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Electron Capture by Protons Passing Through Helium Gas*)

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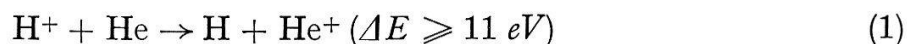
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Abstract. The impact parameter method, in a two-state moving-atom approximation, is applied to the reaction $H^+ + He \rightarrow H(1s) + He^+(1s)$. The effects of distortion and back coupling are taken into account and are shown to improve the predicted value of the total cross-section considerably for energies near that for which the cross-section is maximum. The theory is shown to be inadequate at both high and low energies. Detailed balance is shown to be satisfied by the theory.

I. Introduction

The singly-ionized hydrogen-helium system is of particular interest because of the abundance of these elements in nature, because accurate experimental results can be obtained in collision experiments using helium as the target gas, and because the system is simple enough to be amenable to rather detailed theoretical analysis. As a result, the electron capture reaction



has been studied quite extensively from both experimental¹⁻⁶⁾ and theoretical⁷⁻¹⁴⁾ points of view.

The experimental results for the total capture cross-section (see Figure 1) are characteristic of a non resonant reaction in which the energy defect, ΔE , is rather large. In the energy region 5–40 keV, where a comparison is possible, the results of the two different groups of investigators agree to about 12 percent¹⁵⁾.

Most previous quantitative theoretical investigations have been primarily concerned either with the quasi-adiabatic region⁷⁾ (impact energies below a few keV) or with the higher energy region above about 50 keV where the Born and impulse approximations recommend themselves⁹⁻¹³⁾. Two previous investigations⁸⁾¹⁴⁾ have been concerned with the intermediate energy region where neither the low nor the high energy approximations yield accurate results. While all these investigations have yielded results which are qualitatively correct, good quantitative agreement with the experimental evidence has been obtained only in the energy range 40–400 keV¹¹⁾¹²⁾¹³⁾.

*) This work was supported by the United States Atomic Energy Commission. Reproduction in whole or in part is permitted for any purpose of the U. S. Government.

The purpose of the work reported here is to see if quantitative results can be obtained for the capture cross-section in the intermediate energy range 1–50 keV, using the two-state, moving-atom approximation developed by TAKAYANAGI⁸⁾, GURNEE and MAGEE¹⁶⁾, and particularly by BATES and his coworkers¹⁷⁾¹⁸⁾. In this approximation, the impact parameter method is employed and the time-dependent electron wave function is approximated by a time-dependent linear combination of the initial and final moving-atom states. If the differential equations for the coefficients are solved without further approximations, the approximate wave function remains normalized so that probability is conserved. (What we refer to as probability conservation is sometimes referred to as the allowance for “back coupling” between the final and the initial state.) In addition, detailed balance is satisfied. Finally, the method accounts approximately for distortion, i.e. the energy level shifts which occur during the collision. As will be seen from the results, both back coupling and distortion are important below 50 keV and the inclusion of these effects greatly improves the agreement with experiment in the energy region between about 6 and about 30 keV. At both high and low energies the theory appears to be inadequate.

II. Theory

In the initial state of the colliding He-H⁺ system, the electrons are in the ¹S₀ ground state of He. We neglect the small spin-orbit forces in the hamiltonian and are thus concerned with the time evolution of the exchange-symmetric He ground state wave function under the influence of the passing proton. The basic equations of the theory are therefore just exchange-symmetric, two-electron versions of the ones given for a single electron in reference ¹⁷⁾. The approximate electron wave function, ψ , is written as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = A(t) \chi_A(\mathbf{r}_1, \mathbf{r}_2, t) + B(t) \chi_B(\mathbf{r}_1, \mathbf{r}_2, t). \quad (2)$$

The precise definition of the electron coordinates, $\mathbf{r}_1, \mathbf{r}_2$, is given below Equation (4). The time is designated by t . $A(t)$ and $B(t)$ are expansion coefficients, to be determined as described below.

In Equation (2) the moving-atom wave function¹⁷⁾ for the initial state, A , is given by*)

$$\chi_A(\mathbf{r}_1, \mathbf{r}_2, t) = \varphi_A(\mathbf{r}_{1A}, \mathbf{r}_{2A}) \times \exp \left[-\left(\frac{i}{2}\right) (v z_1 + v z_2) - i \left(E_A + \frac{v^2}{4} \right) t \right], \quad (3)$$

where $\varphi_A(\mathbf{r}_{1A}, \mathbf{r}_{2A})$ is an approximate wave function for the helium ground state. We have taken this wave function to be the two-parameter, open-shell, variational wave function¹⁹⁾,

$$\varphi_A(\mathbf{r}_{1A}, \mathbf{r}_{2A}) = N_A [e^{-(\alpha r_{1A} + \beta r_{2A})} + e^{-(\alpha r_{2A} + \beta r_{1A})}]. \quad (4)$$

The constant N_A normalizes φ_A . The parameters α and β are determined from the variational principle, which yields the values $\alpha = 2.1832$, $\beta = 1.1885$, and the variationally determined energy $E_A = -2.8757^*$). In the above formulae the space coordinates are defined as follows: A designates the helium nucleus; B the hydrogen

*) Atomic units are used except where other units are explicitly introduced.

nucleus. The vectors \mathbf{r}_1 and \mathbf{r}_2 locate the electrons relative to the midpoint of the inter-nuclear line, \mathbf{R} , going from A to B . The vector \mathbf{r}_{1A} goes from A to electron 1, etc. The constant vector \mathbf{v} describes the straight-line motion of B relative to A and is taken along the z -axis in the laboratory frame. The coordinates z_1 and z_2 are defined by $vz_1 = \mathbf{v} \cdot \mathbf{r}_1$ and $vz_2 = \mathbf{v} \cdot \mathbf{r}_2$. The choice of φ_A will be further discussed in Section IV.

