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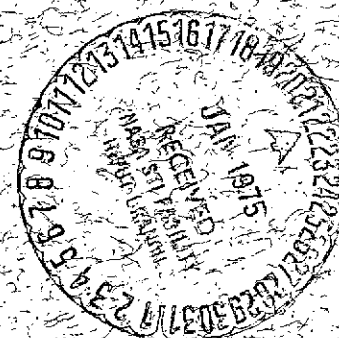
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ABSTRACT

A three body general rearrangement collision is considered where the initial and final bound states are described by the hydrogen like 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 $n/(\mu Z) \gg 1$, where n , μ , and Z are the principal quantum number, the reduced mass, and the nuclear charge of the final state, 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. 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 of 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 in the limit of high n for protons on atomic hydrogen and positrons on atomic hydrogen are given.

I. INTRODUCTION

In 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 super novae explosion in the intersellar media, 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. The 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 McElroy², distorted wave approximation of Bassel and Gerjuoy³, the impulse approximation of McDowell⁴ and Cheshire⁵, the continuum distorted wave approximation of Cheshire⁶, the first order Faddeev-Watson multiple-scattering approximation⁷, the second order Born approximation⁸, 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 Oppenheimer¹⁰, and Brinkman and Kramers¹¹, 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, which from now on we call Oppenheimer, Brinkman and Kramers, or for short OBK, approximation was done for capture into the ground state. Extension to the excited states has been done by May¹², Butler, May, and Johnson¹³, Hiskes¹⁴, and Omidvar¹⁵. More elaborate calculation for the first few low lying states has been done by Mapleton¹⁶, using the full first Born, Coleman and Trelease¹⁷, using the impulse, and Cheshire, Gallaher and Taylor¹⁸, using the pseudostate expansion, approximations.

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). In this paper by expanding the exchange amplitude 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 in the text. It is worth mentioning that a recent measurement by Macdonald et al²⁰ 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 of the order of the squared of the 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 independent of this potential.^{23,8} It is also significant to note that the second Born provides the asymptotically leading term with respect to the incident energy.^{23,24}

The above consideration for the $p + H$ system applies to an exact solution of the problem. It was suggested by Jackson and Schiff²⁵, 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 the full Born for the incident energies above 50 KeV is in excellent agreement with the measured cross section, while the OBK results are by a factor of 5 to 2 larger than either the full Born or the experimental results²⁵.

In the formulation that follows for the sake of generality charges $Z_1 e$ and $Z_2 e$ are assigned to the projectile and the target nucleus. 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 calculations of these authors can not be considered a new method, this terminology is not being used here.

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 unlike 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 $Z_1 e, Z_2 e, -Z_3 e$, 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 $\hbar k_1$ and $\hbar k_2$. Then the conservation of energy implies that

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

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

where μ_i is the reduced mass of the system, $E(i, j)$ is the energy of $(i + j)$ state with the principal quantum number n , R is the rydberg unit of energy, and m_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

$$T(i, f) = \frac{q_1 q_2}{2\pi \hbar^4} \left(\frac{R_2}{R_1} \right) \int |T(i, f)|^2 d(-\hat{k}_1 \cdot \hat{k}_2) \quad (3)$$

$$\begin{aligned} T(i, f) &= \langle \psi(\underline{r}_1, \underline{r}_2, \underline{r}_3) | V_{12} + V_{13} | \exp(i \underline{k}_1 \cdot \underline{r}_1) \phi(i, \underline{r}_{23}) \rangle \\ &= \langle \exp(i \underline{k}_2 \cdot \underline{r}_2) \phi(f, \underline{r}_{13}) | V_{12} + V_{23} | \psi(\underline{r}_1, \underline{r}_2, \underline{r}_3) \rangle \end{aligned} \quad (4)$$

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

Different orders of the Born approximation is 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 $n\ell m$ state, with $n\ell m$ the hydrogenic quantum numbers, in the first Born approximation (4) reduces to²⁵

$$T(n\ell m, V_{23}) = (2\pi)^3 \left[E(2,3) - \frac{\hbar^2 B^2}{2\mu_{23}} \right] U(n\ell m, \underline{c}) U(100, \underline{B}) \quad (5)$$

$$T(n\ell m, V_{12}) = 4\pi Z_1 Z_2 e^2 \int U(n\ell m, \underline{c} - \underline{\hbar}) U(100, \underline{B} - \underline{\hbar}) \frac{d\underline{\hbar}}{\hbar^2} \quad (6)$$

where $U(n\ell m, \underline{p})$ is the Fourier transform of $\phi(n\ell m, \underline{r})$ defined by

$$U(n\ell m, \underline{p}) = (2\pi)^{3/2} \int e^{i \underline{p} \cdot \underline{r}} \phi(n\ell m, \underline{r}) d\underline{r} \quad (7)$$

and

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

The explicit form of $U(n \ell m, \underline{p})$ for the atomic hydrogen can be found elsewhere.²⁹ We modify this form to describe the arbitrary hydrogenlike atoms.

