Asymptotic form of the charge-exchange cross section in three-body rearrangement collisions

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A three-body general-type rearrangement collision is considered where the initial and final bound states are described by hydrogenlike wave functions. The solution obtained is for the first Born approximation where the full interaction potential is taken into account. When the initial state is the ground state, it is shown that for $n/\mu Z \ge 1$, where n,μ , and Z are, respectively, the principal quantum number, the reduced mass, and the nuclear charge of the formed atom, the capture cross section at all incident energies and for capture into the s, p, and d angular momentum states behaves as $C/n^3 + O(1/n^5)$, where C depends on masses and charges of the particles, the final angular momentum, and the incident energy. An analytic expression for C is given. It is shown that for the low-lying levels the $1/n^3$ scaling law at all incident energies is only approximately satisfied. The only exception is for capture into the s states according to the Oppenheimer-Brinkman-Kramers approximation. The case for the symmetric collisions is considered and it is shown that for high n and high incident energy E, the cross section behaves as $1/E^3$. Zeros and minima in the differential cross sections are given in the limit of high n for electron capture by protons from atomic hydrogen, and for positronium formation by proton-atomic hydrogen collisions.

I. INTRODUCTION

In the passage of charged particles through gases, the main process for neutralizing the charged particles is the capture of electrons from the surrounding gas. Such passages occur naturally, for example, in the diffusion of charged particles produced by a supernova explosion in the interstellar medium, or in the diffusion of the solar wind through the planetary atmospheres. Similarly, by passing a beam of protons through a gas, highly excited states of atomic hydrogen are produced. The atoms through an electric field are consequently ionized to produce a highly ionized plasma. The recently observed so-called exotic atoms, such as positronium, muonium, and protonium, are other examples where rearrangement collisions play an important role in their formations.

In the examples mentioned above the capture takes place not only in the ground state, but in the excited states as well. A large number of the calculational methods which deal with the problem of the rearrangement collisions more rigorously and realistically than the first Born approximation are mainly for capture into the ground state, and occasionally the first few excited states. In this respect mention should be made of the close-coupling approximation of Bates¹ and McElroy,² the distorted-wave approximation of Bassel and Gerjuoy,³ the impulse approximation of McDowell⁴ and Cheshire,⁵ the continuum distorted-wave approximation of Cheshire,⁶ the first-order Faddeev-Watson multiple-scattering approximation,⁷ the second-order Born approximation,⁸ and the correspondence-principle method of Abrines and Percival.⁹ In all these references, except Ref. 9, capture into the ground state of the formed atom is considered, and except Refs. 5 and 7, the system considered is electron capture by protons from the atomic hydrogen.

The most commonly used calculation for capture into the excited state is based on a method which is due to Oppenheimer,¹⁰ and Brinkman and Kramers,¹¹ whereby the first Born approximation is used, but the repulsive potential between the projectile and the target nucleus is neglected. The calculation of these authors (the Oppenheimer-Brinkman-Kramers, or for short OBK, approximation) was done for capture into the ground state. Extension to the excited states has been done by May,¹² Butler, May, and Johnson,¹³ Hiskes,¹⁴ and this author.¹⁵ More elaborate calculations for the first few low-lying states have been done by Mapleton¹⁶ (using the full first Born approximation). Coleman and Trelease¹⁷ (using the impulse approximation), and Cheshire, Gallaher, and Taylor¹⁸ (using the pseudostate-expansion approximation.

It was predicted by Oppenheimer that when capture takes place into s states of the excited states, at sufficiently high incident energies the cross section falls as $1/n^3$. This implies that at sufficiently high energies the total cross section also falls as $1/n^3$. On the other hand, the same cross section according to the binary encounter theory should fall as $1/n^2$ (Ref. 18a). It can be shown without any difficulty that in the OBK approximation the capture cross section for capture into any final angular momentum falls as $1/n^3$ for sufficiently high energies. It similarly has been shown

(Ref. 18b) that for rearrangement collisions with heavy projectile and target nucleus, where the second Born term at extremely high energies dominates the first Born term, and the leading term contributing to the cross section does not involve the repulsive potential, the cross section also falls as $1/n^3$. The energy region where the second Born term dominates is above 100 MeV for protons on atomic hydrogen, and is seldom encountered in a practical situation.

It then becomes of interest to find the asymptotic behavior with respect to n of a general-type rearrangement collision in the first full Born approximation. In this paper by expanding the exchange amplitude in this approximation in inverse powers of n, it is shown conclusively that the cross section for capture into the s, p, and d states, and for the sum over all the angular momentum states, falls as $1/n^3$. An error in a previous article by the author¹⁹ has been corrected in the Appendix, and the corrected result is in agreement with the results presented here. It is worth mentioning that a recent measurement by Macdonald *et al.*²⁰ favors the $1/n^3$ over the $1/n^2$ behavior.

The question of validity of the first Born approximation for rearrangement collisions has been the subject of substantial studies. However, almost all of these studies are restricted to the case of the heavy particle projectile, where the trajectory can be described classically, and the heavy target nucleus. In summary it has been shown that in an exact calculation for the p + H system the contribution of the repulsive potential to the cross section is on the order of the squared ratio of the mass of the electron to the mass of the proton. and therefore is insignificantly small.^{21,22} Also it has been shown that for high incident energies and the forward scattering angles, where the main contribution to the total cross section comes from, the terms containing the repulsive potential in the sum of the first and second Born amplitudes cancel out, making the cross section up to the second Born term independent of this potential.^{8,23} It is also significant to note that the second Born provides the asymptotically leading term with respect to the incident energy.^{23,24,24a}

The above consideration for the p + H system applies to an exact solution of the problem. It was suggested by Jackson and Schiff,²⁵ and Bates and Dalgarno²⁶ that as long as an approximate wave function, as is the case in the first Born, is used, the full Born is preferable to the OBK approximation. This is substantiated by the result that for the p + H system the cross section according to the full Born for the incident energies above 50 keV is in excellent agreement with the measured cross section, while the OBK results are larger by a

factor of 5 to 2 than either the full Born or the experimental results.^{25,26a}

In the formulation that follows, for the sake of generality charges Z_1e and Z_2e are assigned to the projectile and the target nucleus, and hydrogenlike wave functions are used for the bound systems. In applying this to a particular problem, the approximate nature of the calculation should be kept in mind.

It should be mentioned that sometimes the first Born approximation is called the method of Jackson and Schiff. However, since the calculation of these authors cannot be considered a new method, this terminology is not being used here.

In summary, in the calculation that follows it is shown that the first Born amplitude for charge exchange can be expanded at all incident energies in terms of the inverse powers of n. The related cross section is proportional to $1/n^3$ plus terms proportional to higher inverse odd powers of n. This implies that the low-lying levels cannot be scaled according to the $1/n^3$ law, irrespective of the value of the incident energy. From the practical point of view, the analytic form for the exchange amplitude given in the text would allow an order of magnitude estimate for the cross section for a general-type rearrangement collision cross section with capture into arbitrary states. This estimate is specially useful for cases where no other calculation is available.