The final state wave function χ_B has the form

$$\chi_B(\mathbf{r}_1, \mathbf{r}_2, t) = \frac{1}{\sqrt{2}} \left\{ \Psi_A(\mathbf{r}_{1A}) \Psi_B(\mathbf{r}_{2B}) \times \exp \left[-\frac{i}{2} (v z_1 - v z_2) - i \left(\varepsilon_A + \varepsilon_B + \frac{v^2}{4} \right) t \right] \right. \\ \left. + \text{exc}(1, 2) \right\}. \quad (5)$$

In Equation (5) Ψ_A and Ψ_B are 1s wave functions for He^+ and H respectively; the quantities ε_A and ε_B are the energies of these states. The symbol $\text{exc}(1, 2)$ means repeat the preceding expression, interchanging the roles of the two electrons. While χ_A is normalized at all times, χ_B is normalized only when the heavy particles are far apart ($R \rightarrow \infty$). In addition, χ_A and χ_B are not orthogonal except in the limit $R \rightarrow \infty$.

The differential equations satisfied by $A(t)$ and $B(t)$ are obtained by requiring that the equations*),

$$\left(\chi_A, \left(\mathbf{H} - i \frac{\partial}{\partial t} \right) \Psi \right) = 0, \quad (6a)$$

and

$$\left(\chi_B, \left(\mathbf{H} - i \frac{\partial}{\partial t} \right) \Psi \right) = 0, \quad (6b)$$

be satisfied at all times. In Equations (6) \mathbf{H} is the complete hamiltonian operator for the two electrons in the field of the two nuclei. As will be demonstrated later in this section the theory is invariant with respect to the addition to \mathbf{H} of an arbitrary function of t^{17}). It is not hard to show, using Equation (6) and the hermiticity of \mathbf{H} , that Ψ remains normalized at all times.

For each impact parameter, ϱ , the differential equations are to be integrated from $t = -\infty$ to $t = \infty$ with the initial conditions

$$A(-\infty) = 1, \quad B(-\infty) = 0. \quad (7)$$

The probability of capture, $P(\varrho, v)$, for relative velocity v and impact parameter ϱ is given by

$$P(\varrho, v) = |B(\infty)|^2. \quad (8)$$

The total cross-section $Q(v)$ for capture without excitation is then

$$Q(v) = 2\pi \int_0^\infty \varrho P(\varrho, v) d\varrho. \quad (9)$$

*) The notation $(\chi_1, 0\chi_2)$ means: "Apply the operator 0 to the wave function χ_2 and integrate the result with the complex conjugate of the wave function χ_1 ".

In the above version of the theory (which is the usual one) it is difficult to show that detailed balance is satisfied*). For this reason it is convenient to orthogonalize the states in the expansion of Equation (2) and to rewrite Equation (2) in the form,

$$\Psi = A'(t) \chi'_A + B'(t) \chi'_B, \quad (10)$$

where

$$\begin{aligned} \chi'_A &= \chi_A, \\ \chi_B &= \chi_B - (\chi_A, \chi_B) \chi_A, \\ A' &= A + (\chi_A, \chi_B) B, \\ B' &= B \end{aligned} \quad (11)$$

Because the new functions χ'_A and χ'_B are orthogonal at all times, the differential equations for $A'(t)$ and $B'(t)$ are simpler than those for $A(t)$ and $B(t)$. The overlap integral (χ_A, χ_B) vanishes as $|t| \rightarrow \infty$. Hence in this limit the primed and unprimed coefficients are equal. The differential equations satisfied by A' and B' are obtained from Equation (10) and the conditions expressed by substituting χ'_A for χ_A and χ'_B for χ_B in Equations (6a) and (6b). These equations are

$$\begin{aligned} i \frac{dA'}{dt} &= C'_A A' + D'_A B', \\ i \frac{dB'}{dt} &= D'_B A' + C'_B B, \end{aligned} \quad (12)$$

where

$$\begin{aligned} C_A &= \left(\chi'_A, \left(H - i \frac{\partial}{\partial t} \right) \chi'_A \right), \\ D'_A &= \left(\chi'_A, \left(H - i \frac{\partial}{\partial t} \right) \chi'_B \right), \\ C'_B &= \frac{\left(\chi'_B, \left(H - i \frac{\partial}{\partial t} \right) \chi'_B \right)}{(\chi'_B, \chi'_B)}, \\ D'_B &= \frac{\left(\chi'_B, \left(H - i \frac{\partial}{\partial t} \right) \chi'_A \right)}{(\chi'_B, \chi'_B)}. \end{aligned} \quad (13)$$

*) In reference 17 detailed balance is shown to be satisfied in the above approximation under the additional assumption $A(t) = 1$. In the course of the present work it was discovered that the restriction $A(t) = 1$ is not necessary. The proof for the two state case is given in the present paper. A different proof, valid for the n -state approximation, has been worked out and will be submitted for publication in the near future.

It is not hard to prove that the same value of $P(\rho, v)$ is obtained from either the primed or the unprimed expansion¹⁸). The self-coupling terms in Equation (12) are eliminated through the substitutions,

$$\begin{aligned} A' &= A'' \exp \left[-i \int_{-t_0}^t C'_A(t) dt \right], \\ B' &= B'' \exp \left[-i \int_{-t_0}^t C'_B(t) dt \right], \end{aligned} \quad (14)$$

where t_0 is some fixed time. The new differential equations are

$$i \frac{dA''}{dz} = v^{-1} D'_A e^{-i\phi} B'', \quad i \frac{dB''}{dz} = v^{-1} D'_B e^{i\phi} A''. \quad (15)$$

In Equation (15) the space variable z ($z = vt$) has been introduced in place of the time t . (The internuclear separation R is given in terms of z by $R = (\rho^2 + z^2)^{1/2}$.) The function ϕ is given by

$$\phi(z) = v^{-1} \int_{-z_0}^z (C'_B - C'_A) d\xi; \quad z_0 = vt_0. \quad (16)$$

It is readily seen from Equation (13) that D'_A , D'_B , and $C'_B - C'_A$ are invariant with respect to the addition of a function of t (such as the internuclear repulsion) to H . As a result the only effect of the addition of a real function of t to H is a phase change (see Equation (14)) in ψ which is of no physical consequence.

