Charge transfer in proton-hydrogen collisions

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A nonperturbative approach to the problem of charge transfer in proton-hydrogen collisions is developed in which the wave function corresponding to the outgoing scattered wave in the incident channel is evaluated by solving the Schrödinger equation it satisfies. The present formulation has the advantage of bringing into the theory not only the effects that are due to the Coulomb distortions but also those due to the polarization of the target atom. Our calculation of the capture cross section $(1s \rightarrow 1s)$, which has been done with neglect of the polarization effect, agrees well with experiment in the low-energy region betweem 8 and 100 keV. A new interesting feature of our theory is that the cross section for capture shows a maximum at an energy of 9 keV. For proton energies below this value the cross section starts decreasing, finally approaching zero. For higher energies it starts falling with increasing energy in the usual way.

I. INTRODUCTION

Theoretical study of the charge-transfer reaction^{1,2} in proton-hydrogen collisions has been of great interest to physicists for a long time. In spite of its long history of development, the problem is still not completely settled. In the study of this problem the methods that have been most used are confined to the Born approximation,^{1,3-5} the impulse approximation,⁶ and other equivalent firstorder approximations. Recently there also have been attempts to apply higher-order approximations to investigate this problem.

In one of the earliest works on rearrangement collisions, Oppenheimer⁷ showed that the scalar product of the initial and the final wave functions was small for fast collisions, so that they could be considered to be approximately orthogonal. Following Oppenheimer, Brinkman and Kramers (BK)¹ calculated the capture cross section for protons passing through hydrogen by using the Born approximation and neglecting the proton-proton interaction term. They found that the cross section was four times the experimental result for proton energies around 100 keV and even larger for lower energies. The calculations by Jackson and Schiff (JS)⁴ and also by Bates and Dalgarno(BD),³ which included the proton-proton interaction term and used the Born approximation, showed that their results agreed with the experimental results for proton energies above 25 keV at which $e^2/\hbar v \leq 1$, v being the velocity of the incident proton. It was pointed out by Wick⁸ that by an appropriate canonical transformation the proton-proton term could be removed from the total Hamiltonian in the limit $M/m \rightarrow \infty$. In view of Wick's remark it looks surprising that the JS result agreed well with experiment. Also it is not easy to see why the BK result should not agree with experiment. On the other hand, it was shown by Mapleton⁵ that the inclusion of the internuclear potential had a very considerable effect, and it led to a significant reduction of the cross sections at all energies.

To improve the understanding of this process, many approaches have been adopted. We compare a few of those here in brief to create a perspective. Using the distorted-wave method for rearrangement collisions,⁹ Bassel and Gerjuoy¹⁰ (BG) eliminated the proton-proton interaction term from the perturbation Hamiltonian. Their cross section for electron capture was in good agreement with experiment between 35 and 100 keV. Bates,¹¹ in an earlier attempt to overcome the defects associated with the nonorthogonality of the initial and final wave functions in the case of charge-transfer reactions, had used an effective potential instead of any post form of the interaction potential for computing the cross section. The form of the effective potential was found to be identical with the one obtained later on by BG except for a multiplicative factor. The methods of Bates and of BG were equivalent over a wide range of energies. Bates' method also showed that the role of the internuclear potential was negligible. The calculation of the cross section for charge transfer using the effective potential of Bates was very difficult. However, McCarroll¹² evaluated it numerically with the help of a computer. In doing this he did not actually use the formula derived from the wave-mechanical treatment. Rather, he used an equivalent formula obtained by Bates¹¹ using the coupled-state impactparameter approach in the two-state approximation. The results of McCarroll¹² agreed with experiment at very low energies only, i.e., around 2 keV. Later on the calculation of McElroy,¹³ which included captures into the excited states 2s and 2p, was found to agree reasonably well with the experimental data between 25 and 50 keV. Beyond this

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energy range the cross section was much higher than that in the experiment. In the opinion of Lovell and McElroy^{14,15} the coupling was weak above 25 keV; consequently, the two-state approximation was inadequate, and it was necessary to include the cross sections for capture into excited states. The calculations of Wilets and Gallaher¹⁶ using a many-state wave-function expansion agreed well with experiment from 2 to 15 keV, but fell below the experimental value at 30 keV. This decrease in the cross section for energies around 30 keV and above did not agree with the theoretical results of McElroy. The expansion method used by Wilets and Gallaher was a slowly convergent one. To improve upon this Cheshire, Gallaher, and Taylor¹⁷ calculated the charge-exchange cross section using the close-coupling method with suitable additions of orthogonal pseudostates. Their results agreed reasonably well with experiments up to 50 keV.

The impulse approximation was first applied by Pradhan⁶ to the problem of electron capture by protons from hydrogen. He showed that the proton-proton interaction had zero matrix element for transition from the initial to the final state, which was in keeping with Wick's remark. This happened because the improved initial wave function was found to be orthogonal to the final wave function in the limit of an infinitely heavy incident ion. In this case agreement with experiment was obtained for proton energies above 25 keV. In the matrix element used by Pradhan for calculating the cross section, the actual interaction potential had been replaced by the electron-nuclear part of the prior interaction. This was corrected for by McDowell¹⁸ using the correct interaction potential. However, he introduced an approximation in the momentum distribution of the unperturbed hydrogen-atom wave function. Later, Cheshire¹⁹ evaluated the capture cross section without imposing this approximation to the momentum distribution. His results agreed with the Born 1s-state calculation of JS around 95 keV, but gave results significantly higher than the Born estimate at 30 keV. His calculations also showed that the proton-proton interaction term did not make any significant contribution to the cross section. Interestingly, as regards the behavior of the cross section¹⁹ in this energy range (30-1100 keV), it was found that the energy dependence of the cross section was similar to that of the Born approximation of the JS type and differed considerably from those of Pradhan⁶ and McDowell.18