Then it follows that

$$U(n \ell m, \underline{p}) = F(n \ell, \underline{p}) Y(\ell m, \hat{\underline{p}}) \quad (9)$$

$$F(n \ell, \underline{p}) = \left[\frac{2}{\pi} \frac{(n-\ell-1)!}{(n+\ell)!} \right]^{1/2} \frac{2^{\ell+2} \ell! \sqrt{n} \alpha (\alpha \underline{p})^{\ell}}{(\underline{p}^2 + \alpha^2)^{\ell+2}} C_{n-\ell-1}^{\ell+1} \left(\frac{\underline{p}^2 - \alpha^2}{\underline{p}^2 + \alpha^2} \right) \quad (10)$$

$$\alpha = \mu_{ij} Z_i Z_j / (m_e n a_0) \quad (11)$$

where $C_n^\nu(z)$ represents the Gegenbauer function.

$F(n \ell, \underline{p})$ can be expressed as a polynomial by considering the expansion³⁰

$$\frac{1}{(\underline{h} - \underline{h}_-)^{\nu} (\underline{h} - \underline{h}_+)^{\nu}} = \sum_{n=0}^{\infty} \underline{h}^n C_n^{\nu}(\underline{\delta}), \quad \underline{h}_{\pm} = \underline{\delta} \pm \sqrt{\underline{\delta}^2 - 1} \quad (12)$$

By making a Taylor's expansion of the left hand side, (12) leads to

$$C_n^{\nu}(\underline{\delta}) = \frac{1}{n!} \frac{d^n}{d \underline{h}^n} (\underline{h} - \underline{h}_-)^{-\nu} (\underline{h} - \underline{h}_+)^{-\nu} \Big|_{\underline{h}=0} \quad (13)$$

By evaluating the right hand side we find that

$$C_n^\nu(\beta) = \frac{1}{n!} (h_- h_+)^{-\nu} \sum_{\lambda=0}^n \binom{n}{\lambda} \frac{\Gamma(\nu+\lambda)\Gamma(\nu+n-\lambda)}{\Gamma(\nu)\Gamma(\nu)} h_-^{-(n-\lambda)} h_+^{-\lambda} \quad (14)$$

By means of (10) and (14) $F(n, l, p)$ can be explicitly expressed in terms of its arguments:

$$F(n, l, h) = \left[\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!} \right]^{1/2} \frac{2^{2l+2} l! \sqrt{n} \alpha^{5/2} (\alpha h)^l}{(h^2 + \alpha^2)^{l+2}} \times R_e \sum_{\gamma=0}^{\lfloor (n-l-1)/2 \rfloor} \left[2 - \delta\left(\gamma, \frac{n-l-1}{2}\right) \right] \binom{l+\gamma}{\gamma} \binom{n-1-\gamma}{n-l-1-\gamma} \left(\frac{h+i\alpha}{h-i\alpha} \right)^{n-l-1-2\gamma} \quad (15)$$

Through (9) and (15) and the identity²⁵

$$E(2, 3) - \frac{\hbar^2 B^2}{2 \mu_{23}} = E(1, 3) - \frac{\hbar^2 C^2}{2 \mu_{13}} \quad (16)$$

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:

$$T(n, l, m, V_{23}) = - 2^{6+2l} \pi^{3/2} (\mu_{13}/\mu_{23}) Z_2 Z_3 e^2 \times (\alpha_0 \alpha)^{3/2} (n \alpha)^{l+1} l! [(2l+1)!]^{-1} C^{-l-l-6} J(l, C) Y(l, m, \hat{C}) \quad (17)$$

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

$$\zeta(\ell, c) = \binom{n+\ell}{n-\ell-1} \sum_{\nu=1}^{n-\ell} \binom{\ell+\nu-1}{\nu-1} \binom{n-\nu}{n-\ell-\nu} \times \cos[2(n-\ell+1-2\nu)\varphi], \quad \varphi = \tan^{-1} d/c, \quad n \rightarrow \infty \quad (18)$$

By its definition ϕ lies in the first quadrant. Eq. (18) then shows that $\zeta(\ell, c)$ lies always between zero and one. In particular we have the following limiting values:

$$\zeta(\ell, c) \rightarrow 1, \quad c \gg 1 \quad (19)$$

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

$$\varphi \approx \frac{d}{c} \left(1 - \frac{d^2}{3c^2}\right) + O\left(\frac{d^5}{c^5}\right), \quad \frac{d}{c} \ll 1 \quad (20)$$

we see that

$$\zeta(\ell, c) \approx 1 + O(1/n^2) \quad (21)$$

Through (17) we then find that for small ℓ

$$T(n, \ell, m, V_{23}) \propto n^{-3/2} + O(n^{-7/2}), \quad d/c \ll 1 \quad (22)$$

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

$$\zeta(0, c) \approx 1 - \frac{2}{3} \left(\frac{d}{c}\right)^2 + \frac{4}{9} \left(\frac{d}{c}\right)^4 n^{-2} + O(n^{-4}) \quad (23)$$

It should be noted that αn is independent of n .

