result of JS is obtained by replacing ω_{23} by unity:

$$R_{ba}(\mathrm{JS})=\langle\phi_b|U_{12}+U_{13}|u_a\rangle. \tag{47}$$

Actually this is not a bad approximation here, but it has the unfortunate effect of distorting the physics rather badly. The point is that

$$\langle\phi_b|U_{12}|\omega_{23}u_a\rangle=0$$

in the limit of infinite proton mass as already mentioned. Thus we obtain

$$R_{ba}=\langle\phi_b|U_{13}|\omega_{23}u_a\rangle.$$

We see then that Wick's assertion that the proton-proton interaction should play no role is verified and that the proton-electron interaction alone is needed. The critical point is that one can no longer replace ω_{23} by unity, since Eq. (32) is then badly wrong. What happens is that in our case the reduction of the BK result

$$R_{ba}(\mathrm{BK})=\langle\phi_b|U_{13}|u_a\rangle$$

is brought about by the use of an improved wave function ($\omega_{23}u_a$ instead of u_a); in the work of JS, $R_{ba}(\mathrm{BK})$ is reduced by the fact that $\langle\phi_b|U_{12}|u_a\rangle$ interferes destructively with $\langle\phi_b|U_{13}|u_a\rangle$. The difference between our result and those of BK and JS may be written as

$$R_{ba}-R_{ba}(\mathrm{JS})=\langle\phi_b|U_{13}+U_{12}|(\omega_{23}-1)u_a\rangle,$$
$$R_{ba}-R_{ba}(\mathrm{BK})=\langle\phi_b|U_{13}|(\omega_{23}-1)U_a\rangle.$$

Clearly all these results coincide in the limit as $\omega_{23}\rightarrow 1$, but the significant criterion for the agreement of all three is the extent to which the influence of $\langle\phi_b|U_{12}|u_a\rangle$ in $\langle\phi_b|U_{12}+U_{13}|u_a\rangle$ is negligible.

Unfortunately the difference $R_{ba}-R_{ba}(\mathrm{JS})$ is of the same order of magnitude as the terms neglected in deriving R_{ba} so that no definite conclusion can be reached as to which result is really more accurate. It is our feeling that our errors are not as great as are incurred in the Born approximation; if the latter is valid, our results are of course also correct. In addition our approach has the advantage of giving a more satisfactory physical picture of the capture process.

6. COMPARISON WITH EXPERIMENT AND CONCLUSIONS

Experimental data on capture of electrons by protons in hydrogen are available in the energy range from 2 to 150 kev. There is no data above 150 kev. We are concerned with the high-energy region (above 25 kev) and in this energy range the data[11–14] are quite good. Cross sections calculated from the present work are given in Table I and are plotted in Fig. 3, along with experimental data of different workers. It is seen from the plot that the agreement with experiment is good for energies above 25 kev. It should, however, be mentioned that we have calculated the cross section of capture into ground state alone whereas experimental data is for the total capture, i.e., capture into all the discrete states. We also show JS and BK curves for cross section of capture into the ground state alone. It is seen that the curves of JS and the present theory approach each other as one goes to higher energies. According to discussions in Sec. 5, our results should also go over to the BK result at high energy. However, at such energies that the BK approximation becomes valid, the capture cross section is essentially zero.

At low energies the agreement with experiment is not good. This is understandable since our approximation, which consisted of keeping the direct capture process only, is not valid at low energy. We have made no attempt to study the low-energy problem.

TABLE I. Capture cross sections from present theory.

E(kev)	$\sigma\times10^{17}$(cm^2)	E(kev)	$\sigma\times10^{17}$(cm^2)
9	260.3670	144	0.1974
16	100.0000	169	0.0928
25	42.1268	196	0.0430
36	18.2912	225	0.0186
49	8.3792	256	0.0080
64	4.0852	289	0.0053
81	1.8914	324	0.0019
100	0.8808	361	0.0004
121	0.4213		

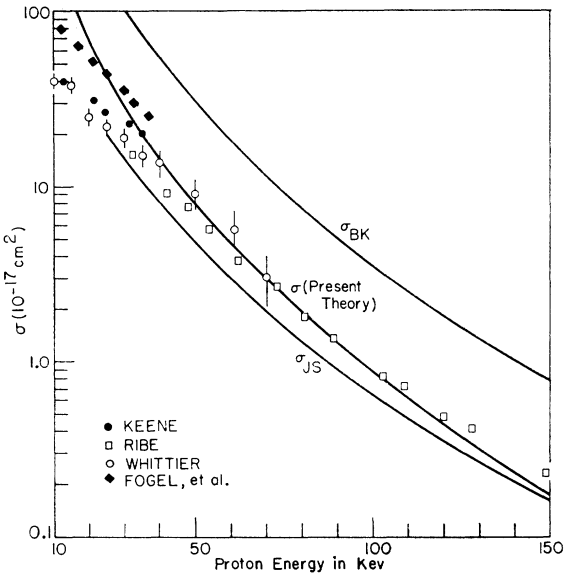

FIG. 3. Capture cross section as function of incident proton energy. Solid lines give theoretical values. Experimental values obtained by different workers are shown by the various symbols.