A later calculation by Cheshire²⁰ based on the continuum-distorted-wave (CDW) approximation also showed that the cross section was independent of the internuclear potential. His results agreed with the JS-type Born calculation at 95 keV, but were higher by a factor of 2.2 than the Born results at 30 keV. In the earlier work Cheshire¹⁹ had shown that the cross section had an asymptotic energy dependence given by $(0.2946 + 5\pi E^{1/2})$ $\times\, 2^{\text{-10}})Q_{\text{BK}}, \ \text{where} \, E \, \text{was the energy of the incident}$ proton in units of 100 keV and $Q_{\rm BK}$ was the BK cross section. The calculation of Drisko²¹ in the second Born approximation showed that the capture cross section behaved in the high energy as (0.2946 + $5\pi E^{1/2}2^{-11}$) $Q_{\rm BK}$. Further estimates by him in the third Born approximation showed this behavior to be $(0.319 + 5\pi E^{1/2}2^{-11})Q_{BK}$. From this it followed that the earlier calculation of Cheshire¹⁹ was somewhat comparable to the second Born approximation of the above type.²¹ His CDW approximation was a calculation going beyond the usual second-order method where the cross section had the same asymptotic behavior as his earlier work. McCarroll and Salin²² investigated the high-energy behavior of cross section for this reaction using a method which was shown to be the guantal equivalent of the CDW approximation of Cheshire. From this they concluded that the first-order methods were inadequate in the high-energy limit. Later on, Salin²³ explicitly showed the connection between the CDW approximation and the method of McCarroll and Salin. He concluded that the CDW approximation was not a good approximation for energies lower than 500 keV. For energies higher than 400 keV he computed the cross sections and found that his results agreed with those of the impulse approximation.²⁴

Recently, the problem of electron capture by protons has been studied by Sil, Chaudhuri, and $Ghosh^{25}$ using the Fadeev approach. Since in this method they have solved an integral equation for the three-body transition amplitude numerically, their calculation appears to be of a higher order than the usual second-order calculations. Here it is found that at low and intermediate energies the experimental points for the cross section lie between the two sets of results obtained by the authors with the proton-proton interaction and without it. Therefore the controversy regarding the role of the nucelus-nucleus interaction in rearrangement collisions appears to remain unsettled.

In the present paper we have made an attempt to study the above problem using a different kind of approximate procedure in which the exact outgoing scattering wave function in the incident channel is expanded in a complete orthogonal set of hydrogenatom wave functions with coefficients that are functions of the coordinate variable. It is seen that these coefficients satisfy the equation of motion of a free particle having a certain effective mass moving relative to the hydrogen atom in the ground state. It is observed that the field in which this particle moves consists of the potential energy of the proton in the field of the undisturbed hydrogen atom plus the term that is due to the polarization of the atom. Both these potential-field effects follow as natural consequences of our theory.

We have made numerical calculations of the capture cross section for energies up to 100 keV. In doing this we have neglected the polarization part of the potential and the part that falls off exponentially. Since the agreement between the theoretical results and the experiment is not good at low energies, we have confined ourselves to energies up to 100 keV. From our results we find that our theory gives good agreement with experiment for the energy range from 8 to 90 keV. It also indicates that the proton-proton interaction plays an important role in rearrangement collisions. For bigger energies (i.e., beyond 90 keV) it is expected that our theory would give better agreement with the experiment. An interesting and unusual feature of our theory is that our cross section for capture into the 1s state increases with incident proton energies and attains a maximum value around 9 keV. When the energy of the incident proton increases further, the cross section decreases. Such behavior in the capture cross section has been observed in the case of captures into excited states.24,26

In Sec. II we derive the requisite formulas for the capture cross section for the following reaction:

$$p + \mathbf{H} \to \mathbf{H} + p \,. \tag{1}$$

Section III is devoted to the solution of the Schrödinger equation to determine the scattering wave function corresponding to the outgoing state. In Sec. IV we obtain the expression for the differential-scattering cross section, and using this we write down the expression for the total cross section. Section V deals with the discussions of the results and the approximations involved therein, and also gives a comparison of our results with the results of a few theoretical calculations and those of recent experiments.

II. FORMULATION OF THE SCATTERING AMPLITUDE

To start with we consider the scattering of a particle in a potential field V. Let the Hamiltonian of the system be denoted by

$$H = H_0 + V \,. \tag{2}$$

The matrix element corresponding to the transition from the initial state ϕ_a to the final state ϕ_b is now defined as

$$T_{a \to b} = \langle \phi_{b} | T | \phi_{a} \rangle = \langle \phi_{b} | V | \Psi_{a}^{(+)} \rangle ,$$

where T is called the transition matrix, and $\phi_a z = \phi_b$ are the eigenstates of H_0 . The state vector $\Psi_a^{(+)}$ represents the stationary outgoing scattering wave function such that

$$(H - E_a + i\eta)\Psi_a^{(+)} = 0.$$
(3)

If the potential *V* is such that

$$V = U_1 + W_1 , (4)$$

we can write

$$H = H_1 + W_1 , \qquad (5a)$$

where

$$H_1 = H_0 + U_1$$
 (5b)

We shall assume that U_1 and V go to zero faster than 1/r. Treating W_1 as a small perturbation the transition matrix now splits up into the sum of two parts²⁷:

$$\begin{aligned} T_{a \to b} &= \langle \phi_b \left| U_1 \left| \chi_a^{(+)} \right\rangle + \langle \Psi_b^{(-)} \left| W_1 \left| \chi_a^{(+)} \right\rangle \\ &= \langle \phi_b \left| U_1 \left| \chi_a^{(+)} \right\rangle + \langle \chi_b^{(-)} \left| W_1 \left| \Psi_a^{(+)} \right\rangle , \end{aligned} \end{aligned}$$
(6)

where $\chi_a^{(+)}$ and $\Psi_b^{(-)}$ are defined by the equations

$$(H_1 - E_a \pm i\eta)\chi_a^{(\pm)} = 0$$

and (*H* –

$$(H - E_b - i\eta)\Psi_b^{(-)} = 0.$$
⁽⁷⁾

For reactions of the type described by Eq. (1) the total Hamiltonian can be written in either the initial system or the final system as (see Fig. 1)

$$H = H_{\alpha} + V_{\alpha} = H_{\beta} + V_{\beta}, \qquad (8)$$

where

$$H_{\alpha} = K + U_{13}, \quad V_{\alpha} = U_{12} + U_{23},$$

$$H_{a} = K + U_{22}, \quad V_{a} = U_{12} + U_{12},$$
(9)

K being the kinetic energy operator for the system of three particles, the incident proton and the electron plus the proton of the hydrogen atom, and the U's being the various interaction potentials. In the case of rearrangement collisions for which $V_{\alpha} \neq V_{\beta}$, one can write the transition matrix in the form²⁷

$$T_{a \to b} = \langle \phi_b | V_\beta | \Psi_a^{(+)} \rangle = \langle \Psi_b^{(-)} | V_\alpha | \Psi_a \rangle, \qquad (10)$$



FIG. 1. (a) Before the collision; (b) after the collision.

where

$$(E_a - H \pm i\eta)\Psi_a^{(\pm)} = 0,$$

$$H_{\beta}\phi_b = E_b\phi_b, \quad H_{\alpha}\Psi_a = E_a\Psi_a.$$
(11)