Evaluation of $T(V_{12})$ is algebraically more complicated. In this case we introduce $q = c - p$. Then with the help of (9) and (15) Eq. (6) can be written

$$\begin{aligned}
 T(nlm, V_{12}) = & 2^{6+2l} \pi^{-1/2} z_1 z_2 e^2 (\alpha_0 \alpha)^{5/2} \\
 & \times l! \left[\frac{n(n-l-1)!}{(n+l)!} \right]^{1/2} (-)^{n-l-1} \\
 & \times \sum_{\mu=0}^{\leq (n-l-1)/2} \left[2 - \delta(\mu, \frac{n-l-1}{2}) \right] \binom{l+\mu}{\mu} \binom{n-1-\mu}{n-l-1-\mu} \operatorname{Re} J(nlm\mu)
 \end{aligned} \quad (24)$$

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

$$J(nlm\mu) = \int_0^\infty \frac{(\alpha - i q)^{n-2l-3-2\mu}}{(\alpha + i q)^{n+1-2\mu}} (\alpha q)^l q^2 f(lm, q) dq \quad (25)$$

$$f(lm, q) = \int \frac{Y(lm, \hat{q}) d\hat{q}}{(\underline{c} - \underline{q})^2 [\alpha_0^2 + (\underline{A} + \underline{q})^2]^2}, \quad \underline{A} = \underline{B} - \underline{c} \quad (26)$$

By separating the real part of the integrand on the right hand side of (24) we obtain

$$\begin{aligned}
 \operatorname{Re} J(nlm\mu) = & \sum_{\nu=0}^{n-l-1-2\mu} \binom{2(n-l-1-2\mu)}{2\nu} (-)^\nu \alpha^{2(n-l-1-2\mu-\nu+)} \\
 & \times J(nlm\mu\nu)
 \end{aligned} \quad (27)$$

$$J(n, l, m, \nu) = \int_0^{\infty} \frac{q^{2+2\nu+l} dq}{(a^2 + q^2)^{n+1-2\nu}} f(l, m, q) \quad (28)$$

Let us consider a parameter q_0 such that $a \ll q_0 \ll 1$. Then (28) can be written

$$J(n, l, m, \nu) = \int_0^{q_0} \frac{q^{2+2\nu+l} dq}{(a^2 + q^2)^{n+1-2\nu}} f(l, m, q) + \int_{q_0}^{\infty} \frac{f(l, m, q) dq}{q^{2(n-2\nu-l/2)}} , \quad a \ll q_0 \ll 1 \quad (29)$$

We notice from (27) that the minimum value of $n - 2\nu - l/2$ is equal or greater than 1. Also as $q \rightarrow 0$, or $q \rightarrow \infty$, the value of $f(l, m, q)$ approaches a finite value independent of q , or zero. Then the value of the second integral in (29) 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 a , the integrand in the first integral in (29) is of the order of $a^{-2[n-2\nu-l/2]}$. Then the value of this integrand is of the order of $a^{-\omega}$, where again ω is greater or equal to one. The second integral in (29) can then be neglected compared to the first one.

Since in the first integral in (29) q lies between 0 and q_0 , we are justified to make a Taylor's expansion of $f(l, m, q)$ in the integrand.

$$f(l, m, q) = \sum_{N=0}^{\infty} \frac{1}{N!} f^{(N)}(l, m, 0) q^N \quad (30)$$

It follows that

$$J(nlm\mu\nu) = \sum_{N=N_0}^{\infty} \frac{1}{N!} f^{(N)}(lm, 0) J^{(N)}(nlm\mu\nu) \quad (31)$$

$$J^{(N)}(nlm\mu\nu) = \int_0^{q_0} \frac{q^{2+2\nu+l+N} dq}{(\alpha^2 + q^2)^{n+1-2\mu}} , \quad \alpha \ll q_0 \ll 1 \quad (32)$$

where N_0 corresponds to the first non-vanishing term of the series.

We introduce now $y = \alpha^2 + q^2$, and obtain

$$J^{(N)}(nlm\mu\nu) = \frac{1}{2} \sum_{\lambda=0}^{\infty} \binom{\nu + \frac{1}{2}(l+N+1)}{\lambda} (-\alpha^2)^{\lambda} \times \int_{\alpha^2}^{q_0^2} \frac{dy}{y^{n+1-2\mu-\nu-\frac{1}{2}(l+N+1)+\lambda}} \quad (33)$$

The minimum value of the power of y in the denominator of the integrand in (33) is $1/2 (3 + l - N)$. Evaluating the integral in (33), and combining (27), (31), and (33) leads to

$$\text{Re } J(nlm\mu) = \sum_{N=N_0}^{\infty} \frac{\alpha^{N-1}}{2 N!} f^{(N)}(lm, 0) C(nl\mu) \quad (34)$$

$$C(nl\mu) = \sum_{\nu=0}^{n-l-1-2\mu} \binom{2(n-l-1-2\mu)}{2\nu} (-)^{\nu} \quad (35)$$

$$\times \sum_{\lambda} \binom{\nu + \frac{1}{2}(l+N+1)}{\lambda} \frac{(-)^{\lambda}}{n-2\mu-\nu-\frac{1}{2}(l+N+1)+\lambda}$$

For $N > l$, and some values of λ , ν , and μ , logarithmic terms occur in (33). This does not create particular difficulty. But since the leading term in the amplitude arises from $N \leq l$, the case $N > l$ will not be treated here.