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APPENDIX A

Here we shall prove that $\langle\phi_b|U_{12}|\omega_{23}u_a\rangle=0$ in the limit $M/m\rightarrow\infty$. We have, from Eq. (39) in the text, in this limit, when $a=1$,

$$\omega_{23}u_a=\frac{e^{i\mathbf{k}_0\cdot\mathbf{R}}}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{K}N(K)G_{1s}(\mathbf{K})e^{i\mathbf{K}\cdot(\mathbf{R}+\mathbf{r}_0)}\times F(is/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0),$$

and so

$$\langle\phi_b|U_{12}|\omega_{23}u_a\rangle=\frac{e^2}{(2\pi)^3}\int d\mathbf{K}N(K)G_{1s}(\mathbf{K})\int d\mathbf{r}_0\int d\mathbf{R}\varphi_{1s}^*(\mathbf{r}_0)\frac{1}{R}\times\exp[i(\mathbf{K}+\mathbf{p})\cdot\mathbf{R}+i\mathbf{K}\cdot\mathbf{r}_0]F(is/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0).$$

[11] F. L. Ribe, Phys. Rev. **83**, 1217 (1951).
[12] Fogel, Krupnik, and Safronov, J. Exptl. Theoret. Phys. U.S.S.R. **28**, 589 (1955) [Soviet Phys. JETP **1**, 415 (1955)].
[13] J. P. Keene, Phil. Mag. **40**, 369 (1949).
[14] A. C. Whittier, Canadian J. Phys. **32**, 275 (1954); P. M. Stier and C. F. Barnett, Phys. Rev. **103**, 896 (1956).

On performing the $\mathbf{R}$ integration, we get

$$\langle\phi_b|U_{12}|\omega_{23}u_a\rangle=\frac{e^2}{2\pi^2}\int d\mathbf{K}\frac{G_{1s}(\mathbf{K})}{(\mathbf{K}+\mathbf{p})^2}\int d\mathbf{r}_0\varphi_{1s}^*(\mathbf{r}_0)\times N(K)e^{i\mathbf{K}\cdot\mathbf{r}_0}F(is/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0)$$
$$=\frac{\sqrt{2}e^2}{\sqrt{\pi}}\int d\mathbf{K}\frac{G_{1s}(\mathbf{K})J(\mathbf{K})}{(\mathbf{K}+\mathbf{p})^2},$$

where

$$J(\mathbf{K})=\frac{1}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{r}_0\varphi_{1s}^*(\mathbf{r}_0)N(K)e^{i\mathbf{K}\cdot\mathbf{r}_0}\times F(is/K,1,iKr_0-i\mathbf{K}\cdot\mathbf{r}_0)$$
$$=\langle\varphi_{1s}(\mathbf{r}_0)|\mathcal{U}_c(\mathbf{K},\mathbf{r}_0)\rangle=0,$$

since $\varphi_{1s}(\mathbf{r}_0)$ and $\mathcal{U}_c(\mathbf{K},\mathbf{r}_0)$ are orthogonal to each other. Thus $\langle\phi_b|U_{12}|\omega_{23}u_a\rangle=0$.

APPENDIX B

We shall prove here that to a fairly reasonable approximation

$$\langle\phi_b|U_{13}|\omega_{23}u_a\rangle\cong\langle\phi_b|U_{23}|\omega_{23}u_a\rangle.$$

For this purpose we expand the state vector $\omega_{23}u_a$ in the complete set of eigenfunctions u_{am} of the operator $(K+U_{13})$. The suffix stands for all possible variables, continuous and discrete, needed to describe the complete set. To be more specific,

$$u_{am}=\frac{1}{(2\pi)^{\frac{3}{2}}}\exp[i\mathbf{K}_{13,2}\cdot(a\mathbf{r}-\mathbf{r}_0)]\varphi_n(\mathbf{r}),$$

where m stands for all possible continuous $\mathbf{K}_{13,2}$ values and all possible discrete as well as continuous n values of hydrogen atom formed by 1 and 3.