In the Born approximation (the JS or, equivalently, the BD version), one has

$$T_{a \to b}^{(\text{Born})} = \langle \phi_{b} | V_{\beta} | \mathfrak{u}_{a} \rangle = \langle \phi_{b} | V_{\alpha} | \mathfrak{u}_{a} \rangle.$$
(12)

We now break up V_{α} and V_{β} as follows:

$$V_{\alpha} = U_{\alpha} + W_{\alpha} , \quad V_{\beta} = U_{\beta} + W_{\beta}$$
(13)

where

$$U_{\alpha} = U_{23}, \quad U_{\beta} = U_{13}, \quad W_{\alpha} = W_{\beta} = U_{12}.$$
 (14)

With the help of (6) we can write²⁷

$$T_{a \to b} = \langle \phi_b | V_\beta | \Psi_a^{(+)} \rangle = \langle \phi_b | U_{13} | \chi_a^{(+)} \rangle + \langle \Psi_b^{(-)} | U_{12} | \chi_a^{(+)} \rangle$$
(15)

where

$$(E_a + i\eta - H_\alpha - U_\alpha) \left| \chi_a^{(+)} \right\rangle = 0.$$
 (16)

If U_{12} has a weak effect, the $\chi_a^{(+)}$ will differ little from $\Psi_a^{(+)}$. One can also obtain an alternative expression for $T_{a \to b}$ using the stationary solutions of the Hamiltonian $(H_{\beta} + U_{\beta})$. In the present case we shall, however, restrict ourselves to the matrix element given by (15) which we shall denote by $R_{ba}^{(+)}$. To simplify our calculation, we approximate $\Psi_b^{(+)}$ by ϕ_b in the first step. This is being done in the spirit of the impulse approximation, where one neglects the two-step capture processes.²⁸ Now the matrix element $R_{ba}^{(+)}$ approximately becomes

$$R_{ba}^{(\star)} \cong \langle \phi_b | (U_{13} + U_{12}) | \chi_a^{(\star)} \rangle .$$
(17)

III. EVALUATION OF THE SCATTERING WAVE FUNCTION $\chi_{\alpha}^{(+)}$

To determine $\chi_a^{(+)}$ we have to solve the Schrödinger equation satisfied by $\chi_a^{(+)}$ corresponding to the Hamiltonian

$$H_{\chi} = H_{\alpha} + U_{\alpha} = K + U_{13} + U_{23} \tag{18}$$

before the collision. The situations before and after the collision are schematically shown in Fig. 1. We choose the coordinate system to describe the geometry of the relative coordinates as shown in Fig. 2. The Hamiltonian H_x which corresponds to the situation before the collision assumes the following form in the center-of-mass system of the three particles:

$$H_{\chi} = -\frac{\hbar^2}{2\mu} \nabla_r^2 - \frac{\hbar^2}{2\mu'} \nabla_{r'}^2 - \frac{e^2}{r} - \frac{e^2}{|\tilde{a}\tilde{r} - \tilde{r}'|}, \quad (19)$$



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

where

$$\mu = \frac{Mm}{M+m} , \quad \mu' = \frac{M(M+m)}{2M+m} ,$$

$$\tilde{a} = M/(M+m), \quad \tilde{r}' = \tilde{a}\tilde{r} - \tilde{r}_0.$$
⁽²⁰⁾

The Schrödinger equation satisfied by $\chi_a^{(\star)}$ is given by

$$\left(-\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{\hbar^2}{2\mu'}\nabla_r^2, -\frac{e^2}{r} - \frac{e^2}{|\vec{a}\vec{\mathbf{r}} - \vec{\mathbf{r}}'|}\right) |\chi_a^{(+)}\rangle = E_a |\chi_a^{(+)}\rangle.$$
(21)

We are interested in the scattering solution of (21). We now expand $\chi_a^{(+)}$ in terms of the hydrogen atomic wave functions $\varphi_{\nu}(\mathbf{\hat{r}})$ with coefficients which are functions of $\mathbf{\hat{r}}'$. That is,²⁹

$$\chi_{a}^{(+)}(\vec{\mathbf{r}},\vec{\mathbf{r}}') = \sum_{\nu} \varphi_{\nu}(\vec{\mathbf{r}}) f_{\nu a}^{(+)}(\vec{\mathbf{r}}')$$
(22)

where ν includes the sum over the discrete states and integration over the continuum variables. Substituting (22) into (21) and then multiplying both sides by $\varphi_{\nu}^{*}(\mathbf{\hat{r}})$, one gets after integration over $\mathbf{\hat{r}}$

$$-\frac{\hbar^2}{2\mu'} \nabla^2_{r'} f_{\nu_a}^{(*)}(\mathbf{\tilde{r}}') + \sum_{\nu'} \langle \varphi_{\nu}(\mathbf{\tilde{r}}) | H' | \varphi_{\nu'}(\mathbf{\tilde{r}}) \rangle f_{\nu'a}^{(*)}(\mathbf{\tilde{r}}')$$
$$= (E_a - \epsilon_{\nu}) f_{\nu a}^{(*)}(\mathbf{\tilde{r}}') = E_{\nu} f_{\nu a}^{(*)}(\mathbf{\tilde{r}}') \quad (23)$$

where

$$H' = -e^2 / |\tilde{a}\tilde{r} - \tilde{r}'|$$
 (24)

In arriving at (23) we have used the relation

$$\left[-(\hbar^2/2\mu)\nabla_r^2 - e^2/r\right] \left|\varphi_{\nu}(\mathbf{\dot{r}})\right\rangle = \epsilon_{\nu} \left|\varphi_{\nu}(\mathbf{\dot{r}})\right\rangle.$$
(25)

Here $\chi_a^{(*)}$ is the eigenfunction of the Hamiltonian (19) which has the following asymptotic behavior:

$$\chi_{a}^{(*)} \xrightarrow[r' \to \infty]{} \varphi_{0}(\vec{\mathbf{r}}) \left(e^{i\vec{\mathbf{k}}_{0} \cdot \vec{\mathbf{r}}'} + h_{0a}(\Omega) \frac{e^{ik_{0}r'}}{r'} \right)$$
$$+ \sum_{\nu \neq 0} \varphi_{\nu}(\vec{\mathbf{r}}) h_{\nu a}(\Omega) \frac{e^{ik_{\nu}r'}}{r'}, \qquad (26)$$

where \mathbf{k}_0 is the wave vector associated with the particle having an effective mass μ' . Here the sub-