Making use of the properties of the binomial coefficients, the sums with respect to λ in (35) can be closed. We find that

$$C(nl\mu) = \frac{(2j)!}{(l+j+1)!} \sum_{\nu=0}^j \frac{(-)^{\nu} \Gamma(\frac{1}{2}(l+N+1)+\nu+1) \Gamma(\frac{1}{2}(l-N+1)+j-\nu)}{(2\nu)! (2j-2\nu)!}$$

$$j = n-l-1-2\mu \quad (36)$$

Combination of (24) and (34) now leads to

$$T(nlm, V_{12}) = \sum_{N=N_0}^{\infty} \frac{2^{2l+5}}{\sqrt{\pi} N!} Z_1 Z_2 e^2 \alpha_0^{5/2} \alpha^{3/2+N} l!$$

$$\times \left[\frac{n(n-l-1)!}{(n+l)!} \right]^{1/2} (-)^{n-l-1} S(nl) f^{(N)}(lm, 0) \quad (37)$$

$$S(n, l) = \sum_j (2 - \delta_{j,0}) \binom{\frac{1}{2}(n+l-1-j)}{l} \binom{\frac{1}{2}(n-1+l+j)}{l} C(n, l, \mu) \quad (38)$$

where now j replaces the summation with respect to μ .

Equations (36) - (38) together with (17) and (18) provide an expansion in terms of α , or $1/n$, for the first Born amplitude. In the following we restrict ourself to the leading term of the expansion.

For evaluation of $f^{(N)}(l, m, 0)$, which are the coefficients of the Taylor's expansion of $f(l, m, q)$, with respect to q , we choose the z axis of the integration along C . Then by a straight forward calculation we find that

$$f^{(0)}(0, 0, 0) = \frac{\sqrt{4\pi}}{C^2(\alpha_0^2 + A^2)^2} \quad (39)$$

$$f^{(0)}(1, m, 0) = 0$$

$$f^{(1)}(1, m, 0) = 2\sqrt{\frac{4\pi}{3}} \left[\frac{\delta(m, 0)}{C^3(\alpha_0^2 + A^2)^2} - \frac{2\sqrt{4\pi/3} AY(1, m, \hat{A})}{C^2(\alpha_0^2 + A^2)^3} \right] \quad (40)$$

$$f^{(0)}(2, m, 0) = f^{(1)}(2, m, 0) = 0$$

$$f^{(2)}(2, m, 0) = 16\sqrt{\frac{4\pi}{5}} \left[\frac{\frac{1}{3}\delta(m, 0)}{C^4(\alpha_0^2 + A^2)^2} - \frac{\frac{1}{3}\sqrt{4\pi(4-m^2)/3} AY(1, m, \hat{A})}{C^3(\alpha_0^2 + A^2)^3} + \frac{\sqrt{4\pi/5} A^2 Y(2, m, \hat{A})}{C^2(\alpha_0^2 + A^2)^4} \right] \quad (41)$$

These equations show that for $\ell = 0, 1$, and 2 , $N_0 = \ell$. Putting $N = N_0 = \ell$ in (36) and using the properties of the binomial coefficients, the summation in (36) with respect to ν can be closed. We find that

$$\begin{aligned} C(n0) &= \frac{\pi}{4} [2 \delta(j,0) - \delta(j,1)] \\ C(n1) &= \frac{\pi}{16} [6 \delta(j,0) - 4 \delta(j,1) + \delta(j,2)] \\ C(n2) &= \frac{\pi}{64} [20 \delta(j,0) - 15 \delta(j,1) + 6 \delta(j,2) - \delta(j,3)] \end{aligned} \quad (42)$$

Substituting these values of $C(n\ell)$ in (38), the summation with respect to j in (38) can similarly be closed. This results in the following expressions:

$$\begin{aligned} S(n0) &= (-1)^{n-1} \pi/2 \\ S(n1) &= (-1)^{n-2} n^2 \pi/8 \\ S(n2) &= (-1)^{n-3} n^4 \pi/128 \end{aligned} \quad (43)$$

Substituting the values of $f^{(N)}(\ell m, 0)$ and $S(n\ell)$ from (39) through (41), and (43), we finally obtain the following results:

$$T(n00, V_{12}) = \frac{32 \pi Z_1 Z_2 e^2 d_0^{5/2} \alpha^{3/2}}{c^2 (d_0^2 + A^2)^2} \quad (44)$$

$$T(n1m, V_{12}) = \frac{64\pi}{\sqrt{3}} Z_1 Z_2 e^2 d_0^{5/2} d^{3/2} (dn) \\ \times \left[\frac{\delta(m, 0)}{C^3 (d_0^2 + A^2)^2} - \frac{2\sqrt{4\pi/3} A Y(1m, \hat{A})}{C^2 (d_0^2 + A^2)^3} \right] \quad (45)$$

$$T(n2m, V_{12}) = \frac{128\pi}{\sqrt{5}} Z_1 Z_2 e^2 d_0^{5/2} d^{3/2} (dn)^2 \\ \times \left[\frac{\frac{1}{3} \delta(m, 0)}{C^4 (d_0^2 + A^2)^2} - \frac{\frac{1}{3} \sqrt{4\pi(4-m^2)/3} A Y(1m, \hat{A})}{C^3 (d_0^2 + A^2)^3} \right. \\ \left. + \frac{\sqrt{4\pi/5} A^2 Y(2m, \hat{A})}{C^2 (d_0^2 + A^2)^4} \right] \quad (46)$$