II. BASIC DERIVATION

A. General expression for the amplitude

1. Capture into a fixed angular momentum state

For generality let us consider two like-charged structureless particles 1 and 2, and one oppositely charged structureless particle 3. The rearrangement collision is represented by $1 + (2+3) \rightarrow (1+3) + 2$, where (2+3) and (1+3) stand for the bound hydrogenlike states of 2, 3, and 1, 3 respectively.²⁷ Let us assume that the masses and charges of the particles are given by m_1 , m_2 , m_3 , and Z_1e , Z_2e , $-Z_3e$, where e is the absolute value of the electronic charge. Similarly, let the initial and final relative momenta in the center of masses be given by $\hbar \vec{k}_1$ and $\hbar \vec{k}_2$. Then the conservation of energy implies that

$$\frac{\hbar^2 k_2^2}{2\mu_2} = \frac{\hbar^2 k_1^2}{2\mu_1} + E(2,3) - E(1,3), \quad \mu_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k},$$
(1)

$$\frac{E(i,j)}{R} = -\frac{\mu_{ij}(Z_iZ_j)^2}{m_e n^2}, \quad \mu_{ij} = \frac{m_i m_j}{m_i + m_j}, \quad (2)$$

where μ_1 and μ_2 are the initial and final reduced masses of the system, E(i,j) is the energy of the (i+j) state with the principal quantum number n, R is the rydberg unit of energy, and $m_{\rm e}$ is the electronic mass.

The exact charge-exchange cross section $\sigma(i, f)$ for transition between states i, f is related to the exact wave function for the three-particle system by

$$\sigma(i,f) = \frac{\mu_1 \mu_2}{2\pi \hbar^4} \frac{k_2}{k_1} \int |T(i,f)|^2 d(-\hat{k}_1 \cdot \hat{k}_2), \qquad (3)$$

$$T(i,f) = \langle \psi(\mathbf{\tilde{r}}_{1}, \mathbf{\tilde{r}}_{2}, \mathbf{\tilde{r}}_{3}) | V_{12} + V_{13} | \exp(i\mathbf{\tilde{k}}_{1} \cdot \mathbf{\tilde{r}}_{1})\phi(i, \mathbf{\tilde{r}}_{23}) \rangle$$

= $\langle \exp(i\mathbf{\tilde{k}}_{2} \cdot \mathbf{\tilde{r}}_{2})\phi(f, \mathbf{\tilde{r}}_{13}) | V_{12} + V_{23} | \psi(\mathbf{\tilde{r}}_{1}, \mathbf{\tilde{r}}_{2}, \mathbf{\tilde{r}}_{3}) \rangle$, (4)

where $\psi(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, \vec{\mathbf{r}}_3)$ is the wave function of the system with $\vec{\mathbf{r}}_i$ the position vector of the *i*th particle, V_{ij} is the potential between the *i* and *j* particles, and $\phi(i, \vec{\mathbf{r}}_{jk})$ is the eigenfunction of the (j+k) particles in state *i*.

Different orders of the Born approximation are obtained from the above expression.²⁸ The first Born approximation is obtained by replacing the total wave function by either its initial or final asymptotic form. The two forms of T(i, f) then become equivalent.²⁵ If we assume that initially the atom is in the ground state and finally in the excited nlm state, with nlm the hydrogenic quantum numbers, in the first Born approximation (4) reduces to²⁵

$$T(nlm, V_{23}) = (2\pi)^{3} [E(2, 3) - \hbar^{2} B^{2} / 2\mu_{23}]$$
$$\times U^{*}(nlm, \vec{C}) U(100, \vec{B}),$$
(5)

$$T(nlm, V_{12}) = 4\pi Z_1 Z_2 e^2 \int U^*(nlm, \vec{\mathbf{C}} - \vec{\mathbf{p}}) \times U(100, \vec{\mathbf{B}} - \vec{\mathbf{p}}) \frac{d\vec{\mathbf{p}}}{p^2}, \quad (6)$$

where $U(nlm, \mathbf{p})$ is the Fourier transform of $\phi(nlm, \mathbf{r})$ defined by

$$U(nlm,\mathbf{\bar{p}}) = (2\pi)^{-3/2} \int e^{i\mathbf{\bar{p}}\cdot\mathbf{\bar{r}}} \phi(nlm,\mathbf{\bar{r}}) d\mathbf{\bar{r}}$$
(7)

and

$$\vec{\mathbf{B}} = (\mu_{23}/m_3)\vec{\mathbf{k}}_1 - \vec{\mathbf{k}}_2, \quad \vec{\mathbf{C}} = \vec{\mathbf{k}}_1 - (\mu_{13}/m_3)\vec{\mathbf{k}}_2.$$
(8)

The explicit form of $U(nlm, \mathbf{p})$ for the atomic hydrogen can be found elsewhere.²⁹ We modify this form to describe the arbitrary hydrogenlike atoms. Making use of the generating function for the Gegenbauer functions, we find the following convenient form for $U(nlm, \mathbf{p})$:

$$U(nlm, \mathbf{\hat{p}}) = F(nl, p) Y(lm, \hat{p}),$$

$$F(nl, p) = \left(\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!}\right)^{1/2} \frac{2^{2l+2} l! \sqrt{n} \alpha^{5/2} (\alpha p)^{l}}{(p^{2}+\alpha^{2})^{l+2}} \operatorname{Re}^{\leq (n-l-1)/2} \left[2 - \delta\left(\mu, \frac{n-l-1}{2}\right)\right] \times \left(\binom{l+\mu}{\mu} \binom{n-1-\mu}{n-l-1-\mu} \left(\frac{p+i\alpha}{p-i\alpha}\right)^{n-l-1-2\mu},$$

$$(10)$$

$$\alpha = \mu_{ij} Z_{i} Z_{j} / (m_{e} na_{0}).$$

$$(11)$$

Through (9) and (10) and the identity²⁵

$$E(2,3) - \hbar^2 B^2 / 2\mu_{23} = E(1,3) - \hbar^2 C^2 / 2\mu_{13}, \qquad (12)$$

the amplitude due to the attractive potential or the OBK amplitude, Eq. (5), in the limit of large n will reduce to the following simple form:

$$T(nlm, V_{23}) = -2^{6+2l}\pi^{3/2}(\mu_{13}/\mu_{23})Z_2Z_3e^2$$

$$\times (\alpha_0\alpha)^{3/2}(n\alpha)^{l+1}l![(2l+1)!]^{-1}$$

$$\times C^{-l-6}\zeta(l, C)Y(lm, \hat{C}), \qquad (13)$$

where α_0 and α refer to the initial and final bound states, respectively, and

$$\begin{aligned} \zeta(l,C) &= \binom{n+l}{n-l-1}^{-1} \sum_{\nu=1}^{n-l} \binom{l+\nu-1}{\nu-1} \binom{n-\nu}{n-l-\nu} \\ &\times \cos[2(n-l+1-2\nu)\phi], \\ \phi &= \tan^{-1}\alpha/C, \quad n \to \infty. \end{aligned}$$

By its definition ϕ lies in the first quadrant. Equation (14) then shows that $\zeta(l, C)$ lies always between zero and one. In particular, we have the following limiting value:

$$\zeta(l,C) \to 1, \quad C \gg 1. \tag{15}$$

Another point of interest is the expansion of $T(nlm, V_{23})$ in inverse powers of *n* for $n \rightarrow \infty$. Making use of the expansion

$$\phi \approx (\alpha/C)(1 - \alpha^2/3C^2) + O(\alpha^5/C^5), \quad \alpha/C \ll 1$$
 (16)

we see that

$$\zeta(l,C) \approx 1 + O(1/n^2)$$
. (17)

Through (13) we then find that for small l

$$T(nlm, V_{23}) \propto n^{-3/2} + O(n^{-7/2}), \quad \alpha/C \ll 1.$$
 (18)

For future reference we give the expansion of $\zeta(0, C)$ to two terms in *n*:

$$\xi(0,C) \approx 1 - \frac{2}{3} \left(\frac{\alpha n}{C}\right)^2 + \frac{4}{9} \left(\frac{\alpha n}{C}\right)^4 n^{-2} + O(n^{-4}).$$
(19)

It should be noted that αn is independent of n_{\circ} .