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script *a* implies the incident channel and the subscript 0 means the initial state. From (26) it follows that $f_{\mu}^{(+)}$ satisifies the boundary conditions:

$$f_{0a}^{(+)}(\mathbf{\bar{r}}') \xrightarrow[\mathbf{r'} \to \infty]{} e^{i\mathbf{\bar{k}}_{0}\cdot\mathbf{\bar{r}}'} + h_{0a}(\Omega) e^{ik_{0}\mathbf{r'}}/\mathbf{r}',$$

$$f_{\nu a, \ \nu\neq 0}^{(+)}(\mathbf{\bar{r}}') \xrightarrow[\mathbf{r'} \to \infty]{} h_{\nu a}(\Omega) e^{ik_{\nu}\mathbf{r'}}/\mathbf{r}'.$$
(27)

Since during the process of capture the target atom is assumed to remain in the ground state, one has the additional boundary condition³⁰

$$r' f_{\nu a}^{(+)}(\vec{\mathbf{r}}') \xrightarrow[\tau' \to \infty]{} 0 \quad \text{for } \nu \neq 0.$$
(28)

A similar condition also applies to the continuum part of the atomic wave functions. Equation (23) together with the boundary conditions given in (27) determines $f_{\nu a}^{(*)}$. The momentum k_{ν} appearing in (26) is such that

0 0 /-

0~0/-

$$E_{\nu} = \hbar^{2} k_{\nu}^{2} / 2 \mu' = \hbar^{2} k_{0}^{2} / 2 \mu' + \epsilon_{0} - \epsilon_{\nu} , \quad \nu \neq 0 ,$$

$$E_{\nu} = \hbar^{2} \tilde{k}_{0}^{2} / 2 \mu' = \hbar^{2} k_{0}^{2} / 2 \mu' , \quad \nu = 0 .$$
(29)

One can rewrite (23) in the form

$$\left(\nabla_{r'}^{2} + \tilde{k}_{\nu}^{2}\right) f_{\nu a}^{(+)}(\mathbf{\tilde{r}}') = \sum_{\nu'} V_{\nu\nu'}(\mathbf{\tilde{r}}') f_{\nu' a}^{(+)}(\mathbf{\tilde{r}}')$$
(30)

where

$$\tilde{k}_{\nu}^2 = 2\,\mu' E_{\nu}/\hbar^2$$

and

$$V_{\nu\nu'}(\mathbf{\tilde{r}}') = (2\,\mu'/\hbar^2) \langle \varphi_{\nu}(\mathbf{\tilde{r}}) | H' | \varphi_{\nu'}(\mathbf{\tilde{r}}) \rangle$$
$$= (2\,\mu'/\hbar^2) H'_{\nu\nu'}(\mathbf{\tilde{r}}') . \tag{31}$$

From (30) it appears that the function $f_{\nu a}^{*}$ describes the motion of a particle of mass μ' moving relative to the hydrogen atom in the state ν .

The matrix element $H'_{\nu\nu}(\mathbf{\dot{r}}')$ before the collision is evaluated using the wave functions of the hydrogen atom. In atomic units, one obtains

$$H_{\nu\nu'}'(\mathbf{\bar{r}}') = \exp\left(\frac{-2r'}{\bar{a}}\right) \left(\frac{1}{r'} + \frac{1}{\bar{a}}\right) - \frac{1}{r'}, \quad \nu = 1s , \quad \nu' = 1s ,$$

$$= \frac{1}{\sqrt{2}} \exp\left(\frac{-3r'}{2\bar{a}}\right) \left(-\frac{8}{27\bar{a}} - \frac{4r'}{9\bar{a}^2}\right), \quad \nu = 1s , \quad \nu' = 2s ,$$

$$= \left(\frac{8\pi}{27}\right)^{1/2} Y_1^m(\mathbf{\bar{r}}') \left(\exp\left(\frac{-3r'}{2\bar{a}}\right) \left(\frac{2}{3\bar{a}^2} + \frac{8}{9\bar{a}r'} + \frac{16}{27r'^2}\right) - \frac{16}{27r'^2}\right), \quad \nu = 1s , \quad \nu' = 2p$$
(32)

where Y_l^m is the well-known spherical harmonics. For $\nu = 0$, Eq. (30) can be written as

$$(\nabla_{r'}^{2} + k_{0}^{2})f_{0a}^{(+)}(\mathbf{\ddot{r}}') = V_{00}(\mathbf{\ddot{r}}')f_{0a}^{(+)}(\mathbf{\ddot{r}}') + \sum_{\nu'\neq 0} V_{0\nu'}(\mathbf{\ddot{r}}')f_{\nu'a}^{(+)}(\mathbf{\ddot{r}}')$$
(33)

where $V_{00}(\vec{r}')$ is obtained from (31) and (32) in atomic units as

$$V_{00}(\mathbf{\tilde{r}}') = 2\,\mu' \left[\exp\left(\frac{-2r'}{\tilde{a}}\right) \left(\frac{1}{r'} + \frac{1}{\tilde{a}}\right) - \frac{1}{r'} \right] \,. \tag{34}$$

Here the subscript 0 stands for the 1s state. In general, it is extremely difficult to evaluate the second term on the right-hand side of (33). However, one can evaluate it in the limit of large r' because in this limit $f_{\nu'a}^{(+)}(\vec{r}\,')$ can be written down explicitly in terms of $f_{0a}^{(+)}(\vec{r}\,')$. From (32) one finds that as $r' \to \infty$

$$V_{0\nu'} \sim 1/r' \text{ for } \nu' = 1s ,$$

 $\sim (1/r')^{l+1} \text{ for } \nu' \neq 1s , l \neq 0 ,$
 $\sim 0 \text{ (exponentially) for } \nu' \neq 1s , l = 0.$ (35)

From the above it is thus seen that for all atomic states ν and ν' including the continuum states (except for $\nu = \nu' = 1s$) $V_{\nu\nu'}(\vec{r}')$ decreases at least as fast as $1/r^2$ for $r' \to \infty$. In view of the above boundary conditions for large r' and $\nu \neq 0$, the only

term³⁰ of importance on the right-hand side of each of the equations (30) is that connecting the channel ν with the open channel 0. Hence,

$$(\nabla_{r'}^2 + \bar{k}_{\nu}^2) f_{\nu a}^{(+)}(\bar{r}') \cong V_{\nu 0}(\bar{r}') f_{0a}^{(+)}(\bar{r}')$$
 for large r' . (36)

From this we have

 $(\nabla_{\tau'}^2 + \tilde{k}_0^2) f_{0a}^{(*)}(\mathbf{\tilde{r}}') = V_{00}(\mathbf{\tilde{r}}') f_{0a}^{(*)}(\mathbf{\tilde{r}}') \text{ for large } r', \quad (37)$ which is the same as

$$\nabla_{r'}^2 f_{0a}^{(+)}(\vec{r}\,') = -\,\vec{k}_0^2 f_{0a}^{(+)}(\vec{r}\,') + O(1/\gamma\,') \,. \tag{38}$$