From Equation (13) it can be shown that the imaginary part of ϕ is related to the normalization of χ'_A and χ'_B . Designating the real part of ϕ by ϕ_1 we find that

$$\phi = \phi_1 - i \ln [(\chi'_B, \chi'_B)^{1/2}], \quad (17)$$

provided z_0 is chosen to be sufficiently great that $(\chi'_B, \chi'_B) = 1$ at $z = -z_0^*$. Expressed in terms of ϕ_1 , Equation (15) now reads

$$i \frac{dA''}{dz} = v^{-1} \{D'_A(\chi'_B, \chi'_B)^{-1/2}\} e^{-i\phi_1} B'', \quad (18a)$$

$$i \frac{dB''}{dz} = v^{-1} \{D'_B(\chi'_B, \chi'_B)^{1/2}\} e^{i\phi_1} A''. \quad (18b)$$

The quantities in the braces in Equations (18a) and (18b) can be shown to be complex conjugates of each other. From Equation (13), taking account of the fact that H is a hermitian operator, it is seen that

$$\{D'_A(\chi'_B, \chi'_B)^{-1/2}\} - \{D'_B(\chi'_B, \chi'_B)^{1/2}\}^* = -i(\chi'_B, \chi'_B)^{-1/2} \frac{d}{dt} (\chi'_A, \chi'_B) = 0. \quad (19)$$

The last equality follows from the orthogonality of χ'_A and χ'_B .

*) In the calculations z_0 was taken to be large enough that (χ'_B, χ'_B) was equal to unity to at least 6 figures. Professor D. R. BATES has kindly pointed out that because the coefficients in Equation (14) depend on t_0 , the solution $\Psi(r_1, r_2, t)$ depends on t_0 . Hence the argument given in the text only guarantees that detailed balance is satisfied for a particular interval $(-t_0, t_0)$ and not necessarily for all sufficiently large t_0 as should be the case. Using the formulae given in the text it can be shown that for all sufficiently large t_0 the t_0 -dependence of Ψ is entirely contained in the multiplicative phase factor $\exp(-i \int_{-t_0}^0 dt C'_A)$ which does not influence the transition probabilities. From this it can be seen that detailed balance is actually satisfied for all sufficiently large t_0 .

Equations (18a) and (18b), simplified through the use of Equation (19), were used to obtain the numerical results presented in Section IV. The capture probabilities were calculated for each impact parameter, ρ , and velocity, v , by integrating Equation (18) from $z = -z_0$ to $z = +z_0$, with the initial conditions

$$A'' = 1, \quad B'' = 0. \quad (20)$$

The capture probability was taken to be

$$P(\rho, v) = |B''(z_0)|^2. \quad (21)$$

The choice of a symmetric interval of integration is essential for the compatibility of Equations (20) and (21) with Equations (7), (8), (11), and (14). According to Equation (14) the moduli of the primed and double-primed quantities are equal at $t = -t_0$. The symmetric interval guarantees that they are also equal to $t = +t_0$. This follows from the evaluation of the coefficients C'_A and C'_B from Equations (13), (5), and (3), which shows that for each ρ and v , the real parts of C'_A and C'_B are even functions of t and their imaginary parts are odd functions of t . In Equation (14) the imaginary parts of C'_A and C'_B therefore integrate to zero over the symmetric interval $(-t_0, t_0)$.

From Equation (11) it is also seen that the compatibility of Equations (20) and (21) with Equations (7) and (8) requires that z_0 be large enough that (χ_A, χ_B) be negligible compared to unity. This condition was respected in the numerical work to 5 figures or better.

The fact that the approximation represented by Equation (2) or, equivalently, Equation (10) is compatible with detailed balance follows from Equation (19), as a consequence of which Equations (18a) and (18b) can be transformed, one into the other, through the process of complex conjugation and the substitutions $A'' \rightarrow (B'')^*$ and $B'' \rightarrow -(A'')^*$. Thus if $A''(z)$, $B''(z)$ is the unique solution of Equation (18) for the initial conditions $A''(-z_0) = 1$, $B''(-z_0) = 0$, and $A'''(z)$, $B'''(z)$, is the unique solution for the initial conditions $A'''(-z_0) = 0$, $B'''(-z_0) = 1$, the transformation just described guarantees that $|A'''(z_0)|^2 = |B'''(z_0)|^2$. This shows that detailed balance is satisfied.

III. Numerical Application of the Theory

The computations were carried out with the aim of obtaining $Q(v)$ to four figures. The main steps in the evaluation of $Q(v)$ are:

1. The evaluation of the coefficients C'_A , C'_B , D'_A , D'_B , as functions of v , ρ , and z .
2. The integration of Equation (18) to find $P(\rho, v)$ from Equation 21.
3. The integration of $P(\rho, v)$ over impact parameter to find $Q(v)$. (See Equation (9).)

It is convenient to discuss these steps in reverse order.

The impact parameter quadrature was carried out over the intervals $(0, R_1)$ and (R_1, R_2) using Gauss-Legendre quadrature formulae with N_1 points in the first interval and N_2 points in the second interval. Preliminary studies of the accuracy of the quadrature scheme were carried out for a test function of the form $P(\rho, v) = e^{-\sigma \rho} \cos^2(\tau \rho)$, where σ and τ were adjustable constants. In these trials, for five figure

accuracy or better in the ρ quadrature, it was always sufficient to have three or four quadrature points on each loop of the oscillating integrand. For the actual calculations, an initial choice of R_1 , R_2 , N_1 and N_2 was made, using as a guide the $\rho P(\rho, v)$ curves of McCARROLL²⁰) for the reaction $H^+ + H \rightarrow H + H^+$. The actual shape of the calculated $\rho P(\rho, v)$ curve was then used to decide whether this initial choice was adequate to guarantee four-figure accuracy in $Q(v)$. The cases $v = 0.5$ and $v = 0.2$ were partially recomputed. In the other cases the initial choice was judged to be adequate.