Evaluation of $T(V_{12})$ is algebraically more complicated. In this case we introduce $\bar{q} = \vec{C} - \vec{p}$. Then with the help of (9) and (10), Eq. (6) can be written

$$T(nlm, V_{12}) = 2^{6+2l} \pi^{-1/2} Z_1 Z_2 e^2(\alpha_0 \alpha)^{5/2} l! \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{1/2} (-)^{n-l-1} \times \sum_{\mu=0}^{\leq (n-l-1)/2} \left[2 - \delta\left(\mu, \frac{n-l-1}{2}\right)\right] {l+\mu \choose \mu} {n-1-\mu \choose n-l-1-\mu} \operatorname{Res}(nlm\mu),$$
(20)

where Re stands for the real part of a quantity, and

$$\operatorname{Res}(nlm\mu) = \sum_{\nu=0}^{n-l-1-2\mu} \binom{2(n-l-1-2\mu)}{2\nu} (-)^{\nu} \alpha^{2(n-l/2-1-2\mu-\nu)} J(nlm\mu\nu), \qquad (21)$$

$$J(nlm\mu\nu) = \int_0^{q_0} \frac{f(lm,q)q^{2+2\nu+l}dq}{(\alpha^2+q^2)^{n+1-2\mu}} + \int_{q_0}^{\infty} \frac{f(lm,q)dq}{q^{2(n-2\mu-\nu-l/2)}}, \quad \alpha \ll q_0 \ll 1,$$
(22)

$$f(lm,q) = \int \frac{Y(lm,\hat{q})\,d\hat{q}}{(\vec{C} - \vec{q})^2 [\,\alpha_0^2 + (\vec{A} + \vec{q})^2]^2}, \quad \vec{A} = \vec{B} - \vec{C} \quad .$$
(23)

We notice from (21) that the minimum value of $n - 2\mu - \nu - l/2$ is equal or greater than 1. Also as q - 0, or $q - \infty$, the value of f(lm, q) approaches a finite value independent of q, or zero. Then the value of the second integral in (22) is of the order of $q_0^{-\omega}$, where ω is a number greater or equal to 1. Similarly, when q is of the order α , the integrand in the first integral is (22) is of the order of $\alpha^{-2[n-2\mu-\nu-l/2]}$. Then the value of this integrand is of the order of $\alpha^{-\omega}$, where again ω is greater or equal to 1. The second integral in (22) can then be neglected compared to the first one.

Since in the first integral in (22) q lies between 0 and q_0 , and $q_0 \ll 1$, we are justified to make a Taylor expansion of f(lm, q) with respect to q in the integrand of this integral. Then the integral can be evaluated analytically term by term. Introducing $y = \alpha^2 + q^2$, (22) can be written

$$J(nl\,m\mu\,\nu) = \frac{1}{2} \sum_{N=N_0}^{\infty} \frac{1}{N!} f^{(N)}(lm,0) \sum_{\lambda=0}^{\infty} \left(\frac{\nu + \frac{1}{2}(l+N+1)}{\lambda} \right) (-\alpha^2)^{\lambda} \int_{\alpha^2}^{a_0^2} \frac{dy}{y^{n+1-2\mu-\nu-(l+N+1)/2+\lambda}},$$
(24)

where N_0 corresponds to the first nonvanishing term of the series, and $f^{(N)}(lm, 0)$ is the *N*th derivative of f(lm, q) evaluated at q = 0.

Combining (24) and (21) we obtain

$$\operatorname{Res}(nlm\mu) = \sum_{N=N_0}^{\infty} \frac{\alpha^{N-1}}{2N!} f^{(N)}(lm,0)C(nl\mu), \qquad (25)$$

$$C(n l \mu) = \sum_{\nu=0}^{n-l-1-2\mu} {2(n-l-1-2\mu) \choose 2\nu} (-)^{\nu} \\ \times \sum_{\lambda} {\nu+\frac{1}{2}(l+N+1) \choose \lambda} \\ \times \frac{(-)^{\lambda}}{n-2\mu-\nu-\frac{1}{2}(l+N+1)+\lambda} .$$
(26)

For N > l, and some values of λ , ν , and μ , loga-

rithmic terms occur in (24). This does not create particular difficulty. But since the leading term in the amplitude arises from $N \le l$, the case N > l will not be treated here.

Evaluation of $C(nl\mu)$ is straightforward (cf. Ref. 30). For l=0, 1, and 2 we find that

$$C(n0\mu) = \frac{1}{4}\pi [2\delta(j,0) - \delta(j,1)],$$

$$C(n1\mu) = \frac{1}{16}\pi [6\delta(j,0) - 4\delta(j,1) + \delta(j,2)],$$

$$C(n2\mu) = \frac{1}{64}\pi [20\delta(j,0) - 15\delta(j,1) + 6\delta(j,2) - \delta(j,3)],$$

$$j = n - l - 1 - 2\mu. \quad (27)$$

Substituting from (25) into (20), the sum with respect to μ can similarly be closed (cf. Ref. 30). For the moment we consider only the leading term of $T(nlm, V_{12})$ with respect to an expansion in inverse powers of n. For l = 0, 1, and 2 we obtain

$$T(n00, V_{12}) = \frac{32\pi Z_1 Z_2 e^2 \alpha_0^{5/2} \alpha^{3/2}}{C^2 (\alpha_0^2 + A^2)^2}, \qquad (28)$$

$$T(n1m, V_{12}) = \frac{32\pi}{\sqrt{3}} Z_1 Z_2 e^2 \alpha_0^{5/2} \alpha^{3/2} (\alpha n) \left(\frac{\zeta(m, 0)}{C^3 (\alpha_0^2 + A^2)^2} - \frac{2(2\pi)}{C^2 (\alpha_0^2 + A^2)^3} \right),$$
(29)

$$T(n2m, V_{12}) = \frac{1}{\sqrt{5}} Z_1 Z_2 e^2 \alpha_0^{5/2} \alpha^{3/2} (\alpha n)^2 \left(\frac{\frac{3}{3} (m, 0)}{C^4 (\alpha_0^2 + A^2)^2} - \frac{\frac{3}{3} [4\pi (4 - m^2)/3]^2 A Y(1m, A)}{C^3 (\alpha_0^2 + A^2)^3} + \frac{(4\pi/5)^{5/2} A^2 Y(2m, A)}{C^2 (\alpha_0^2 + A^2)^4} \right).$$
(30)

This completes the evaluation of the core amplitudes for l = 0, 1, 2. As is seen, these amplitudes are given analytically in terms of the incident energy and the scattering angle $\theta = \cos^{-1}\hat{k}_1 \cdot \hat{k}_2$.

We notice that the core amplitudes have the same n and energy dependence as the OBK amplitude given by (13). Because of the factor of $\alpha^{3/2}$ in both amplitudes, the cross section for both the OBK and Born behaves as $1/n^3$. The energy dependence can be seen by noticing that at high incident energies C and A behave as $E_0^{1/2}$, where E_0 is the incident energy. Then studies of Eqs. (13) and (28) through (30) show that for capture into the final l states the cross section behaves as E_0^{-6-l} . An exception is the case of the symmetric collisions (Sec. II B) where, for appropriate energy ranges to be discussed later, the cross section falls as E^{-3} for all the angular momentum states.