If we write $V_{\nu 0}(\mathbf{\tilde{r}}') \propto (1/r')^p$ where $p \ge 2$, we have³⁰ $\nabla_{r'}^2 [V_{\nu 0}(\mathbf{\tilde{r}}')f_{0a}^{(+)}(\mathbf{\tilde{r}}')] = [\nabla_{r'}^2 V_{\nu 0}(\mathbf{\tilde{r}}')]f_{0a}^{(+)}(\mathbf{\tilde{r}}')$

+
$$V_{\nu 0}(\mathbf{\bar{r}}') [\nabla^2_{\mathbf{r}'} f^{(+)}_{0a}(\mathbf{\bar{r}}')]$$

$$+2\vec{\nabla}_{r'} V_{\nu 0}(\vec{r}\,')\cdot\vec{\nabla}_{r'} f^{(+)}_{0a}(\vec{r}\,') \,. \eqno(39)$$

Using (38), we get from this

$$\nabla^2_{\mathbf{r}'} \left[V_{\nu 0}(\mathbf{\bar{r}}') f_{0a}^{(+)}(\mathbf{\bar{r}}') \right]$$

$$= -\bar{k}_0^2 \left[V_{\nu 0}(\mathbf{\dot{r}}') f_{0a}^{(+)}(\mathbf{\dot{r}}') + O(1/r'^{p+1}) \text{ for large } r' \right].$$
(40)

On adding the factor $\tilde{k}_{\nu}^2 V_{\nu 0}(\mathbf{\tilde{r}}') f_{0a}^{(+)}(\mathbf{\tilde{r}}')$ to both the sides of (40), we obtain

$$(\nabla_{r'}^{2} + \tilde{k}_{\nu}^{2}) [V_{\nu 0}(\mathbf{\dot{r}}') f_{0a}^{(+)}(\mathbf{\dot{r}}')] \cong (\tilde{k}_{\nu}^{2} - \tilde{k}_{0}^{2}) [V_{\nu 0}(\mathbf{\dot{r}}') f_{0a}^{(+)}(\mathbf{\dot{r}}')]$$

for large r' . (41)

Comparing this relation with (36) we see that the functions $f_{\nu a}^{(*)}(\tilde{\mathbf{r}}')$ have the form

$$f_{\nu a}^{(+)}(\mathbf{\tilde{r}}') \cong (\tilde{k}_{\nu}^{2} - k_{0}^{2})^{-1} V_{\nu 0}(\mathbf{\tilde{r}}') f_{0a}^{(+)}(\mathbf{\tilde{r}}')$$
 for large r' (42)

which is valid for $\nu \neq 0$ only. Substituting this expression for $f_{\nu a}^{(+)}(\vec{r}')$ into the second term of the right-hand side of (33), we find that this term is given by

$$U_{p}({\bf \ddot{r}}')f_{0a}^{(+)}({\bf \ddot{r}}')$$

where

$$U_{p}(\vec{\mathbf{r}}') = \sum_{\nu' \neq 0}^{\infty} \frac{|V_{0\nu'}(\vec{\mathbf{r}}')|^{2}}{\tilde{k}_{\nu'}^{2} - \tilde{k}_{0}^{2}} \text{ for large } r'.$$
(43)

Since the dominant (p wave) terms in $V_{0\nu'}(\mathbf{\bar{r}}')$ vary as $1/r'^2$ for large r', the potential $U_p(\mathbf{\bar{r}}')$ varies as $1/r'^4$ as $r' \rightarrow \infty$. This is the exact long-range potential up to terms of $O(1/r'^6)$. Using (29) the expression for $U_p(\mathbf{\bar{r}}')$ can be rewritten as

$$U_{p}(\mathbf{\tilde{r}}') = \frac{1}{2\mu'} \sum_{\nu' \neq 0} \frac{|V_{0\nu'}(\mathbf{\tilde{r}}')|^{2}}{\epsilon_{0} - \epsilon_{\nu'}}$$
(44)

where

$$V_{0\nu'}(\mathbf{\bar{r}}') = 2\,\mu' \int d\mathbf{\bar{r}} \,\varphi_0^*(\mathbf{\bar{r}}) \left(\frac{-1}{|\mathbf{\bar{a}}\mathbf{\bar{r}} - \mathbf{\bar{r}}'|}\right) \varphi_{\nu'}(\mathbf{\bar{r}}) \,.$$

$$(45)$$

Since the denominator in (44) is always negative, the polarization potential $U_p(\mathbf{r}')$ is attractive. We have seen that for ν' if we use the states 2s, 3s, etc., the matrix element $V_{0\nu'}$, is found to be exponentially decaying. For large r', $|V_{0\nu'}(\mathbf{r}')|^2$ goes to zero much faster than $1/r'^4$, where the $1/r'^4$ behavior is due to the p states. So we see that the pstates are the only dominant contributors. The contributions from the d states and the other higher l states go as $1/r'^{2l+2}$ for large r', and hence, they are much smaller than the p-state contributions. Accounting for all the p-state contributions and putting $\tilde{a} = M/(M+m) \to 1$ (which is true in the limit $M \to \infty$), dipole contributions to the potential $U_p(\mathbf{\bar{r}'})$ are written as

$$U_{p}(\mathbf{\tilde{r}}') = -(\mu'/r'^{4})\alpha_{1} \text{ as } r' \to \infty, \qquad (46)$$

where

$$\alpha_1 = \frac{2}{3} \sum_{n \neq 0} \frac{|\langle R_{1s} | r | R_{np} \rangle|}{\epsilon_n - \epsilon_0}$$

is the dipole polarizability of the hydrogen atom. R_{1s} and $R_{\eta\phi}$ are the radial parts of the wave functions of the hydrogen atom.

For the time being, we shall be interested in the solution of (33) without the second term on the right-hand side whose value for large r' is given by the polarization potential $U_{\rho}(\mathbf{\tilde{r}}')$ given in (46).