The integration of Equation (18) was carried out using a variable step-size, Adams-Moulton integration subroutine, with the maximum relative truncation error set at 10^{-5} , except for $v = 0.2$ where it was set at 10^{-6} . Preliminary trials at $v = 0.2$ and $v = 1.1$ were used to guarantee that the choice of z_0 and the maximum allowable truncation error were such that the resulting values of $P(\rho, v)$ were accurate to four figures or better. For $v \geq 0.5$ the minimum step size required was 0.0125. (It was usually 0.025.) For $v = 0.2$, where distortion is extremely important, ϕ_1 is consequently very large, and as a smaller truncation error is necessary, the minimum step size required was 0.003125. The variable step size feature allows a considerable saving in computer time, especially for low velocities, because the minimum step size, which is required for small values of R , is much less than the average step size required elsewhere on the integration path. The quadrature required for the evaluation of ϕ (see Equation (16)) was done using a 3-point Gauss-Legendre quadrature to advance from one time step in the differential equation subroutine to the next. The differential equation integration times, which depended on ρ and v , ranged from about 1.5 to 2 minutes for $v \geq 0.5$. For $v = 0.2$ the average integration time was about 4.5 minutes*).

The evaluation of the coefficients C'_A , etc. is by far the most timeconsuming part of the numerical calculation. The required formulae, which are readily obtained from Equations (13), (11), (3), (4), and (5), are too lengthy to be recorded here. All but one of the 6-dimensional integrals over the two-electron configuration space can be reduced to three-dimensional integrals which can either be evaluated analytically or which have the form,

$$\int d\mathbf{r} e^{-Ar_A} e^{-Br_B} e^{ivz} g(\mathbf{r}), \quad (22)$$

where A and B are constants (not to be confused with the coefficients $A(t)$, $B(t)$ of Section II) and $g(\mathbf{r})$ is a function like 1, r_A^{-1} , or r_B^{-1} . These integrals are encountered in all calculations of electron capture probabilities using the impact parameter method and can be evaluated numerically, for each value of v , ρ , z by one-dimensional Gauss-Laguerre quadrature²⁰⁾²¹⁾. For $v \leq 2$, 10 quadrature points were used; for $v = 4$, 20 quadrature points were used.

In addition to the above mentioned integrals it is necessary to evaluate the integral

$$M \equiv \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-Cr_{1A}} e^{-Dr_{1B}} e^{-Cr_{2A}} e^{-Dr_{2B}} e^{iv(z_2 - z_1)} (r_{12})^{-1}. \quad (23)$$

In Equation (23) r_{12} is the electron-electron separation and C and D are constants. This integral is a typical two-center exchange integral, modified by a velocity-dependent term which is associated with the relative motion of the centers. This

*) The computations were performed on a Control Data Corporation 1604 computer.

integral was evaluated by introducing spheroidal coordinates and using the Neumann expansion for $(r_{12})^{-1}$ (22). The sixfold integral can then be reduced to the form

$$M = 16 \pi^2 (C + D)^{-5} \exp \left(- (C + D) R \right) \sum_{L=0}^{\infty} \sum_{M=0}^L T_{LM}, \quad (24)$$

where

$$T_{LM} = \varepsilon(M) (-1)^M (2L + 1) \left[\frac{(L-M)!}{(L+M)!} \right]^2 I_{LM},$$

$$\varepsilon(M) = \begin{cases} 1, & M = 0 \\ 2, & M > 0, \end{cases} \quad (25)$$

and

$$I_{LM} = \frac{2}{R(C+D)} \int_0^{\infty} dx_2 e^{-x_2} \int_0^{x_2} dx_1 e^{-x_1} Q_L^M \left(\frac{2x_2}{R(C+D)} + 1 \right) \times$$

$$P_L^M \left(\frac{2x_1}{R(C+D)} + 1 \right) g_L^M(x_1, x_2). \quad (26)$$

In Equation (26) P_L^M and Q_L^M are associated Legendre functions and

$$g_L^M(x_1, x_2) = 2 \operatorname{Re} \{ f_L^M(x_2) f_L^{M*}(x_1) \}, \quad (27)$$

where

$$f_L^M(x) = \left(x + \frac{(C+D)R}{2} \right)^2 P_L^M(\cos \Psi) j_L(\zeta) + \left(\frac{(C+D)R}{2} \right)^2 \sum_J A_J^{LM} P_J^M(\cos \Psi) j_J(\zeta). \quad (28)$$

In Equation (28) j_L is the spherical Bessel function, and the coefficients A_J^{LM} are defined by

$$x^2 P_L^M(x) = \sum_J A_J^{LM} P_J^M(x). \quad (29)$$

The complex quantities $\cos \Psi$ and ζ are solutions of the equations,

$$\zeta \cos \Psi = \frac{i(C-D)R}{2} + \frac{vz}{R(C+D)} \left(x + \frac{R(C+D)}{2} \right),$$

$$\zeta \sin \Psi = \frac{v\varrho}{R(C+D)} \{ x^2 + x(C+D)R \}^{1/2}. \quad (30)$$