It remains to show now that the next higher-order term in $T(nlm, V_{12})$ behaves as $n^{-7/2}$. To show this from (23) we can write

$$f^{(N)}(lm,0) = \int Y(lm,\hat{q})g^{(N)}(\hat{q},0)\,d\hat{q}\,, \qquad (31)$$

where $g^{N}(\hat{q}, q)$ is found through the expansion

$$g(\hat{q}, q) = (C^{2} + q^{2} - 2Cqx)^{-1}(\alpha_{0}^{2} + A^{2} + q^{2} + 2AqX)^{-2}$$
$$= \sum_{N=0}^{\infty} \frac{q^{N}}{N!} g^{(N)}(\hat{q}, q), \quad x = \hat{C} \cdot \hat{q}, X = \hat{A} \cdot \hat{q} . \quad (32)$$

By differentiating the right-hand side of the first line in (32) with respect to q, we find that $g^{N}(\hat{q}, 0)$ is a polynomial in terms of $X^{\mu}x^{\nu}$, where $\mu + \nu = N$. Since both X and x have odd parities with respect

to the reflection of \hat{q} through the origin, the parity of $g^{N}(q, 0)$ with respect to this reflection is N. From (31) it then follows that $f^{N}(lm, 0)$ vanishes unless l+N is even. For a given l, N then takes only odd or even integers. Through (25) we then see that if the leading term of $T(nlm, V_{12})$ behaves as $n^{-3/2}$, the next higher-order term behaves as $n^{-7/2}$.

Since the higher-order term in $T(nlm, V_{23})$ is also proportional to $n^{-7/2}$, the higher-order term in the cross section is proportional to $1/n^5$.

As a check on the validity of the foregoing derivation, and to clarify an error which has led to an erroneous conclusion in a previous publication,¹⁹ Eq. (28) is rederived in the Appendix by a different method.

To find the total cross section, Eq. (3) must be used. By changing the variable of integration from $\hat{k}_1 \cdot \hat{k}_2$ to C^2 , and using the explicit form of T(i, f), the integral in (3) could easily be integrated in terms of elementary functions were it not for the factor $\zeta(l, C)$ in the OBK amplitude. Because of this factor the total cross section should be obtained numerically. However, for the symmetric collisions (Sec. II B) and also when $\zeta(l, C) \rightarrow 1$ (Sec. IIIA), analytic expression for the cross section will be given.

2. Summation with respect to the angular momentum

Using a formula due to Fock³¹ we can sum the squared modulus of the amplitude with respect to lm, and find a closed expression. It will be shown that at high energies the s states dominate, and the total cross section behaves as $1/n^3$. From (6) by introducing $\bar{\mathbf{q}} = \mathbf{\vec{C}} - \mathbf{\vec{p}}$ we obtain

$$\sum_{lm} |T(nlm, V_{12})|^{2} = (4\pi Z_{1}Z_{2}e^{2})^{2} \int \int U(100, \vec{A} + \vec{q})U^{*}(100, \vec{A} + \vec{q}')(\vec{C} - \vec{q})^{-2}(\vec{C} - \vec{q}')^{-2} d\vec{q} d\vec{q}' \\ \times \sum_{lm} U^{*}(nlm, \vec{q})U(nlm, \vec{q}') .$$
(33)

For evaluation of the sum with respect to lm we use the sum rule for the four-dimensional spherical harmonics³¹

$$\sum_{lm} U^*(nlm, \bar{\mathbf{q}}) U(nlm, \bar{\mathbf{q}}') = \frac{8\alpha^5}{\pi^2 (\alpha^2 + q^2)^2 (\alpha^2 + q_1'^2)^2} \frac{n \sin nw}{\sin w} ,$$
(34)

where w is a function of $\overline{\mathbf{q}}$ and $\overline{\mathbf{q}}'$ given by

$$4\sin^2\frac{1}{2}w = (\xi - \xi')^2 + (\eta - \eta')^2 + (\xi - \xi')^2 + (\chi - \chi')^2$$
(35)

and $\xi\eta\xi\chi$ are the Cartesian coordinates of a four-dimensional unit sphere related to \dot{q} by

$$\begin{pmatrix} \xi \\ \eta \\ \xi \end{pmatrix} = \frac{2\alpha q}{\alpha^2 + q^2} \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \quad \chi = \frac{\alpha^2 - q^2}{\alpha^2 + q^2}$$
(36)

with θ and ϕ the angular part of the polar coordinates of \overline{q} .

By finding the form of U(100, p) from (9) and (10), Eq. (33) can now be written

$$\sum_{lm} |T(nlm, V_{12})|^2 = (4\pi Z_1 Z_2 e^2)^2 64\pi^{-4} (\alpha_0 \alpha)^5 n^2 \int \int \frac{f(\mathbf{\bar{q}}, \mathbf{\bar{q}}')}{(\alpha^2 + q^2)^2 (\alpha^2 + q'^2)^2} \frac{\sin nw}{n \sin w} d\mathbf{\bar{q}} d\mathbf{\bar{q}}',$$
(37)

$$f(\mathbf{\bar{q}},\mathbf{\bar{q}}') = (\mathbf{\bar{C}} - \mathbf{\bar{q}})^{-2} (\mathbf{\bar{C}} - \mathbf{\bar{q}}')^{-2} [\alpha_0^2 + (\mathbf{\bar{A}} + \mathbf{\bar{q}})^2]^{-2} [\alpha_0^2 + (\mathbf{\bar{A}} + \mathbf{\bar{q}}')^2]^{-2} .$$
(38)

The function $f(\bar{\mathbf{q}}, \bar{\mathbf{q}}')$ remains finite as $\alpha \rightarrow 0$. Following the argument given in Sec. II A 1, we make a Taylor's expansion of $f(\bar{\mathbf{q}}, \bar{\mathbf{q}}')$, and keep the zero-order term, f(0, 0). On the right-hand side of (37) the only term which depends on the angular coordinates of $\bar{\mathbf{q}}$ and $\bar{\mathbf{q}}'$ is $\sin nw/\sin w$. Realizing that $\sin nw/\sin w$ is a scalar quantity, for integration over the angles of $\bar{\mathbf{q}}$ and $\bar{\mathbf{q}}'$ we can take the z axis along $\bar{\mathbf{q}}$. Then, introducing $\cos\gamma = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}'$,

$$\iint \frac{\sin nw}{n\sin w} \, d\hat{q} \, d\hat{q}' = \frac{8\pi^2}{n} \int_0^\pi \frac{\sin nw}{\sin w} \sin \gamma \, d\gamma \,. \tag{39}$$

The variable of integration can be changed from γ to w through the relationship³¹

 $\cos w = \cos\beta\cos\beta' + \sin\beta\sin\beta'\cos\gamma,$

$$\beta = \cos^{-1} \left(\frac{\alpha^2 - q^2}{\alpha^2 + q^2} \right) \,. \tag{40}$$

When the integration is carried out, we find that

$$\iint \frac{\sin nw}{n\sin w} \, d\hat{q} \, d\hat{q'} = \left(\frac{4\pi}{n}\right)^2 \frac{\sin n\beta}{\sin\beta} \frac{\sin n\beta'}{\sin\beta'} \,. \tag{41}$$

Equation (37) can now be written

$$\sum_{lm} |T(nlm, V_{12})|^2 = 2^{12} (Z_1 Z_2 e^2)^2 \alpha_0^5 \alpha^3 f(0, 0) \\ \times \left(\int_0^\infty \frac{\sin(n\beta)q \, dq}{\alpha^2 + q^2} \right)^2.$$
(42)

For evaluation of the integral in (42) we break up the range of integration into ranges 0 to q_0 and q_0 to ∞ , where q_0 is chosen such that $\alpha \ll q_0 \ll 1$. An argument similar to one given following Eq. (23) then shows that the integral due to the second range compared to one due to the first range can be neglected. The latter integral can be evaluated and in the limit $\alpha \rightarrow 0$ it approaches the value $(-1)^{n-1}\pi/2$. It then follows that

$$\sum_{lm} |T(nlm, V_{12})|^2 = \frac{(32\pi Z_1 Z_2 e^2)^2 \alpha_0^5 \alpha^3}{C^4 (\alpha_0^2 + A^2)^4} .$$
(43)

Comparison of this with (28) indicates that for the zero-order expansion of $f(\mathbf{\bar{q}}, \mathbf{\bar{q}}')$, the total cross section is equal to the *s* capture cross section. The higher-order terms of expansion of $f(\mathbf{\bar{q}}, \mathbf{\bar{q}}')$ with respect to $\mathbf{\bar{q}}$ and $\mathbf{\bar{q}}'$, as can be seen from (38), lead to results which fall faster with respect to energy compared to the zero-order term, and therefore can be neglected.