This polarization potential is of importance in the limit of very low energies. With the inclusion of this, it is almost impossible to obtain an analytic solution for Eq. (40). Since the expression for $V_{00}(\mathbf{\tilde{r}}')$ contains a factor which falls off exponentially with r' (goes to zero very rapidly with increasing r'), this can be assumed to be of relatively less importance than the factor 1/r'. Also, on dropping this term we are able to obtain an exact analytical solution for $f_{0a}^{(+)}(\mathbf{\tilde{r}}')$ from the Schrödinger equation:

$$\left(\nabla_{r'}^{2} + k_{0}^{2}\right)f_{0a}^{(+)}(\vec{\mathbf{r}}\,') = -\left(2\,\mu\,'/r\,'\right)f_{0a}^{(+)}(\vec{\mathbf{r}}\,')\,,\tag{47}$$

which is valid for all values of r'. This being the case of an attractive Coulomb potential, the scattering solutions of (47) can be written as³¹

$$f_{0a}^{(+)}(\mathbf{\bar{r}}') = N(k_0) \exp(i\vec{\mathbf{k}}_0 \cdot \mathbf{\bar{r}}') F(i\mu'/k_0, \mathbf{1}, ik_0r' - i\vec{\mathbf{k}}_0 \cdot r')$$
(48)

where

$$N(k_0) = \exp(\pi \mu'/2k_0)\Gamma(1 - i\,\mu'/k_0) \,. \tag{49}$$

To write (48) the normalization is assumed to be done inside a cubical box of unit volume. In this equation F stands for the confluent hypergeometric functions, the arguments of which are properly chosen so as to correspond to the outgoing waves.

Since here we shall be calculating the cross section for capture into the ground state of the hydrogen atom, following (22) we have

$$\chi_{a}^{(+)}(\mathbf{r},\mathbf{r}') = f_{0a}^{(+)}(\mathbf{r}')\varphi_{1s}(\mathbf{r})$$

which, with the help of (48), is written as

$$\chi_a^{(+)}(\mathbf{\vec{r}},\mathbf{\vec{r}}') = N(k_0) \exp(i\mathbf{\vec{k}_0}\cdot\mathbf{\vec{r}}')$$

$$\times F(i\,\mu\,'/k_0,\mathbf{1},ik_0r\,'-i\mathbf{\vec{k}_0}\cdot\mathbf{\vec{r}}')\varphi_{1s}(\mathbf{\vec{r}}).$$
(50)

To determine the wave function ϕ_b one has to solve the Schrödinger equation (11), where H_β is given by (9). This being the unperturbed Hamiltonian which corresponds to the situations after the collision, the Schrödinger equation satisfied by ϕ_b in the center-of-mass frame of the three-particle system is written as

$$\left(-\frac{\hbar^2}{2\mu'} \nabla_{r''}^2 - \frac{\hbar^2}{2\mu} \nabla_{r_0}^2 - \frac{e^2}{r_0}\right) \left|\phi_b\right\rangle = E_b \left|\phi_b\right\rangle, \quad (51)$$

where $\tilde{\tau}'' = \tilde{\tau} - \tilde{a}\tilde{\tau}_0$. If \tilde{k}_s is the wave vector associated with the particle of an effective mass μ' after scattering, the solution of (51) is given as

$$\phi_{b}(\vec{r}_{0},\vec{r}^{\,\prime}) = \exp(i\vec{k}_{s}\cdot\vec{r}^{\,\prime\prime})\varphi_{1s}(\vec{r}_{0}) \tag{52}$$

such that $E_b = k_s^2/2\mu' + \epsilon_0$ for capture into the ground state. Since scattering connects the states characterized by $E_a = E_b$, where $E_a = k_0^2/2\mu' + \epsilon_0$, we have $|\vec{\mathbf{k}}_s| = |\vec{\mathbf{k}}_0|$.

IV. COMPUTATION OF THE CROSS SECTION FOR CAPTURE

With the help of the transition matrix, the differential-scattering cross section for capture is now given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{ba} = \left(\frac{\mu'}{2\pi}\right)^2 \left|R_{ba}^{(+)}\right|^2 \frac{v_b}{v_a},\tag{53}$$

where v_a and v_b are the relative velocities before and after the collision, and this ratio is 1 in the present case. Hereafter we shall drop the superscript (+) from $R_{ba}^{(+)}$ and subscript *a* from $f_{0a}^{(+)}$. Following (18) and using the expressions for $\chi_a^{(+)}$ and ϕ_b as given in (50) and (52), respectively, the transition matrix element is written in the atomic units as

 $R_{ba} = R_{ba}^{(1)} + R_{ba}^{(2)} , \qquad (54)$

where

$$R_{ba}^{(1)} = \langle \phi_b | U_{13} | \chi_a^{(+)} \rangle$$

$$= \int \int d\vec{\mathbf{r}} d\vec{\mathbf{r}}_0 \exp(-i\vec{\mathbf{k}}_s \cdot \vec{\mathbf{r}}) \exp(i\vec{a}\vec{\mathbf{k}}_s \cdot \vec{\mathbf{r}}_0)$$

$$\times \varphi_{1s}^*(\vec{\mathbf{r}}_0)(-1/r)\varphi_{1s}(\vec{\mathbf{r}})f_0^{(+)}(\vec{\mathbf{r}}') ,$$

$$\vec{\mathbf{r}}' = \vec{a}\vec{\mathbf{r}} - \vec{\mathbf{r}}_0 , \qquad (55)$$

and

$$R_{ba}^{(2)} = \langle \phi_b | U_{12} | \chi_a^{(*)} \rangle$$
$$= \int \int d\mathbf{\bar{r}} d\mathbf{\bar{r}}_0 \exp(-i\mathbf{\bar{k}}_s \cdot \mathbf{\bar{r}}) \exp(i\vec{a}\mathbf{\bar{k}}_s \cdot \mathbf{\bar{r}}_0)$$
$$\times \varphi_{1s}^*(\mathbf{\bar{r}}_0) \left(\frac{1}{|\mathbf{\bar{r}} - \mathbf{\bar{r}}_0|}\right) \varphi_{1s}(\mathbf{\bar{r}}) f_0^{(*)}(\mathbf{\bar{r}}') .$$
(56)

Now we shall introduce the Fourier transform of $f_0^{(+)}(\mathbf{\tilde{r}}')$ as

$$f_0^{(+)}(\vec{\mathbf{r}}') = \left(\frac{1}{2\pi}\right)^3 \int d\vec{\mathbf{k}} \exp(i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}')g(\vec{\mathbf{k}}) , \qquad (57)$$

where $g(\vec{k})$ is given by the inverse Fourier transform:

$$g(\vec{\mathbf{k}}) = \int d\vec{\mathbf{r}}' \exp(-i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}') f_0^{(+)}(\vec{\mathbf{r}}') .$$
 (58)