The evaluation of M was carried out by truncating the series in Equation (24) after the terms for $L = 4$. The double integrals I_{LM} were done by dividing the region $0 \leq x_2 < \infty$ into two regions (0,1) and (1, ∞). A 10 point Gauss-Legendre quadrature was used in the first interval and a 10 point Gauss-Laguerre quadrature was used in the second. The indefinite integral over x_1 was built up from each x_2 quadrature point to the next through the use of a 3 point Gauss-Legendre quadrature. For $v = 0$, $R = 1$ and $v = 0$, $R = 5$ the computed value of M was compared with the value obtainable from the tables in reference 23, using the same number of terms from the tables in the sum over L . The results agreed to a few parts in the sixth figure. For $\varrho = 0$, $z = 10^{-5}$, and $v = 0, 0.8, 2$, and 6 the value of M was compared with the value calculated for $R = 0$ from an exact analytic formula. The agreement was exact to 5 figures for $v = 0$ and 0.8 ; the difference was 2 in the fifth place for $v = 2$ and was about 5 percent for $v = 6$. The magnitude of the error introduced by the truncation

of the series of Equation (24) increases with increasing R and v . It was estimated by observing the magnitude of the contributions to M from terms with $L = 3$ and $L = 4$. For $v = 1$ we believe the truncation error to be less than one in the fifth place for $R < 1.5$, to be of the order of one in the fourth place for $R \sim 2$, one in the third place for $R \sim 4$, and 2 in the 3rd place for $R \sim 5$.

Fortunately, D'_A does not involve the exchange integral. Thus the exchange integral influences the results only through its contribution to $\text{Re} \{C'_B\}$ in the expression for ϕ_1 . (See Equations (16) and (17).) Now in Equation (18) the factor, $\exp(-i \Delta E t) = \exp(-i (\epsilon_B + \epsilon_A - E_A) z/v)$, can (and should) be factored out of D'_A and combined with the distortion factor $\exp(-i \phi_1)$. It is then seen from Equation (16) that the exchange integral influences the calculation through its effect on the sum $C'_B - C'_A + (\epsilon_B + \epsilon_A - E_A) \sim C'_B - C'_A + 0.4$. Consequently the inaccuracy in M for large R and v , where it is small compared to 0.4, is reflected in a considerably smaller inaccuracy in the function $\gamma(z) = \phi_1(z) + (\epsilon_B + \epsilon_A - E_A) z/v$. Because of its smallness compared to 0.4 at large R , $C'_B - C'_A$ was set equal to zero for $|z| > 5.8$.

About 15 sec. are required to compute the value of M for one set of values of v , ϱ , and z . Once M has been computed, about 3 sec are required to evaluate D'_A , C'_A , and C'_B . In order to reduce the required computer time, for each value of v and ϱ , interpolation in z was used to provide values of M at an arbitrary z from a table of values computed in advance. These values were then used to compute a table of coefficients from which, by interpolation, the values of the coefficients at an arbitrary z could be obtained. In the case of M , interpolation of the logarithm turned out to be the most efficient method. The interpolation schemes were chosen as functions of ϱ and z in such a way as to maximize the interpolation mesh sizes without introducing further inaccuracies in M and the coefficients due to the interpolation. In the case of M , from 14 to 20 interpolation points were used; in the case of the coefficients from 60 to 100 points were used.

A considerable effort was made to insure that the coupling coefficient $D'_A(\chi'_B, \chi'_B)^{-1/2}$ and the function $\gamma(z)$ were accurate to 5 figures or better. We believe this to be the case except for $v \leq 0.5$ and $\varrho \leq 3$ where $\gamma(z)$ is likely to be in error by 1 or 2 in the fourth place. Several computations of the direct and inverse reaction probabilities were carried out at $v = 0.5$ and $v = 1.1$ by solving the differential equations for the original coefficients $A(t)$, $B(t)$. (See Equations (2), (6), (7), and (8).) The probabilities agreed with each other and with the probability calculated from Equation (21) to 3 parts in the fifth figure or better. Since the coefficients in the differential equations for the two versions of the theory are very different, we feel that the agreement constituted a good check against blunders and on the overall accuracy of the numerical procedures.

IV. Results and Discussion

A. The Total Cross Section

The results of the calculations are given in Table I and in Figure 1. At each value of v , except at $v = 4$, four values, $Q_i(v)$, $i = 1-4$, are presented*). These are instructive in connection with the relative importance of distortion and probability conservation.

*) At $v = 4$ only Q_1 and Q_2 were computed.

The cross-sections Q_1 and Q_2 were calculated by quadrature using the small-probability approximation, $A'' = 1$, in Equation (18b). (See reference 17), Equation (31).) In Q_1 distortion was neglected, i.e. ϕ_1 was set equal to zero; in Q_2 it was included. The cross-sections Q_3 and Q_4 were calculated by solving Equations (18) so that probability was actually conserved. In Q_3 distortion was again neglected; in Q_4 it was included. Naturally, Q_4 is to be considered as the final prediction of the theory.

Table 1

Total Capture Cross-Sections. In Q_1 both distortion and probability conservation are neglected; in Q_2 just probability conservation is neglected; in Q_3 just distortion is neglected; in Q_4 both distortion and probability conservation are taken into account. The cross-sections are given in units of 10^{-16} sq. cm

[E keV]	Q_1	Q_2	Q_3	Q_4
1.00	7.852×10^{-1}	5.862×10^{-3}	1.815×10^{-1}	3.553×10^{-3}
6.25	4.571×10^0	1.025×10^0	1.950×10^0	7.48×10^{-1}
30.2	2.393×10^0	2.274×10^0	2.015×10^0	1.916×10^0
100	2.666×10^{-1}	2.897×10^{-1}	2.553×10^{-1}	2.756×10^{-1}
400	3.412×10^{-3}	3.543×10^{-3}		