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B. Symmetric collisions

We refer to the charge-exchange collisions as symmetric when $m_1 = m_2$. The resonance collisions as defined by Bates and Dalgarno²⁶ refer to the case when $m_1 = m_2$, $Z_1 = Z_2$, and the capture takes place into the ground state. The resonance collision is then a special case of the symmetric collisions. In treating this case we keep in mind that quantum mechanically we cannot separate the exchange from the direct amplitude. The following treatment is valid provided there is no considerable overlap between the particles' 1 and 2 wave functions.

It was first recognized by Mapleton³² that in a resonance collision, in particular in electron capture by protons from the atomic hydrogen, the cross section at high energies behaves as $1/E^3$ instead of the gneral behavior of $1/E^6$. However, the $1/E^3$ behavior does not appear until the incident energy is well above 100 MeV. Below this energy the $1/E^6$ behavior dominates. The similar case of the exchange collision between positron and positronium has been treated by Chen and Kramer.⁷ The case of exchange collision between electron and atomic hydrogen has been overlooked by both authors. This case will be treated here. In addition, we like to show that the $1/E^3$ behavior also appears for capture into the highly excited states, and probably appears for capture into any excited state. The excited states have not been previously treated in the literature.

We apply the results to the inelastic exchange collision of electrons with atomic hydrogen, and show that the high-energy behavior is given only through the $1/E^3$ behavior.

The $1/E^3$ behavior as shown by Mapleton arises from the backscattering and is due to the core potential. We then consider the cross section due to $T(nlm, V_{12})$ only. Let us introduce $M = \mu_{13}/m_3 = \mu_{23}/m_3$. From the definition of \vec{B} and \vec{C} we find that

$$B^{2} - C^{2} = -\beta \alpha_{0}^{2}, \quad \beta = (1 - M^{2}) \mu_{1} / \mu_{13}.$$
 (44)

With reference to Eqs. (28)-(30), and by taking the z axis along \vec{C} , we see that the cross section as defined by (3) is of the form of a sum with respect to *i* and *j* of an integral I(i, j) defined by

$$I(i,j) = \int_{-1}^{+1} \frac{d(-\hat{k}_1 \cdot \hat{k}_2)}{C^{2i} [\alpha_0^2 + (\vec{B} - \vec{C})^2]^j} .$$
(45)

By changing the variable of integration in the above equation from $\hat{k}_1 \cdot \hat{k}_2$ to C^2 , the integration can be performed by elementary methods. It then is realized that in the high-energy limit the main contribution comes from $\hat{k}_1 \cdot \hat{k}_2 = -1$, which corresponds to back-scattering. In this limit we find that

$$I(i,j) \approx [2(j-1)(1-M)^2(1+M)^{2i}\alpha_0^{2(j-1)}k_1^{2(i+1)}]^{-1}.$$
(46)

Substituting from (28)-(30) into (3), making use of the above equation, and summing the cross section with respect to the magnetic quantum numbers, we find the following high-energy limit capture cross sections:

$$\begin{split} n^{3}\sigma(ns)/\pi a_{0}^{2} &\approx \frac{1}{3}2^{8}\mu_{13}^{2}(m_{e}\mu_{1})^{-1} \\ &\times Z_{1}^{5}Z_{2}Z_{3}^{2}(1+M)^{-4}(1-M)^{-2}(E/R)^{-3}, \\ \sigma(np) &\approx \frac{4}{5}(Z_{1}/Z_{2})^{2}\sigma(ns), \\ \sigma(nd) &\approx \frac{16}{175}(Z_{1}/Z_{2})^{4}\sigma(ns), \\ E/R &\gg Z_{2}^{2}. \end{split}$$

In these equations E/R is the center-of-mass energy in rydberg units related to k_1^2 through $E/R = (m_e/\mu_1)a_0^2k_1^2$ with a_0 the Bohr radius. It should be realized that the restriction on E/R given by (47) is not restrictive enough. For each value of m_1 and m_3 the next-to-leading term in (45) should be worked out, and the validity criterion should be given accordingly. This will be done for p +H and e +H systems in the next section.

An important difference between the symmetric and nonsymmetric collisions is that in the former case capture into any final-state angular momentum l behaves as $1/E^3$, while in the nonsymmetric case this behavior is $1/E^{6+l}$. In the symmetric case all angular momenta contribute to the total cross section, although as it can be seen from (47) the contribution becomes progressively less as lincreases. In the nonsymmetric-case contribution comes from the s states only.

III. APPLICATIONS

A. Protons on atomic hydrogen

In Fig. 1 the differential cross section for capture into states of high s is plotted versus $\cos\theta$, where θ is the scattering angle. It is seen that as is the case for capture into the 1s state the cross section peaks in the forward direction both in the Born and the OBK approximations. The cross section also peaks in the backward direction for high incident energies in the Born approximation as is seen for 2.5 MeV incident energy. The magnitude of the peak for the backward capture is less by about 9 orders of magnitude compared to the forward capture. This can be seen by comparing Figs. 1 and 2. There is no backward peak for the Born approximation at 25 keV, since collisions are not strong enough. Since there is no nuclearnuclear interaction in the OBK approximation, there similarly is no backward peak in this approximation.

In Fig. 2 the differential cross section is plotted for very small scattering angles. In the Born approximation the cross section becomes zero for angles of the order of the electron to proton mass



FIG. 1. Differential cross section for $p + H(1s) \rightarrow H(ns)$ +p, $n^2 \gg 1$. θ is the scattering angle, B and OBK stand for the first Born approximation, and the Oppenheimer-Brinkman-Kramers approximations. 25 keV and 2.5 MeV are the energies of the primary protons.



FIG. 2. Zeros in the differential cross section for small scattering angles and s captures. Notation is the same as for Fig. 1. m_e/M is the ratio of the electron to proton masses.

ratio, and is almost independent of the charge and energy of the projectile. The origin of this zero is due to the fact that the amplitude which results from the attractive and repulsive potentials is real, and for some scattering angle they become equal in magnitude, but opposite in sign. For small angles, corresponding to large impact parameters, the attractive-potential amplitude dominates, while for larger angles, corresponding to close collisions, the nuclear-nuclear amplitude dominates, and zero occurs between the two extremes.

As the target nuclear charge increases, it is expected that the zero will appear at smaller angles. In the limit of very high Z_2 the zero does not appear at all. Because of the simplicity of the model, the foregoing charge dependence of the zero angle may not provide a true picture of the actual protonmultielectron-atom charge-exchange collisions. It is more applicable to the electron capture by protons from the isoelectronic sequence of atomic hydrogen.

The zero in the differential cross section has been the subject of extensive investigation by many authors. But most of these investigations are restricted to capture into the ground state. For such capture Kramer⁸ has shown that in the place of the zero in the first Born, only a minimum appears in the second Born approximation. Measurement of the structure of the differential cross section at small angles should provide a clue to the accuracy of different calculational models.

In Fig. 3 the differential cross section for 1s



FIG. 3. Differential cross section for np and nd captures, $n^2 \gg 1$, for the first Born approximation. Notation is the same as for Fig. 1.