This completes the evaluation of the core amplitude for $\ell = 0, 1, 2$. 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 (17). Due to 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. (17) and (44) through (46) show that for capture into the final ℓ state the cross section behaves as $E_0^{-6-\ell}$.

It remains to show that the higher order term in $T(n^\ell m, V_{12})$ behaves as $n^{-7/2}$. To show this from (26) and (30) we can write

$$f^{(N)}(\ell m, 0) = \int Y(\ell m, \hat{q}) g^{(N)}(\hat{q}, 0) d\hat{q} \quad (47)$$

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

$$\begin{aligned} g(\hat{q}, q) &= (C^2 + q^2 - 2CqX)^{-1} (C_0^2 + A^2 + q^2 + 2AqX)^{-2} \\ &= \sum_{N=0}^{\infty} \frac{q^N}{N!} g^{(N)}(\hat{q}, q), \quad X = \hat{C} \cdot \hat{q}, \quad X = \hat{A} \cdot \hat{q} \end{aligned} \quad (48)$$

By differentiating the middle term in (48) 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 (47) it then follows that $f^N(\ell m, 0)$ vanishes unless $\ell + N$ is even. For a given ℓ , N then takes only odd or even integers. Through (34) we then see that if the leading term of $T(n^\ell m, V_{12})$ behave as $n^{-3/2}$, the next higher order term behaves as $n^{-7/2}$.

Since the higher order term in $T(n^\ell m, V_{23})$ 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 publication¹⁹, Eq. (44) is rederived in the Appendix by a different method.

To find the total cross section equation (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 $\zeta(\ell, c)$ in the OBK amplitude. Due to this factor the total cross section should be obtained numerically. However, for the symmetric collisions, Sec. II. 3, and also when $\zeta(\ell, c) \rightarrow 1$, (Sec. III. 1), 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 $q = C - p$ we obtain

$$\begin{aligned} \sum_{\ell m} |T(n \ell m, V_{12})|^2 &= (4\pi Z_1 Z_2 e^2)^2 \\ &\times \iint U(100, \underline{A} + \underline{q}) U^*(100, \underline{A} + \underline{q}') (\underline{C} - \underline{q}) (\underline{C} - \underline{q}')^{-2} d\underline{q} d\underline{q}' \\ &\times \sum_{\ell m} U^*(n \ell m, \underline{q}) U(n \ell m, \underline{q}') \end{aligned} \quad (49)$$

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

$$\sum_{\ell m} U^*(n \ell m, \underline{q}) U(n \ell m, \underline{q}') = \frac{8 \alpha^5}{\pi^2 (\alpha^2 + q^2)^2 (\alpha^2 + q'^2)^2} \frac{n \sin n\alpha}{\sin w} \quad (50)$$

where w is a function of q and q' given by

$$4 \sin^2 \frac{w}{2} = (\xi - \xi')^2 + (\eta - \eta')^2 + (\zeta - \zeta')^2 + (\chi - \chi')^2 \quad (51)$$

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

$$\begin{pmatrix} \xi \\ \eta \\ \zeta \\ \chi \end{pmatrix} = \frac{2\alpha\beta}{\alpha^2 + \beta^2} \begin{pmatrix} \sin\theta \cos\varphi \\ \sin\theta \sin\varphi \\ \cos\theta \\ \chi \end{pmatrix}, \quad \chi = \frac{\alpha^2 - \beta^2}{\alpha^2 + \beta^2} \quad (52)$$

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

By finding the form of $U(100, \mathbf{p})$ from (9) and (10), Eq. (49) can now be

written

$$\sum_{lm} |T(nlm, V_{12})|^2 = (4\pi Z_1 Z_2 e^2)^2 64 \pi^{-4} (\alpha_0 \alpha)^5 n^2 \times \iint \frac{f(\underline{q}, \underline{q}')}{(\alpha^2 + \beta^2)^2 (\alpha'^2 + \beta'^2)^2} \frac{\sin n w}{n \sin w} d\underline{q} d\underline{q}' \quad (53)$$

$$f(\underline{q}, \underline{q}') = (\underline{C} - \underline{q})(\underline{C} - \underline{q}')^{-2} [\alpha_0^2 + (\underline{A} + \underline{q})^2]^{-2} [\alpha_0^2 + (\underline{A} + \underline{q}')^2]^{-2} \quad (54)$$