$$\omega_{23}u_a=\sum_m u_{am}\langle u_{am}|\omega_{23}u_a\rangle,$$

and hence

$$\langle\phi_b|K+U_{13}|\omega_{23}u_a\rangle=\sum_m\langle\phi_b|K+U_{13}|u_{am}\rangle\langle u_{am}|\omega_{23}u_a\rangle$$
$$=\sum_m E_m\langle\phi_b|u_{am}\rangle\langle u_{am}|\omega_{23}u_a\rangle, \quad (B1)$$

where

$$E_m=(\hbar^2K_{13,2}^2/2\mu)-\epsilon_n,$$

ϵ_n being the binding energy of the hydrogen atom state n. Now

$$\langle\phi_b|u_{am}\rangle\sim G_{1s}(\mathbf{k}_s-\mathbf{K}_{13,2})G_n(\mathbf{k}_s-\mathbf{K}_{13,2}),$$

and since these G's sharply peaked[15] about $\mathbf{k}_0$ in the $\mathbf{K}_{13,2}$ space, we can put:

$$E_m\cong(\hbar^2k_0^2/2\mu)-\epsilon_n\cong(\hbar^2k_0^2/2\mu)\cong E_b. \quad (B2)$$

This is possible since ϵ_n is of the order of few electron volts, whereas $\hbar^2k_0^2/2\mu$ is of the order of 10^2 kev. For state n lying in the continuum with large ϵ_n, $\langle\phi_b|u_{am}\rangle$ becomes very small so that these states are not very important in the series in Eq. (B1). As a consequence of Eq. (B2), it is possible to pull E_m outside the summation sign in Eq. (B1). Consequently we get

$$\langle\phi_b|K+U_{13}|\omega_{23}u_a\rangle\cong E_b\sum_m\langle\phi_b|u_{am}\rangle\langle u_{am}|\omega_{23}u_a\rangle=E_b\langle\phi_b|\omega_{23}u_a\rangle. \quad (B3)$$

Also we have

$$\langle\phi_b|K+U_{23}|\omega_{23}u_a\rangle=E_b\langle\phi_b|\omega_{23}u_a\rangle. \quad (B4)$$

Comparing Eqs. (B3) and (B4), we get

$$\langle\phi_b|K+U_{23}|\omega_{23}u_a\rangle\cong\langle\phi_b|K+U_{13}|\omega_{23}u_a\rangle,$$

from which it follows that

$$\langle\phi_b|U_{23}|\omega_{23}u_a\rangle\cong\langle\phi_b|U_{13}|\omega_{23}u_a\rangle. \quad (B5)$$

In this connection it might be noted that

$$\langle\phi_b|U_{13}|u_a\rangle=\langle\phi_b|U_{23}|u_a\rangle.$$

This relation has been proved in Sec. 2 and is exact whereas relation (B5) is approximate.

Another point deserves comment in connection with Eq. (B4). It has been assumed in this equation that K is Hermitian. Here K appears between ϕ_b and $\omega_{23}u_a$ and one might worry that because of the presence of the singular Møller matrix ω_{23}, this may not be the case. Fortunately the state vector $\omega_{23}u_a$ contains bound states of the hydrogen atom as a factor which makes it vanish at infinity, assuring thereby the Hermiticity of K.

APPENDIX C

Here we shall give a method of evaluating integrals of the type occurring in Sec. 4, Eq. (41). The integral in question is of the type:

$$I=\int d\mathbf{r}e^{-\lambda r}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{r}F(ia,1,ipr-i\mathbf{p}\cdot\mathbf{r}). \quad (C1)$$

We use the convenient integral representation for the confluent hypergeometric function[16]:

$$F(ia,1,z)=\frac{1}{2\pi i}\oint^{(0^+,1^+)}dt\,t^{ia-1}(t-1)^{-ia}e^{zt}. \quad (C2)$$

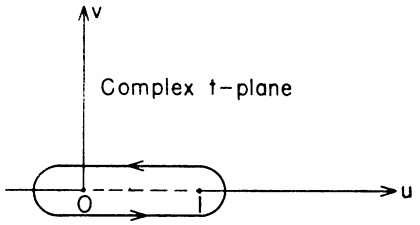

FIG. 4. Contour for the integral representation of the confluent hypergeometric function.

[15] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), first edition, p. 1680.

[16] A. Nordsieck, Phys. Rev. **93**, 785 (1954).

The contour is closed and encircles each of the two points 0 and 1 in the t plane once anticlockwise as shown in Fig. 4. There is a branch cut between points $t=0$ and $t=1$ on the real axis.