With the help of (57), $R_{bg}^{(1)}$ becomes

$$R_{ba}^{(1)} = -\left(\frac{1}{2\pi}\right)^3 \int d\vec{k} g(\vec{k}) G_1(\vec{p}) G_2(\vec{q}) , \qquad (59)$$

where

$$G_{1}(\vec{p}) = \int d\vec{r} \, \frac{\varphi_{1s}(\vec{r})}{\gamma} \exp(i\vec{p}\cdot\vec{r}) = \frac{4\pi^{1/2}}{1+p^{2}} \,, \tag{60}$$

$$G_{2}(\mathbf{\bar{q}}) = \int d\mathbf{\bar{r}}_{0} \varphi_{1s}(\mathbf{\bar{r}}_{0}) \exp(-i\mathbf{\bar{q}} \cdot \mathbf{\bar{r}}_{0}) = \frac{8\pi^{1/2}}{(1+q^{2})^{2}}, \qquad (61)$$

having

$$\vec{p} = \vec{a}\vec{k} - \vec{k}_s, \quad \vec{q} = \vec{k} - \vec{a}\vec{k}_s$$

Using the results of (60), (61), and (58), we have

$$R_{ba}^{(1)} = -\frac{4}{\pi^2} \exp\left(\frac{\pi \mu'}{2k_0}\right) \Gamma(1 - i \mu'/k_0)$$

$$\times \int \int d\vec{\mathbf{r}}' d\vec{\mathbf{k}} \exp(i\vec{\mathbf{k}}_0 \cdot \vec{\mathbf{r}}') \exp(-i\vec{\mathbf{k}} \cdot \vec{\mathbf{r}}')$$

$$\times F(i \mu'/k_0, 1, ik_0 r' - i\vec{\mathbf{k}}_0 \cdot \vec{\mathbf{r}}')$$

$$\times (1 + p^2)^{-1} (1 + q^2)^{-2}. \qquad (62)$$

To perform the integrations involved in (62) analytically is extremely difficult. To reduce the difficulty of dealing with multidimensional integrals, we shall make an approximation by putting $|\mathbf{\tilde{q}}| \cong |\mathbf{\tilde{p}}|$. Since $\tilde{a} = M/(M+1)$, and $M \gg 1$, such an approximation seems to be a reasonably good one. This is further justified by the fact that this does not disturb the BK result¹ which is obtained in the limit

$$N(k_0)F(i\mu'/k_0,1,ik_0r'-i\vec{\mathbf{k}}_0\cdot\vec{\mathbf{r}}') \rightarrow 1,$$

that is, in the Born approximation. With the above substitution the \vec{k} integration in (62) can be done analytically without any difficulty. One then gets

$$R_{ba}^{(1)} \cong -\exp\left(\frac{\pi\mu'}{2k_0}\right) \Gamma(1-i\mu'/k_0)\tilde{a}^{-3}$$

$$\times \int d\vec{\mathbf{r}}' \exp i\left(\vec{\mathbf{k}}_0 \cdot \vec{\mathbf{r}}' - \frac{\vec{\mathbf{k}}_s \cdot \vec{\mathbf{r}}'}{\tilde{a}}\right)$$

$$\times \left(\frac{r'}{\tilde{a}} + 1\right) \exp\left(\frac{-r'}{\tilde{a}}\right)$$

$$\times F(i\mu'/k_0, 1, ik_0r' - i\vec{\mathbf{k}}_0 \cdot \vec{\mathbf{r}}'). \tag{63}$$

Proceeding in the manner similar to that which we have used in evaluating $R_{ba}^{(1)}$, we find that the expression for $R_{ba}^{(2)}$ can be written as

$$R_{ba}^{(2)} = \frac{4}{\pi^4} \int d\vec{t} t^{-2} \int d\vec{k} g(\vec{k}) (1 + p'^2)^{-2} (1 + q'^2)^{-2} , \quad (64)$$

where

$$\vec{p}' = \vec{a}\vec{k} - \vec{k}_s - \vec{t} \ , \ \vec{q}' = \vec{k} - \vec{a}\vec{k}_s - \vec{t} \ .$$

As before, we replace $|\mathbf{q}'| \cong |\mathbf{p}'|$. With this approximation $R_{ba}^{(2)}$ becomes

$$R_{ba}^{(2)} \cong \frac{4}{\pi^4} \int \frac{d\vec{t}}{t^2} \int d\vec{r}' f_0^{(+)}(\vec{r}') \\ \times \int d\vec{k} \exp(-i\vec{k} \cdot \vec{r}') (1+p'^2)^{-4} .$$
(65)

After doing the \vec{k} integration first and then the \vec{t} integration, $R_{ba}^{(2)}$ becomes

$$R_{ba}^{(2)} \cong \tilde{a}^{-2} \int d\vec{\mathbf{r}}' f_0^{(+)}(\vec{\mathbf{r}}') \exp\left(\frac{-i\vec{\mathbf{k}}_s \cdot \vec{\mathbf{r}}'|}{\tilde{a}}\right) \\ \times \left(\frac{1}{r'} + \frac{1}{\tilde{a}} + \frac{r'}{3\tilde{a}^2}\right) \exp\left(\frac{-r'}{\tilde{a}}\right).$$
(66)

Using the results of (63) and (66), the total matrix element R_{ba} is given by

$$R_{ba} \approx \exp(\frac{1}{2}\pi\alpha)\Gamma(1-i\alpha)\lambda^{3}$$

$$\times \int d\vec{\mathbf{r}}' \exp[i(\vec{\mathbf{k}}_{0}\cdot\vec{\mathbf{r}}'-\lambda\vec{\mathbf{k}}_{s}\cdot\vec{\mathbf{r}}')] \left(\frac{1}{\lambda r'}-\frac{2r'\lambda}{3}\right)$$

$$\times \exp(-\lambda r')F(i\alpha,1,ik_{0}r'-i\vec{\mathbf{k}}_{0}\cdot\vec{\mathbf{r}}'), \quad (67)$$

where

$$\lambda = 1/\tilde{a}, \quad \alpha = \mu'/k_0.$$

To do the \vec{r}' integration in (67), we consider the integral which is represented by

$$I = \int d\vec{\mathbf{r}} \exp(i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}) [\exp(-\lambda r)/r]$$
$$\times F(i\alpha, \mathbf{1}, ipr - i\vec{\mathbf{p}}\cdot\vec{\mathbf{r}}) .$$
(68a)

These are the integrals which one comes across in the study of the atomic collision theory. Such integrals are evaluated by contour integration using the technique adopted by Nordsieck.³² The value of this integral is given as

$$I = 4\pi (\lambda^2 + q^2)^{i\,\alpha - 1} (\lambda^2 - 2i\lambda p + q^2 - 2\vec{p} \cdot \vec{q})^{-i\,\alpha} \,. \tag{68b}$$

With the help of (68) R_{ba} is written from (67) as

$$R_{ba} = \exp(\frac{1}{2}\pi\alpha)\Gamma(1-i\alpha)\lambda^3 \left(\frac{1}{\lambda}I - \frac{2\lambda}{3}\frac{d^2I}{d\lambda^2}\right).$$
 (69)