 $\neg np$ and $1s \neg nd$, when $n^2 >> 1$, is plotted versus $\cos \theta$. For these cases the peaks in the backward capture appears not at 180° , but very close to 180° .

In Fig. 4, similar to Fig. 2, the differential cross section for $1s \rightarrow np$ transitions, $n^2 >> 1$, is shown for small scattering angles. Unlike $1s \rightarrow ns$ transitions, there are no zeros in the differential cross sections, but minima in the Born approximation.



FIG. 4. Minima in the differential cross section for small scattering angles and np captures. Notation is the same as for Fig. 2.

The OBK cross sections, similar to the previous cases, are monotonically decreasing functions of the scattering angle.

In Fig. 5 the differential cross sections for small scattering angles are shown for $1s \rightarrow nd$, $n^2 >> 1$ transitions, and for the Born approximation. The curve for 25 keV peaks not at zero, but at an angle close to zero. The curve for 2.5 MeV is a monotonically decreasing function of the scattering angle.

In Fig. 6 the total cross section for 1s - nl, $n^2 >> 1$, l=0,1,2 transitions in the OBK approximation, and also the total cross section summed over all the angular momenta, are plotted versus the square of the relative velocity in units of the Bohr velocity. It is of interest to see that capture into the *p* states for incident energies up to about 100 keV has larger cross section compared to capture into the *s* states. A similar trend is shown for the first Born approximation as will be seen in Fig. 7. It is difficult to understand the physical reason for this behavior, and an experimental verification of this behavior is desirable.

The determination of $\sigma(nl)$, $n^2 >> 1$, was first made by Butler, May, and Johnson.¹³ Although they use a different method to calculate their cross section, it is found out that their results are graphically identical to the OBK results shown in Fig. 6. Their cross section is for capture into all the excited states varying from a lower limit N to infinity. Making use of the expression



FIG. 5. Differential cross section for small scattering angles and nd captures. Notation is the same as for Fig. 2.

$$\sum_{n=N}^{\infty} \frac{1}{n^3} \approx \frac{1}{2N^2} + O\left(\frac{1}{N^3}\right), \quad N >> 1 ,$$

we see that when the ordinate of Fig. 6 is multiplied by $\frac{1}{2}$, their cross section will result. This implies that their calculation is equivalent to an impact parameter calculation. The peaks in Fig. 6 are broad and do not occur at $v/v_0 = 1$. This makes the designation of these peaks as resonances by Butler *et al.*, which should occur when $v = v_0$, difficult to understand.

Figure 7 shows capture into nl, $n^2 >> 1$, l=0,1, and 2 in the Born approximation. Similar to the OBK case, for low impact energies the l=1 dominates. At high energies l=0 contribution dominates and it approaches σ_B (total). It should be noted that σ_B (total) here is not the sum of all l contribution, but only l=0,1, and 2.

Figure 8 has a special significance, for it shows how the $1/n^3$ law is obeyed for the p + H system. In this figure the ratio of $n^3\sigma(1s \rightarrow nl)$ to $n_0^3\sigma(1s \rightarrow n_0l)$, where $n^2 >> 1$, and $n_0 = l + 1$ is the lowest member of the $1s \rightarrow nl$ transition, is plotted for the OBK and the first Born approximations as a function of the energy for a range of the incident energies from 0 to 2.5 MeV. Each curve in this



FIG. 6. Total cross section for *ns*, *np*, *nd*, and $n \Sigma l$ capture in the OBK, or the impact parameter, approximation as function of the square of the relative velocity v. v_0 is the Bohr velocity, and $(v/v_0)^2 = 1$ corresponds to about 25-keV incident proton energy.



FIG. 7. Total cross section for ns, np, nd, and their sum in the Born approximation as a function of the square of the relative velocity.



FIG. 8. Ratio of the $\sigma(1s \rightarrow nl)/\sigma(1s \rightarrow n_0l)$, $n^2 \gg 1$, where $n_0 = l + 1$, as a function of the squared of the relative velocity. The lower three curves are due to the OBK approximation, and the upper three curves are due to the first Born approximation.

figure provides an upper limit to an envelope of curves bounded from below by the x axis, each curve within the envelope designating the ratio of the cross section for a particular transition to the cross section for the lowest member of the transition.

If the excited-state cross sections at sufficiently high energies were scalable from those of the ground state by the $1/n^3$ law, the ordinates of all the curves should approach unity in this energy limit. However, except for the s captures according to the OBK, this limit is not reached, indicating the approximate nature of the $1/n^3$ law for the low-lying states in other cases.

Making use of the results which will be derived shortly [cf. Eq. (50)] and the results of Ref. 12, we can show that

$$\frac{n^{3}\sigma_{OBK}(1s \rightarrow ns)}{\sigma_{OBK}(1s \rightarrow 1s)} \rightarrow 1, \quad \frac{n^{3}\sigma_{OBK}(1s \rightarrow np)}{8\sigma_{OBK}(1s \rightarrow 2p)} \rightarrow \frac{4}{3} ,$$

$$\frac{n^{3}\sigma_{OBK}(1s \rightarrow nd)}{27\sigma_{OBK}(1s \rightarrow 3d)} \rightarrow 2.025, \quad n \rightarrow \infty, \quad v/v_{0} \rightarrow \infty .$$
(48)

Similarly, making use of (51) and a result of Ref. 25, we can show that

$$\frac{n^3 \sigma_B(1s-ns)}{\sigma_B(1s-1s)} \to 1.23, \quad n \to \infty, \quad v/v_0 \to \infty \quad . \tag{49}$$

Equations (48) and (49) substantiate the nonscalability of the low-lying levels. The ratios in the Born approximation for the p and d captures cannot be found, since the high-energy limits of $\sigma_B(1s \rightarrow 2p)$ and $\sigma_B(1s \rightarrow 3d)$ are not available.

Another useful aspect of Fig. 8 is in throwing some light on the simplifying assumption of Bates and Dalgarno (cf. Ref. 26) that the scalings in the Born and the OBK approximations are the same. While this assumption simplifies many calculations, Fig. 8 clearly shows that this assumption is not being satisfied.

It is of interest to show the connection between the capture cross sections for the low-lying levels, as worked out by other authors, and the asymptotic capture cross sections as obtained here. In Figs. 9-11 the scaled cross sections $n^3\sigma/(\pi a_0^2)$ for the p+H system and for the final s, p, and d angular momentum states are plotted versus $(v/v_0)^2$. As expected from the statement preceding Eqs. (48) and (49) and these equations, the cross sections due to the low-lying levels don't approach their asymptotic forms with respect to n even at high energies. However, it is not understood why the 2s, 3s, 4s, and 5s curves converge into a single curve at high energies. The same can be said of the 3p and 4p curves.

Recently Khayrallah *et al.*³³ and Bayfield *et al.*³⁴ have measured electron capture by protons from



FIG. 9. Total cross section for capture into s states in the first Born approximation. The results for capture into 1s through 5s states are obtained from the calculation of Mapleton (Ref. 16), the result for capture into $ns, n \rightarrow \infty$ states is due to the present calculation. The asymptotic cross section with respect to energy is shown by the dashed line.

the atomic hydrogen, where the capture takes place within the quantum numbers n = 13 to n = 30. Their results are shown in Fig. 12. Their experimental uncertainty is $\pm 30\%$. In the same figure results obtained by the impact-parameter approximation of Butler and Johnston,³⁵ and May³⁶ are also shown. Shown also are the OBK results. The impact parameter and the OBK results are almost identical, and cannot be distinguished on the graph. Finally, using asymptotic form with respect to n, the cross section due to the first Born approximation is also shown. As was shown in Sec. II, correction to the asymptotic form is of the order of $1/n^2$. It will also be shown later³⁷ for n = 13, by what percentage the Born cross section has converged to its asymtotic form. The discrepancy of more than a factor

of 3 between the first Born and the experiment cannot be due to the use of the asymptotic form. In the light of the fact that in the range 40-60 keVincident energy the first Born is in excellent agreement with measurement when capture takes place to all *n* values from 1 to infinity,²⁵ the lack of agreement in Fig. 8 is puzzling. This disagreement suggests that the criterion for validity of the first Born for capture into the highly excited states is different compared to that for capture into the ground state, and better agreement may be obtained at higher energies. It should also be noted that Jackson and Schiff scale the ground state according to the $1/n^3$ law to obtain the excited states capture cross sections, therefore underestimating these cross sections (cf. Fig. 8).