Substituting the integral representation (C2) into Eq. (C1), we get

$$I=\frac{1}{2\pi i}\oint dt t^{ia-1}(t-1)^{-ia}V(t),$$

where

$$V(t)=\int d\mathbf{r}\frac{e^{-\lambda r+i\mathbf{q}\cdot\mathbf{r}+it(pr-\mathbf{p}\cdot\mathbf{r})}}{r}$$

$$=\frac{4\pi}{|\mathbf{q}-\mathbf{p}t|^2-(pt+i\lambda)^2}=\frac{-2\pi}{(\alpha+\gamma)t-\alpha},$$

where

$$\alpha=\tfrac{1}{2}(q^2+\lambda^2),\quad \gamma=\mathbf{p}\cdot\mathbf{q}+i\lambda p-\alpha,$$

so that

$$I=\frac{i}{\alpha+\gamma}\oint dt\frac{t^{ia-1}(t-1)^{-ia}}{t-t_0},$$

where $t_0=\alpha/(\alpha+\gamma)$. The integrand has simple poles at $t_1=0$ and at $t_0=\alpha/(\alpha+\gamma)$. Since there are branch points at $t=0$ and $t=1$ on the real axis, to evaluate the complex integral by Cauchy's theorem, the contour is suitably deformed as shown in Fig. 5 (since there are no other

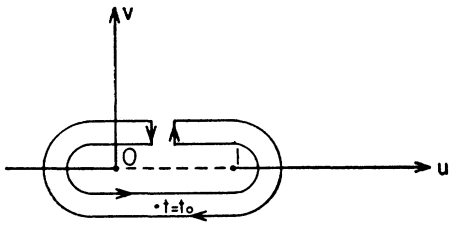

FIG. 5. Deformed contour for the evaluation of I, employing Cauchy theorem.

poles) so as to enclose the pole at $t=t_0$. The pole at $t=0$ as well as the branch cut then lie outside the contour. The deformed contour is clockwise with respect to the point $t=t_0$. This is compensated by putting a negative sign in the integrand. From simple

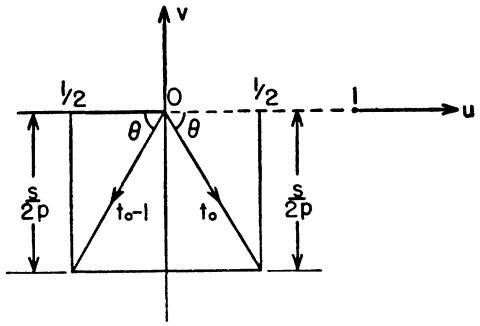

FIG. 6. Relative phases of vectors t_0 and (t_0-1) in the complex t-plane.

Cauchy theorem, we then get

$$I=\frac{2\pi}{\alpha+\gamma}[\text{Residue at } t=t_0]$$

$$=\frac{2\pi}{t_0(\alpha+\gamma)}\left(\frac{t_0}{t_0-1}\right)^{ia}. \tag{C3}$$

In Eq. (41), $\mathbf{p}=\mathbf{q}$, $\lambda=s$, and $a=s/p$, so that

$$\alpha=\tfrac{1}{2}(p^2+s^2),\quad \alpha+\gamma=p^2+isp.$$

Since $(t_0-1)^{-ia}$ and $(t_0)^{ia}$ in Eq. (54) are multivalued, proper care must be taken to fix the correct value of I. For this it is enough to know the relative phases to t_0 and (t_0-1). In the present case [Eq. (41)], we have

$$t_0=\tfrac{1}{2}-(is/2p),\quad t_0-1=-\tfrac{1}{2}-(is/2p).$$

The vectors t_0 and (t_0-1) are shown in Fig. 6. It is clear from the figure that

$$\arg(t_0)=(2\pi-\theta),\quad \arg(t_0-1)=[2\pi-(\pi-\theta)]=\pi+\theta,$$

where $\tan\theta=s/p$; and the phase at the point infinitely close to positive real axis, but lying below the branch cut, is arbitrarily put as 2π since we only need relative phases of t_0 and t_0-1. We also have $|t_0|=|t_0-1|$, so that $t_0/(t_0-1)=e^{i(\pi-2\theta)}$. Using this in Eq. (C3), we get

$$I=\int d\mathbf{r}e^{-r_0 s}\frac{e^{ip\cdot r_0}}{r_0}F(is/p,1,ipr_0-ip\cdot\mathbf{r}_0)$$

$$=\frac{2\pi}{(\alpha+\gamma)t_0}\exp\left(\frac{2s\theta}{p}-\frac{\pi s}{p}\right)$$

$$=\frac{4\pi}{s^2+p^2}\exp\left[\frac{2s}{p}\arctan\left(\frac{s}{p}\right)-\frac{\pi s}{p}\right].$$