The function $f(\mathbf{q}, \mathbf{q}')$ remains finite as $\alpha \rightarrow 0$. Following the argument given in the previous section, we make a Taylor's expansion of $f(\mathbf{q}, \mathbf{q}')$, and keep the zero order term, $f(0, 0)$. On the right hand side of (53) the only term which depends on the angular coordinates of \mathbf{q} and \mathbf{q}' is $\sin n w / \sin w$. Realizing

that $\sin n w / \sin w$ is a scalar quantity, for integration over the angles of \mathbf{q} and \mathbf{q}' we can take the z-axis along \mathbf{q} . Then, introducing $\cos \gamma = \hat{\mathbf{q}} \cdot \hat{\mathbf{q}}'$,

$$\iint \frac{\sin n w}{n \sin w} d\hat{\mathbf{q}} d\hat{\mathbf{q}}' = \frac{8\pi^2}{n} \int_0^\pi \frac{\sin n w}{\sin w} \sin \gamma d\gamma \quad (55)$$

The variable of integration can be changed from γ to w through the relationship³

$$\cos w = \cos \beta \cos \beta' + \sin \beta \sin \beta' \cos \gamma, \\ \beta = \cos^{-1} \frac{d^2 - g^2}{d^2 + g^2} \quad (56)$$

When the integration is carried out we find that

$$\iint \frac{\sin n w}{n \sin w} d\hat{\mathbf{q}} d\hat{\mathbf{q}}' = \left(\frac{4\pi}{n} \right)^2 \frac{\sin n \beta \sin n \beta'}{\sin \beta \sin \beta'} \quad (57)$$

Equation (53) can now be written

$$\sum_{lm} |T(nlm, V_{12})|^2 = 2'^2 (Z_1 Z_2 e^2)^2 d_0^5 d^3 f(0,0) \\ \times \left[\int_0^\infty \frac{\sin(n\beta) g dg}{d^2 + g^2} \right]^2 \quad (58)$$

The integral on the right hand side similar to the previous section can be evaluated by introducing a parameter $\alpha \ll q_0 \ll 1$. Then the value of the

integral in the limit $\alpha \rightarrow 0$ is equal to $(-1)^{n-1} \pi/2$. It then follows that

$$\sum_{l_m} |T(n l_m, V_{12})|^2 = \frac{(32 \pi Z_1 Z_2 e^2)^2 d_0^5 d^3}{c^4 (d_0^2 + A^2)^4} \quad (59)$$

Comparison of this with (32) indicates that for the zero order expansion of $f(q, q')$, the total cross section is equal to the s capture cross section. The higher order terms of expansion of $f(q, q')$ with respect to q and q' , as can be seen from (54), lead to results which fall faster with respect to energy compared to the zero order term, and therefore can be neglected.

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.

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 general 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 Kramer⁷. The case of exchange collision between electron and atomic hydrogen has been overlooked by both authors. Here 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 arises from the backscattering and is due to the core potential. We then consider cross section due to $T(n \ell m, V_{12})$ only. Let us introduce $M = \mu_{13}/m_3 = \mu_{23}/m_3$. From the definition of B and C we then find that

$$B^2 - C^2 = -\beta d_0^2, \quad \beta = (1 - M^2) \mu_1 / \mu_{13} \quad (60)$$

By means of this equation and using Eqs. (44) - (46) we can show that

$$\begin{aligned} |T(n \ell m, V_{12})|^2 &= \frac{2^{10} \pi^2 Z_1^2 Z_2^2 e^4 d_0^5 d^3 (2d^m)^{2\ell}}{(2\ell+1) d^4 (d_0^2 + A^2)^4} \\ &\times \sum_{i,j} \beta_{i,j} d^{-2i} (d_0^2 + A^2)^{-j}, \\ \ell &= 0, 1, 2, \quad i, j = 0, 1, 2, \dots \quad (61) \end{aligned}$$

where the coefficients β_{ij} are independent of the angle between \mathbf{k}_1 and \mathbf{k}_2 .

To obtain the cross section we change the variable of integration from $\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2$ to C^2 (cf. Eq. (37)). Defining an integral $I(i, j)$ by

$$I(i, j) = \int_{-1}^{+1} \frac{\alpha(-\hat{k}_1 \cdot \hat{k}_2)}{C^{2i} [\alpha_0^2 + (B - C)^2]} d^j \quad (62)$$

Then by an elementary integration we find that

$$I(i, j) = \frac{-1}{2M K_1 K_2} \frac{(-b)^{i-1}}{\alpha^{i+j-1}} \left\{ \sum_{\lambda \neq j-1}^{i+j-2} \binom{i+j-2}{\lambda} \frac{1}{j-1-\lambda} \left(\frac{-b C^2}{a+b C^2} \right)^{j-1-\lambda} + \binom{i+j-2}{j-1} \ln \frac{-b C^2}{a+b C^2} \right\}_{C_{\pm}^2},$$

$$C_{\pm}^2 = (K_1 \mp M K_2)^2 \quad (63)$$

where the coefficients a and b are defined by the equation $\alpha_0^2 + (B - C)^2 = a + b C^2$, and are given by

$$a = (1+M)(1-M)(M^{-1} K_1^2 + K_2^2) + \alpha_0^2, \quad b = -M^{-1}(1-M)^2 \quad (64)$$