Following (69), we find

$$|R_{ba}|^{2} = 16\pi^{2}\lambda^{6}(\pi\alpha/\sinh\pi\alpha)e^{\pi\alpha}(A^{2}+B^{2})^{-2} \\ \times \exp[2\alpha\tan^{-1}(B/A)](\lambda^{2}+q^{2})^{-6}\tilde{G}(\vec{k}_{0},\vec{k}_{s}),$$
(70)

where $\tilde{C}(\vec{k}_0, \vec{k}_s)$ is a very complicated function of \vec{k}_0 and \vec{k}_s , which we have deliberately avoided expanding here. In the above equation

$$\vec{\mathbf{q}} = \vec{\mathbf{k}}_0 - \lambda \vec{\mathbf{k}}_s ,$$

$$A = \lambda^2 (1 + k_0^2) - k_0^2 ,$$

$$B = -2\lambda k_0 .$$

It may be noticed that our expression for $|R_{ba}|^2$ looks very similar to that in Ref. 6. Using this expression for $|R_{ba}|^2$, the differential scattering cross section for the capture can be written down following Eq. (53). Integrating over all the angles, we obtain the total scattering cross section as

$$\sigma = 2\pi \int_0^{\pi} \left(\frac{d\sigma}{d\Omega}\right)_{ba} \sin\theta \, d\theta \,, \tag{71}$$

where θ is the angle of scattering, i.e., the angle between \vec{k}_0 and \vec{k}_s . Evaluation of the integral on the right-hand side of (71) was done numerically using a computer for various incident proton energies between 1 and 100 keV.

V. DISCUSSION OF RESULTS

Though by now there are a large number of experiments available which measure the cross section for the capture of electrons by protons passing through hydrogen, we shall compare our result (quoted in Table I) with the experimental data obtained by McClure³³ in a recent experiment. In Fig. 3 we have plotted the results of our calculations along with those of the Born approximation,⁴ the impulse approximation,¹⁹ the distorted-wave approximation,¹⁰ the close-coupling method,¹⁷ and the experimental data of McClure,³³ for protons with energies less than 100 keV. From among all the available theoretical calculations, we have chosen these as representative results from well-known methods for our range of energies.

Our numerical results quoted in Table I and plotted in Fig. 3 have been obtained ignoring the polarization part of the potential and the part that falls off exponentially with distance. The resultant approximation is somewhat equivalent to the distorted-wave approximation.⁹ However, this is not the same approximation as that of BG.¹⁰ This can be very easily shown by comparing the transition matrix elements in both cases. Here it should be mentioned that the present approximation obviously goes beyond the first Born approximation as we have replaced the initial (or, equivalently, the

TABLE I. Capture cross sections from present theory for different incident proton energies.

Energy (keV)	$\sigma (10^{-17} \text{ cm}^2)$
1.00	0.608
2.00	13.664
3.00	34.565
4.00	53.882
5.00	69.297
6.00	79.342
7.00	84.883
8.00	88.704
9.00	89.990
10.00	87.611
20.00	52.574
30.00	26.844
40.00	13.815
50.00	7.658
60.00	4.798
70.00	3.481
80.00	2.974
90.00	2.684



FIG. 3. Plot of the capture cross sections against the incident proton energies. Theoretical results are shown by I, Born (Ref. 4); II, impulse (Ref. 19); III, distorted wave (Ref. 10); IV, close coupling (Ref. 17); V, present work. Experimental results from the work of McClure (Ref. 33) are indicated by dots.

final) free wave function with a wave function which is closer to the exact solution. To be more specific, we have taken into account the distortion of the outgoing scattered wave by the scattering field in the simplest sense.

To point out the relationship of our present work with the impulse approximation,^{6,18}¹⁹ it may be mentioned here that the outgoing scattering wave function of our theory should be considered to be philosophically similar to the one derived in the impulse approximation. That is because, in the impulse approximation, the outgoing scattering wave function is the one that is evaluated in an approximate way by taking into account the scattering of the incident proton by the wave packet of the electron of the target hydrogen atom having a momentum distribution the same as that of the hydrogen atom in the ground state. In our theory we determine the outgoing scattering wave function by considering the motion of the incident proton moving in a potential field generated due to its motion relative to the hydrogen atom in the 1s state. However, our approximation seems to be a better one than the impulse approximation because we have

been able to determine the outgoing scattering wave function analytically. With the inclusion of the exponentially decaying potential term plus the polarization part, our solution should be considered to be much closer to the exact solution. This is brought out by our calculated results at low energies whereas the impulse approximation results are reasonable only above 25 keV.

It is found that the results from our theory fit well with the experimental results for the entire energy range starting from 8 keV. A new interesting feature of our results is that our calculations show a maximum in the value of the total cross section at an incident proton energy of 9 keV. Below this energy the cross section starts gradually decreasing with decreasing incident proton energy and finally goes to zero for very low energy. Beyond 9 keV it again starts to fall with increasing incident proton energies. This type of behavior of the cross section versus energy has not been observed in any of the theoretical calculations on electron capture by protons into the 1s state for the reaction given in Eq. (1). One, of course, encounters such behavior in the case of other kinds of reactions³⁴ and for capture into the excited states of the target atom.^{24 26} Physically this is to be expected.

At higher energies our theory is expected to give better agreement with experiment. However, it is rather seen that at an energy of 100 keV or above there is a slight departure of our calculated cross section from the experimental value. We observe an increase of up to 30% in the value of our cross section over the experimental result. We do not consider this to be a flaw in our theory. Rather we feel that this happens due to the fact that we have dropped the factor $\exp(-2r'/\tilde{a}) \times (1/r'+1/\tilde{a})$ in $V_{00}(r')$ compared to 1/r' while solving for $f_{0a}^{(+)}(r')$ This factor, which is exponentially decaying, has to be taken into account for large energies. Once we include this term it is not possible to get an analytic solution for $f_{0a}^{(+)}(\vec{r}')$. The other possibility may be our use of the approximation $|\vec{q}| \cong |\vec{p}|$ while doing the \vec{k} integration in (62); although we have seen that such an approximation does not disturb the Born results. We are taking these facts into consideration in our ensuing work on this problem.

We conclude here by saying that according to our observation the internuclear Coulomb interaction plays a significant role in charge-transfer collisions. As a matter of fact, the controversy regarding its role in the rearrangement collisions still remains unsettled. Anyway, ours being a nonperturbative approach, we feel that this would help to clarify many controversies existing regarding charge-transfer reactions. Since in our theory it 596

is possible to take into account the polarizability of the target atom, this would be very useful to explain the experimental data at low energies satisfactorily.

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