FIG. 10. Notations are the same as in Fig. 9, but capture takes place into the p states. The results for capture into 2p, 3p, and 4p states are due to Mapleton (Ref. 16).



FIG. 11. Notations are the same as in Fig. 9, but for capture into d states. The results for capture into 3d and 4d states are due to Mapleton (Ref. 16).

An accurate estimate of the excited-state cross section should modify the total cross section of these authors.

Improvement in the first Born approximation has been obtained by Band,³⁸ who orthogonalizes the initial and final wave functions of the system. In the range 50-60 keV his calculated cross section agrees with the measurement within the experimental errors.

In the limit of high energies the total cross section can be found analytically. The difficulty in carrying out the integration with respect to the scattering angle is the factor $\zeta(l, C)$ in the OBK amplitude given by (14). However, in the limit indicated by (15) the integration can be carried out. For the p +H system the major contribution to the cross section comes from small scattering angles. Then following H. Schiff³⁹ we expand C^2 and $(B-C)^2$, which appear in the integral expression for the cross section, in terms of this angle, and keep the leading terms. We then find the following values for the cross section:

$$\sigma(ns) = \sigma_{OBK}(ns) \left[1 - \frac{5}{24} Z_2 a^2 + \frac{5}{256} Z_2^2 a^4 \right] ,$$

$$\sigma(np) = \sigma_{OBK}(np) \left(1 - \frac{3}{8} Z_2 a^2 + \frac{15}{256} Z_2^2 a^4 \right) ,$$

$$\sigma(nd) = \sigma_{OBK}(nd) \left(1 - 0.4648 Z_2 a^2 + 0.07941 Z_2^2 a^4 \right) ,$$

$$\frac{n^3 \sigma_{OBK}(nl)}{\pi a_0^2} = \frac{2^{6(3+1)} (2l+1)}{5+l} \left(\frac{l!}{(2l+1)!} \right)^2 \frac{Z_1^{5+2l} Z_2^5}{s^{12+2l} a^{10+2l}} ,$$

$$a = 1 + Z_2^2 s^{-2}, \quad s = v/v_0 \gg 1 . \quad (50)$$

In these expressions σ and σ_{OBK} stand for cross sections in the Born and OBK approximations.

For $Z_2 = 1$, which corresponds to the p + H system, (50) simplifies and we get the following ratios:



FIG. 12. Sum of the capture cross sections for $p + H(1s) \rightarrow H(n \Sigma l) + p$, n = 13-30 according to the measurement designated by Ex(BKK) (Refs. 33 and 34), impact parameter designated by IP (Refs. 35 and 36), OBK, and the first Born approximations. The sum designated by σ_* is in units of \mathring{A}^2 . In the figure the normalized data of Ref. 34, which are slightly lower than Ref. 33, have been used. The error in the experimental data shown by the error bars is $\pm 30\%$.

$$\frac{\sigma(ns)}{\sigma_{\rm OBK}(ns)} \approx 0.811, \quad \frac{\sigma(np)}{\sigma_{\rm OBK}(np)} \approx 0.684 ,$$

$$\frac{\sigma(nd)}{\sigma_{\rm OBK}(nd)} \approx 0.615, \quad s >>1 .$$
(51)

It is interesting to compare the first of these equations with a similar expression for capture into the ground state given by Jackson and Schiff, which is $\sigma(1s)/\sigma_{OBK}(1s) \approx 0.661$.

Finally, let us investigate the E^{-3} behavior for capture into the highly excited states. This behavior for capture into the ground state has been investigated by Mapleton.³² Applying Eqs. (47) to the p + H case, we obtain

$$\frac{n^{3}\sigma(ns)}{\pi a_{0}^{2}} \approx \frac{32cZ_{1}^{5}Z_{2}}{3\epsilon (E/R)^{3}} , \quad E/R >> \epsilon^{-5/3} \approx 2.75 \times 10^{5} ,$$
(52)

where the validity condition is obtained by considering the next-to-highest term in (45). c in (52)is the ratio of the target nucleus mass to the proton mass. A similar expression for $\sigma(np)$ and $\sigma(nd)$ can be obtained using (47). It should be noted that the validity condition in (52), consistent with the condition given by Mapleton, indicates the $1/E^3$ behavior appears for energies well above 100 MeV. The result given by Mapleton is

$$\frac{\sigma(1s)}{\pi a_0^2} \approx \frac{1.23 \times 10^3}{(E/R)^3} , \quad E/R >> \epsilon^{-5/3} .$$
 (53)

By putting $c = Z_1 = Z_2 = 1$ in (52) we see that the coefficient of $(E/R)^{-3}$ in (52) is 15.9 times larger than a similar coefficient in (53). This can be taken as an indication that the ground state cannot be scaled to the highly excited states.

Assuming that protons are distinguishable, we can also compare cross sections for direct and exchange excitation for the p + H system with a highly excited final state. For the direct excitation we have $^{40, 41}$

$$\frac{n^{3}\sigma(1s \rightarrow nl)}{\pi a_{0}^{2}} \approx \frac{\mu_{1}Z_{1}^{2}}{m_{e}Z_{2}^{2}E/R} \left(A\left(1s \rightarrow nl\right) \ln \frac{m_{e}E}{\mu_{1}Z_{2}^{2}R} + B\left(1s \rightarrow nl\right) \right), \quad (54)$$

$$A\left(1s \rightarrow nl\right) = \delta\left(l, 1\right) \frac{4}{2} \left| \langle nl | Z_{2}\overline{t}/a_{0} | 1s \rangle \right|^{2},$$

where A(1s + nl) and B(1s + nl) are atomic constants independent of the nuclear charge and μ_1 is the reduced mass of the system. Using the values of these constants,⁴² for $Z_1 = Z_2 = 1$, and an incident energy of 100 MeV, we find that

$$\begin{split} &\sigma^{Ex}(ns)/\sigma^{D}(ns) \approx 0.85 \times 10^{-12} , \\ &\sigma^{Ex}(np)/\sigma^{D}(np) \approx 0.22 \times 10^{-13} , \\ &\sigma^{Ex}(nd)/\sigma^{D}(nd) \approx 0.67 \times 10^{-13} . \end{split}$$

However, as Z_1 and Z_2 increase, the exchange effect becomes more important in a complicated way. Using our simple model, from (47) and (53), the first ratio for example increases as $(Z_1Z_2)^3$.

For relativistic incident and bound electron energies, Mittleman⁴³ has shown that the cross section behaves as 1/E.

For the exchange scattering of electrons from the atomic hydrogen, as will be discussed in the next section, the $1/E^3$ behavior appears at much lower energies, and there is no $1/E^6$ asymptotic behavior.