At high incident energies when $k_1^2 \gg \mu_1 \alpha_0^2 / \mu_{13}$ we find that

$$\left(\frac{-b C_+^2}{a+b C_+^2} \right) \approx \frac{(1-M)^2}{4M}, \quad \left(\frac{-b C_-^2}{a+b C_-^2} \right) \approx \frac{(1-M^2)^2 K_1^2}{M \alpha_0^2},$$

$$K_1^2 \gg 4, \alpha_0^2 / 4, 3 \quad (65)$$

In applying (65) to (63) we realize that the leading term comes from the C_-^2 limit and $\lambda = 0$. Then

$$I(i, j) \approx \left[2(j-1)(1-M)^2(1+M)^2 \alpha_0^{2(j-1)} K_1^{2(i+1)} \right]^{-1} \quad (66)$$

The above equation implies that the leading terms in the cross section arises from the terms with smallest value of i . In (61) we then have to consider the terms with $i = 0$.

Using the form of $T(n, l, m, V_{12})$ given by (44) through (46) we find that

$$\begin{aligned}
 l=m=0, \quad \beta_{00}=1, \quad \beta_{0j}=0 \text{ otherwise.} \\
 l=1, m=0, \quad \beta_{0j}=0, \quad j=0, 1, 2, \dots \\
 l=1, m=\pm 1, \quad \beta_{01}=2, \quad \beta_{02}=-2\alpha_0^2, \quad \beta_{0j}=0 \text{ otherwise,} \\
 l=2, m=0, \quad \beta_{02}=1/4, \quad \beta_{03}=1/2, \quad \beta_{04}=\alpha_0/4, \\
 \beta_{0j}=0 \text{ otherwise,} \\
 l=2, m=\pm 1, \quad \beta_{0j}=0, \quad j=0, 1, 2 \\
 l=2, m=\pm 2, \quad \beta_{03}=3/8, \quad \beta_{04}=-3\alpha_0^2/8, \\
 \beta_{0j}=0 \text{ otherwise.} \quad (67)
 \end{aligned}$$

Combining (67) with (61), and making use of (63), the total cross section as given by (3) can be evaluated. Since the magnetic quantum number m refers to C as the z axis which is not fixed in space, there is no use to list the cross section for each m . We sum with respect to m and we find that

$$\begin{aligned}
 n^3 \sigma(ns) / \pi \alpha_0^2 &\approx \frac{1}{3} 2^8 \gamma_{13}^2 (m_e \gamma_{13})^{-1} Z_1^5 Z_2^2 Z_3^2 \\
 &\quad \times (1+M)^{-4} (1-M)^{-2} (E/R)^{-3}, \\
 \sigma(nh) &\approx \frac{4}{5} (Z_1/Z_2)^2 \sigma(ns),
 \end{aligned}$$

$$\sigma(nd) \approx \frac{16}{175} (Z_1/Z_2)^4 \sigma(ns) \quad (68)$$

In these equations E/R is the center of mass energy in rydberg units related to k_1^2 through

$$E/R = (m_e/m_1) a_0^2 k_1^2 \quad (69)$$

with a_0 the Bohr's radius. It should be realized that the restriction on k_1^2 given by (65) for the validity of Eqs. (68) is not restrictive enough. For each value of m_1 and m_3 the next to the leading term in (63) should be worked out, and the validity criterion be given accordingly. This will be done for $p + H$ and $e + H$ systems in the next section.

As was shown by Mapleton we see that the contribution to the $1/E^3$ behavior comes from the C_2^2 limit, which corresponds to the backscattering.

An important difference between the symmetric and non-symmetric collisions is that in the former case capture into any final state angular momentum ℓ behaves as $1/E^3$, while in the non-symmetric case this behavior is $1/E^{6+\ell}$. In the symmetric case all angular momenta contribute to the total cross section, although as it can be seen from (68) the contribution becomes progressively less as ℓ increases. In the non-symmetric case contribution comes only from the s states.

III. APPLICATIONS

A. Protons on Atomic Hydrogen

In Fig. 1 the differential cross section for capture into the highly s states 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 magnitudes compared to the forward capture. This can be seen by comparing figures 1 and 2. There is no backward peak for the Born at 25 keV, since collisions are not strong enough. Since there is no nuclear nuclear interaction in the OBK approximation, there similarly is no backward peak in this approximation.

In Figure 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 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 due to the attractive and repulsive potentials are 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 appear at smaller angles. In the limit of very high Z_2 the zero does not appear at all. Due to the simplicity of the model, the foregoing charge dependence of the zero angle may not provide a true picture of the actual proton-multielectron atom charge exchange collisions. It is more applicable to the electron capture by protons from the isoelectronic sequence of the 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 Figure 3 the differential cross section for $1s \rightarrow n p$ and $1s \rightarrow n d$, when $n^2 \gg 1$, is plotted versus $\cos \theta$. For these cases the peaks in the backward capture appears not at 180° , but very close to 180° .