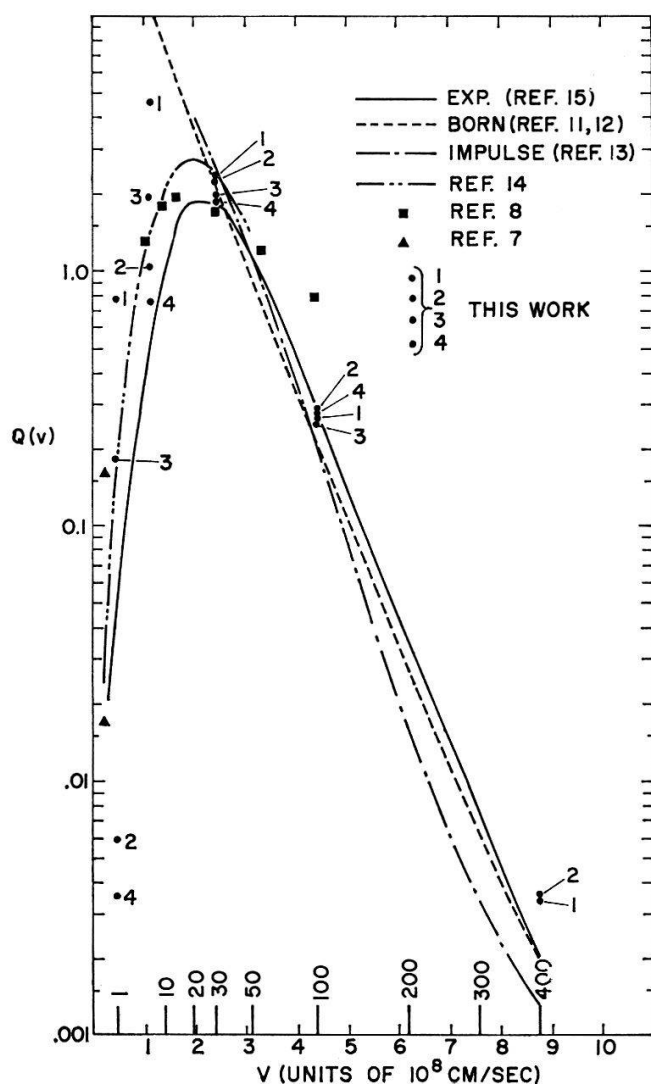


Fig. 1

The Total Cross-Section. The cross-sections are given in units of 10^{-16} cm². The vertical lines at the bottom indicate the impact energy in keV. The points labeled 1-4 correspond to the following approximations to $Q(v)$: in Q_1 both distortion and probability conservation are neglected; in Q_2 just probability conservation is neglected; in Q_3 just distortion is neglected; in Q_4 both distortion and probability conservation are taken into account.

Figure 1 also contains values of $Q(v)$ calculated by different methods, as well as the experimental cross-section Q_e . All the theoretical cross-sections are for capture without excitation. The experimental cross-section Q_e includes capture into excited states and capture with excitation of the residual slow He^+ ion. According to MAPLETON¹¹), $Q(v)$ should lie below Q_e , by from 15 to 22 percent in the energy range covered by the graph. The results may be summarized as follows:

1. Both distortion and probability conservation are very important below 30 keV. Their inclusion in the calculation generally improves the predicted value of $Q(v)$.

2. Allowing for capture into excited states and capture accompanied by excitation of the residual He^+ ion in making the comparison with experiment, the two-state, moving-atom approximation leads to a cross-section which is about 25 percent too high in the energy region 15–100 keV. At higher energies the predicted cross-section is a good deal too high. At energies below 15 keV the theory again becomes quantitatively inaccurate, being too high by about 65 percent at 6 keV and too low by about a factor of 14 at 1 keV.

3. The total cross-section is extremely sensitive to distortion at low energies, with the consequence that even moderately accurate results for the total cross-section will require very accurate information about the interactions which occur during the collision.

The above results appear to the authors to be encouraging with respect to the application of the two state approximation to other non-resonant systems at energies not too far above and below that for which the cross-section is maximum, and discouraging with respect to its application at higher and lower energies.

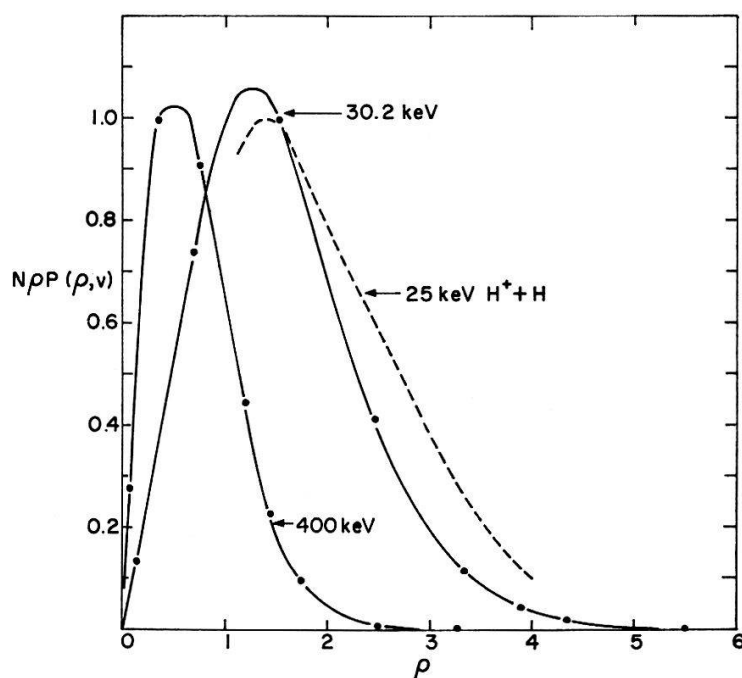


Fig. 2

Capture Probability versus Impact Parameter. The dots indicate the computed values. The curves were drawn freehand from these. The dashed curve is adapted from reference 20. The normalizing factor N has the value 1.855 at 30.2 keV and 526 at 400 keV.

That the theory should work fairly well in the energy range near the cross-section maximum is reasonable since under these circumstances, (a) capture without excitation has a large probability compared with other possible processes, and (b) the important impact parameters for the capture process (see Figure 2 and Figure 3) are not small compared to the diameters of the interacting atoms. These two conditions are certainly necessary for the validity of the two-state, moving atom approximation. In addition, the influence of distortion, while quantitatively important, is not so great as to preclude its calculation by means of an expansion which includes just two atomic states.