B. Exchange scattering of electrons from the atomic hydrogen

Since in this case $m_1 = m_2$, we also are dealing with a symmetric collision. This case has not been treated by Mapleton. A proper treatment for this problem when the electron spins are not polarized, similar to the p + H problem, would be to use an antisymmetrized wave function in which case the direct and exchange cross sections cannot be separated from each other. However, to get an idea about the relative size of the exchange to the direct amplitudes, we use (13) and (47) to get

$$\frac{n^{3}\sigma_{OBK}(ns)}{\pi a_{0}^{2}} \approx \frac{2^{10}Z_{2}^{5}}{(E/R)^{6}},$$

$$\frac{n^{3}\sigma(ns)}{\pi a_{0}^{2}} \approx \frac{2^{6}}{3Z_{2}(E/R)^{3}}, \quad E/R >> 1,$$
(55)

where E/R is the incident energy in rydbergs. Then $1/E^3$ behavior becomes valid at much lower energy compared to the p + H case. Expressions similar to (55) can be found for p and d captures.

Comparison of (55) and (54) shows that the ratio of exchange to direct cross section for the e + Hsystem increases as Z_2 , the nuclear charge of the H isoelectronic sequence. For 20-Ry electrons on atomic hydrogen this ratio is 0.115.

At sufficiently high impact energies where the two electrons of the system are distinguishable we can get the following picture for the differential cross section. For forward scattering angles where the direct scattering dominates the differential cross section behaves as $\ln E/E$ with E being the impact energy.⁴⁰ For the backward direction the exchange scattering with a $1/E^3$ behavior dominates.

C. Exchange scattering of positrons from positronium

This problem has been treated by Chen and Kramer, considering capture into the ground state and applying the first-order Faddeev-Watson multiple-scattering approximation.⁷ As a result of

the $e^+ - e^+$ interaction, they find that at high energy the cross section behaves as $1/E^3$. We like to show that similar behavior is obtained using the first Born approximation and considering capture into the highly excited states. By putting m_1 $= m_2 = m_3 = m_e$ and making use of Eqs. (47), we find that

$$\frac{n^{3}\sigma(ns)}{\pi a_{0}^{2}} \approx \frac{2^{11}}{81(E/R)^{3}} , E/R >> 1 , \qquad (56)$$

where E/R is the center-of-mass energy, equal to $\frac{2}{3}$ of the incident energy. Similar expressions can be obtained for capture into the np and ndstates. If the first Born cross section as given in Ref. 7 for capture into the ground state is found from a graph in this reference, the coefficient of $(E/R)^{-3}$ on the right-hand side of (56) for n=1 is found to be 1.66, while this coefficient in (56) is 25.3. The ratio of the two coefficients is 15.2, almost the same as this ratio for the p +H system.

D. Positronium formation in e^+ +H collisions

The difficulties arising in the first Born approximation in the case of the heavy particle projectiles does not arise in this case, and the validity of this approximation is less known. For capture into the ground state it is found that^{44, 45} the cross section given by the first Born approximation is an order of magnitude smaller than that of OBK. There are some indications from the measurements^{46, 46a} that the first Born cross section is also too large at the threshold of Ps formation.

By putting $m_1 = m_3$ = electron mass, m_2 = proton mass, and $Z_1 = 1$ in the general formula (13) and (28)-(30), and using (3), appropriate cross section for capture into the high *n* can be obtained. The cross sections obtained should provide useful order-of-magnitude estimates for captures into the *s*, *p*, and *d* states.

Unlike the p +H case, few details will be given here. It is of interest, however, that as in the p +H case, the differential cross section for scaptures according to the first Born approximation goes to zero for some scattering angle.

To show this we equate the right-hand sides of (13) and (28) in the limit $\zeta(0, C) \rightarrow 1$. This limit is satisfied if $a_0 C_{\min} >> 1$. From (8) we see that $C^2 = k_1^2 + \frac{1}{4}k_2^2 - k_1k_2\cos\theta$. Therefore $a_0 C_{\min} >> 1$ corresponds to $a_0k_1 >> 1$. Under this condition and $Z_2 = 1$, the angle at which the zero occurs is given by $C^2 = 2\vec{B} \cdot \vec{C}$. Using (8) we then find that

$$d\sigma(ns)/d\theta \approx 0$$
 for $\theta \approx 29^{\circ}$. (57)

The angle is much larger than the similar angle for the p +H case. The experimental verification

of this zero in the differential cross section is of great interest. As the nuclear charge of the target increases, this angle should decrease.

IV. CONCLUSIONS

In the calculation presented two objectives have been achieved. First it has been established that in the full Born approximation the $1/n^3$ scaling law also holds. The main difference from the OBK approximation is that in the latter approximation, and only for capture into the *s* states, the $1/n^3$ law holds for any *n*, provided the incident energy is large enough, while for the full Born the $1/n^3$ law holds only for large *n*.

Secondly, in the limit of high n an analytic expression was obtained for the differential cross section with respect to the scattering angle for a general-type rearrangement collision. The total cross section can be obtained analytically or by means of a single numerical integration. The existing analytic expression will allow, within the validity of the Born approximation, an order-ofmagnitude estimate for capture cross sections into any excited state. As is shown (cf. Fig. 8), for estimating the extreme case of capture into the ground state, or the lowest n value corresponding to capture into the p or d angular momentum states, the estimated cross section in the region of interest is off by a factor of 2 to 3, but the discrepancy decreases as n gets larger, and the error involved is of the order of $1/n^2$.

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APPENDIX

The error in Ref. 19 is in choosing a variable z axis for the evaluation of the integral in (5) of this reference while the integrand is not scalar except for the s states. Here we show that for the s states one can use the results of Ref. 19 to obtain Eq. (28) of the text. Keeping in mind the transformation between the spherical and parabolic hydrogenic wave functions,⁴⁷ we can write

$$T(n00, V_{12}) = \sum_{n_1=0}^{n-1} \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & 0\\ \frac{1}{2}(n_2 - n_1) & \frac{1}{2}(n_1 - n_2) & 0 \end{pmatrix} \times T(nn_10, V_{12}), \qquad (A1)$$

where the large parentheses on the right-hand side denote the 3-j symbol, and $T(nn_10, V_{12})$ is given by Eq. (15) of Ref. 19.

A phase correction should be applied to Eq. (8) of this reference by replacing $2n_1$ in this equation by $n_1 - n_2$. Since $n_1 - n_2$ is even for odd n and is odd for even n, the derivation that follows Eq. (8) is valid for odd n. For even n the derivation should be slightly modified, but the final result is the same as the one which will be given here.

Then for odd n, Eqs. (7) and (15) of Ref. 19 imply that

$$\begin{split} T(nn_2n_1m, V_{12}) &= T^*(nn_1n_2m, V_{12}) \\ &= -T(nn_1n_2m, V_{12}), \quad n_2 \neq n_1 \;. \ \ (A2) \end{split}$$

The interchange of the first two columns of the 3-j symbol is equivalent to the interchange of n_1 and

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 n_2 . This interchange leaves the 3-j symbol invariant. Then the right-hand side of (A1) vanishes unless $n_2 = n_1$. It follows that⁴⁸

$$T(n00, V_{12}) = \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & 0\\ 0 & 0 & 0 \end{pmatrix}$$
$$\times T(nn_1 = n_2 0, V_{12})$$
$$= (-)^{(n-1)/2} \frac{32\pi Z_1 Z_2 e^2 \alpha_0^{5/2} \alpha^{3/2}}{C^2 [\alpha_0^2 + (\vec{B} - \vec{C})^2]^2}, \quad (A3)$$

where for $T(nn_1 = n_20, V_{12})$ Eq. (9) of Ref. 19 has been used. Except for a phase factor, (A3) is the same as (28) in the text.

The error in Ref. 19 was discovered through a correspondence with R. A. Mapleton. Y. B. Band had independently recognized the source of the error (cf. Ref. 38).

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