At lower energies, where an adiabatic approach recommends itself and an expansion in terms of molecular eigenfunctions is to be preferred, the important impact parameters are somewhat smaller than in the energy range where the cross-section is near its maximum, and distortion is extremely important. As a result, even if a two-state *molecular* approach is valid, linear combinations of atomic wave functions cannot be expected to approximate the molecular eigenfunctions with sufficient accuracy to yield a good value for the capture cross-section.

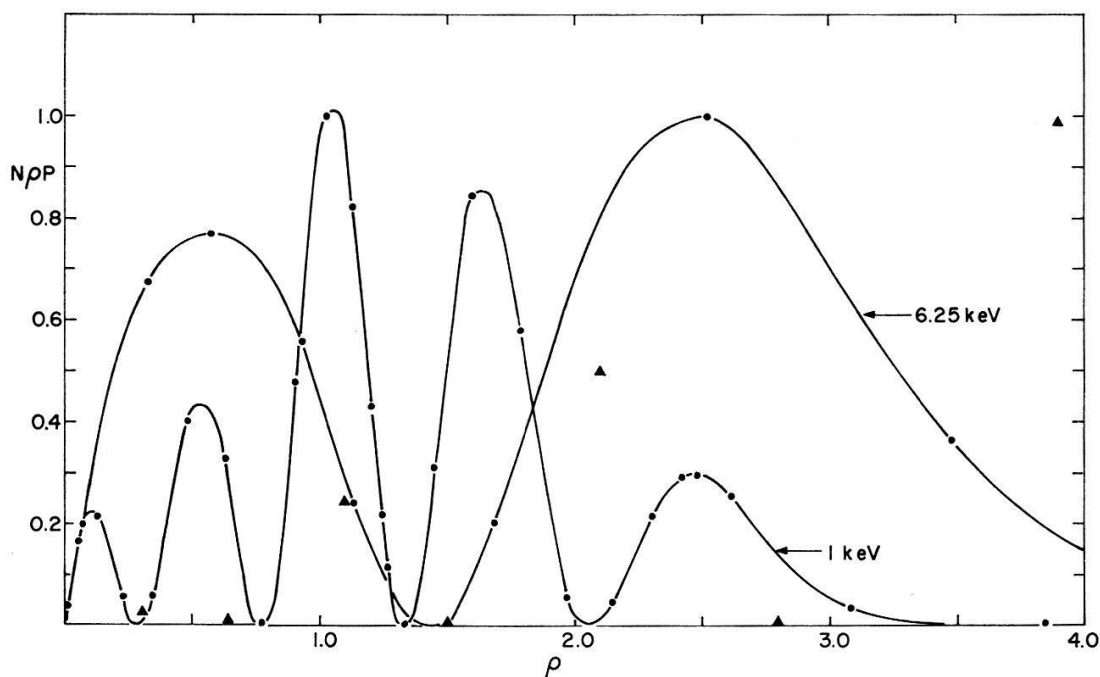


Fig. 3

Capture Probability versus Impact Parameter. The dots indicate the computed values. The curves were drawn freehand from these. The solid triangles show the maxima and minima in the 1 keV curve for $H^+ + H \rightarrow H + H^+$ as given in reference 20. In this latter case the probability is appreciable out to $\rho = 6$. The normalizing factor N has the value 6.67 for 6.25 keV and 449 for 1 keV.

At higher energies where the effects of distortion and back coupling in the two state approximation are negligible, the important impact parameters become small compared to the atomic size, and in addition, inelastic processes (particularly ionization) are important.

Now for small values of R the wave functions χ_A and χ_B are not qualitatively very different. Hence a linear combination of them offers very little flexibility as an expansion set and it is probably unrealistic to hope that it is adequate to describe the actual electron wave function. Other methods are doubtless required at high energies¹²⁾¹³⁾²⁴⁾²⁵⁾²⁶⁾²⁷⁾.

Let us now consider briefly the relation of results obtained in this paper with those obtained previously by the other investigators (See Figure 1).

The two-state, moving atom approximation offers clear advantages over the BORN¹²⁾ and impulse¹³⁾ approximations at energies in the range of roughly 6–40 keV where distortion and probability conservation are important and an atomic wave function expansion is adequate. At higher energies the Born and impulse approximations agree better with experiment; at lower energies none of these approximations can be trusted. It is worth noting that in the case of helium the high energy behavior of the two-state, moving-atom approximation relative to the Born and impulse approximations resembles closely that found for the resonant reaction $H^+ + H \rightarrow H + H^+$ ²⁴⁾, and the non-resonant reaction $He^{2+} + H(1s) \rightarrow He^+(1s) + H^+$ ²⁸⁾.

The other theoretical calculations are most applicable to the low energy side of the cross-section maximum.

MASSEY and SMITH⁷⁾, in a pioneering application of the perturbed stationary state method, evaluated the capture cross-section for the energy range 100–300 eV, using rather crude approximations to the molecular wave functions. It would be of interest to repeat this calculation with more accurate molecular wave functions²⁹⁾.

The calculations of TAKAYANAGI⁸⁾, and those of RAPP and FRANCIS¹⁴⁾ are similar to those of the present paper, in that they are all based on a two-state, atomic wave function expansion. In references⁸⁾ and ¹⁴⁾, the matrix elements are evaluated neglecting the effect of momentum transfer. As is illustrated in Figure 2 of reference²⁰⁾, the neglect of momentum transfer increases the predicted cross-section considerably at energies above a few keV.

In the calculations of TAKAYANAGI, the reaction was treated as a two electron problem and ϕ_A (see Equation (4)) was taken to be $\sim \exp(-1.6875(r_{1A} + r_{2A}))$. Thus TAKAYANAGI's approach differs from ours with respect to the choice of helium wave function and the treatment of momentum transfer. In addition, TAKAYANAGI neglects back coupling and, through his treatment of the heavy ion motion, introduces coefficients C_A and C_B different from those which follow from Equations (2) and (6).

The calculation of RAPP and FRANCIS was done as a single-electron calculation and was intended to provide a means of getting semiquantitative results with a minimum of labor. It is difficult to assess a priori the net result of the many approximation used in their formulation. Perhaps the most important ones are (a) the use of a one-electron formulation, (b) the neglect of distortion, (c) the neglect of momentum transfer, and (d) the use of simplifying asymptotic formulae which are quantitatively valid only for impact parameters much larger than unity. (See Section 5 of their paper.) At low energies, where their neglect of momentum transfer is not too important, distortion is very important, and the important impact parameters are not large enough for the asymptotic formulae to be very accurate.

The extreme sensitivity of the low energy results to distortion is the most likely origin of the wide variation amongst the various theoretical predictions. This can be appreciated by noting¹⁴⁾ that if in Equation (18) $D'_A(\chi'_B, \chi'_B)^{-1/2} \exp(-i\phi_1)$ can be approximated by

$$k_1 \operatorname{sech}(k_2 z) \exp\left(\frac{-i\omega z}{v}\right), \quad (31)$$

where k_1 , k_2 , and ω are independent of z , then

$$P(\varrho, v) = \sin^2\left(\frac{\pi k_1}{(v k_2)}\right) \operatorname{sech}^2\left(\frac{\pi \omega}{(2 k_2 v)}\right). \quad (32)$$

For low velocities, and impact parameters which are not too small, the functional form of Equation (31) fits the actual coefficients in Equation (18) well enough for an order of magnitude discussion. For $v = 0.2$, and $\varrho \sim 1$, the values $k_2 \sim 1$, $k_1 \sim 0.3$ are representative. The quantity ω should be taken as the average of $C'_B - C'_A + \Delta E$ over the values of z which are important in the collision (See Equations (16)–(18).) In the case under discussion it is appropriate to use $\omega \sim 0.8$. For $v = 0.2$ the second term of the product in Equation (32) is then

$$\sim 4 e^{-(\pi \omega / k_2 v)} = 4 e^{-5\pi \omega}. \quad (33)$$

From Equation (33) it is seen that with $\omega \sim 1$, a 20 percent decrease in ω increases the value of expression (33) by a factor of about twenty. It is not surprising, then, that different approximate calculations lead to widely different results.

B. The Variation of $P(\varrho, v)$ with Impact Parameter

The variation of $P(\varrho, v)$ as a function of ϱ for fixed v is of interest (a) because the theoretical values of $P(\varrho, v)$ can be compared with experiment⁶⁾, at least over a restricted range of ϱ , and (b) because a knowledge of which impact parameters are important at a given energy is helpful in determining which approximations should be most valid.

In Figures 2 and 3 $\varrho P(\varrho, v)$ is plotted as a function of ϱ for several energies. In these figures the results obtained by MCCARROLL²⁰⁾ for the resonant reaction $H^+ + H \rightarrow H + H^+$ are also indicated. The shift toward smaller impact parameters which occurs in a non-resonant reaction is quite apparent, and is dramatic at the lowest energy. Because the theory is so sensitive to distortion, the 1 keV curve is very likely to be in violent disagreement with experiment.

The calculations necessary for a comparison of $P(\varrho, v)$ with the experimental results of HELBIG and EVERHART⁶⁾ are being carried out and will be submitted for publication in the near future.

C. The Choice of Helium Wave Function

After a consideration of various possible helium wave functions and some investigation designed to see how difficult it would be to use them for capture calculations³⁰⁾³¹⁾, it was decided to use the two-parameter wave function described by Equation (4). The main reason was that, while the two-parameter function was about as easy to use as the one-parameter function used by TAKAYANAGI, the two-parameter function yields a better value of the energy defect ΔE , and has a physically more reasonable space dependence in the limit in which one electron stays close to the helium nucleus and the other is far away*). Calculations of the matrix elements associated with the expansion described by Equations (2) and (6) were carried out for both wave functions in the approximation $v = 0$ ³¹⁾. These calculations showed that for $R > 4$ and $R < 0.5$ some or all of the matrix elements were quite sensitive to the wave function. The sensitivity at large R is not likely to be very important in the capture calculation because the probabilities which are important in the total cross-section are primarily determined by the interaction at smaller values of R . The sensitivity of the matrix elements for small values of R is caused by cancellations which occur only because the wave functions χ_A and χ_B are not orthogonal, and manifests itself primarily through the appearance of (χ'_B, χ'_B) in Equations (13), (16), and (18). Now for $v = 0.2$ the ratio of (χ'_B, χ'_B) calculated with the one-parameter function to that calculated with the two-parameter function is 1.7, 1.3, 1.2, 1.1, and 1.0 for $R = 0.0, 0.5, 1.0, 1.5$, and 3.0 , respectively. For $v = 0.5$ the corresponding ratios are 1.11, 1.09, 1.07, 1.05, and 1.01.

Thus, at low velocities and small internuclear distances the coefficients in Equations (18) are rather sensitive to the choice of helium wave function while at higher velocities and larger internuclear distances they are not.

It is difficult to translate these observations into rigorous estimates of the effect of the helium wave function on $P(\rho, v)$ and $Q(v)$. Our overall judgement, based on considerations of the type described above, is that at energies above 15 keV the use of a better helium wave function might change $Q(v)$ by up to 20 percent and that $Q(v)$ becomes increasingly sensitive to the choice of wave function as the projectile energy is decreased**).

V. Acknowledgements

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*) With one electron near the helium nucleus, the other electron should see unit charge at large distances, not a charge of 1.6875.

**) MAPLETON (see reference 12) has evaluated the Born approximation with the one-parameter function and with the Hylleras six-parameter function. In the energy range 40–1000 keV the predicted cross-sections differ by between 5 and 15 percent.

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VI. Postscript

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