In Figure 4, similar to Fig. 2, the differential cross section for $1s \rightarrow n p$ transitions, $n^2 \gg 1$, is shown for small scattering angles. Unlike $1s \rightarrow n s$ transitions, there are no zeros in the differential cross sections, but minima in the Born approximation. The OBK cross sections, similar to the previous cases, are monotonically decreasing function of the scattering angle.

In Figure 5 the differential cross sections for small scattering angles are shown for $1s \rightarrow n d$, $n^2 \gg 1$ 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 the 2.5 MeV is a monotonically decreasing function of the scattering angle.

In Figure 6 the total cross section for $1s \rightarrow n\ell$, $n^2 \gg 1$, $\ell = 0, 1, 2$ transitions in the OBK approximation, and also the total cross section summed over all the angular momenta, are plotted versus the squared 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. Similar trend is shown for the first Born as will be seen in Figure 7. It is difficult to understand the physical reason for this behavior, and an experimental verification of this behavior is desirable.

The determination of $\sigma(n\ell)$, $n^2 \gg 1$, was first made by Butler, May, and Johnson¹³. Although they use a different method to calculate their cross section, it is found out that their results graphically are 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

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

we see that when the ordinate of Fig. 6 is multiplied by $1/2$, 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 $n\ell$, $n^2 \gg 1$, $\ell = 0, 1$, and 2 in the Born approximation. Similar to the OBK case, for low impact energies the $\ell = 1$ dominates. At high energies $\ell = 0$ 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 $\ell = 0, 1$, 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 $n^3 \sigma(1s \rightarrow n\ell)$ to $n_0^3 \sigma(1s \rightarrow n_0\ell)$, where $n^2 \gg 1$, and $n_0 = \ell + 1$ is the lowest member of the $1s \rightarrow n\ell$ 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 zero to 2.5 MeV. Each curve in this figure provides an upper limit to an envelop of curves bounded from below by the x axis, each curve within the envelop 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 states cross sections at sufficiently high energies were scalable from that 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. (73)), and the results of Ref. (12) we can show that

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

$$\frac{n^3 \sigma_{OBK}(1s \rightarrow nd)}{27 \sigma_{OBK}(1s \rightarrow 3d)} \rightarrow 2.025, \quad n \rightarrow \infty, \quad v/v_0 \rightarrow \infty \quad (70)$$

Similarly, making use of (74) and a result of Ref. 25 we can show that

$$\frac{n^3 \sigma_B(1s \rightarrow ns)}{\sigma_B(1s \rightarrow 1s)} \rightarrow 1.23, \quad n \rightarrow \infty, \quad v/v_0 \rightarrow \infty \quad (71)$$

The ratios in the Born for the p and d captures cannot be found, since the high energy limits of $\sigma_B(1s \rightarrow 2p)$ and $\sigma_B(1s \rightarrow 3d)$ is 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. Figure 8 clearly shows that this assumption is an approximation.

Recently Khayrallah et al,³³ and Bayfield et al³⁴ have measured electron capture by protons from the atomic hydrogen, where the capture takes place within the quantum numbers $n = 13$ to $n = 30$. Their results are shown in Figure 9. Their experimental uncertainty is $\pm 30\%$. In the same figure results obtained by the impact parameter approximation of Butler and Johnston³⁵, and May³⁶

are also shown. Shown are also the OBK results. The impact parameter and the OBK results are almost identical, and can not be distinguished on the graph. Finally, using asymptotic form with respect to n , the cross section due to the first Born is also shown. As was shown in the previous section, correction to the asymptotic form is of the order of $1/n^2$. It will also be shown later³⁷ that by $n = 13$, the Born cross section has converged to its asymptotic form within a few percent. Then discrepancy of more than a factor of three between the first Born and the experiment can not be due to the use of the asymptotic form. In the light of the fact that in the range 40-60 keV incident energy the first Born is in excellent agreement with measurement when capture takes place in all values of n ²⁵, the lack of agreement in Figure 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. 9). 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 Band³⁸ 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 $\zeta(\ell, C)$ in the OBK amplitude given by (18). However, in the limit indicated by (19) 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. For the sake of generality let us introduce ϵ as the ratio of the mass of the electron to that of the proton. Let the masses of the projectile and target nucleus be given by b/ϵ and c/ϵ , where b and c are the two particle masses in units of the proton's mass. Then using (8) we find that

$$\begin{aligned} a_0^2 C^2 &\approx \frac{s^2}{4} \left[\left(1 - \frac{Z_2^2}{s^2}\right)^2 + \left(\frac{2bc}{b+c}\right)^2 \frac{M^2}{m_e^2} \theta^2 \right] \\ a_0^2 (\tilde{B} - \tilde{C})^2 &\approx s^2 \left[1 - \frac{bc \theta^2}{(b+c)^2} \right] \end{aligned} \quad (72)$$

From the first equation we see that the minimum value of $a_0 C$ is $s/2$. Then through (19) we see $\zeta(\ell, C) \sim 1$ for all the scattering angles if $s \gg 1$. Combining (3), (17), and (44) - (46), making use of (72), and changing the variable of integration to $x = [2bc/(b+c)]^2 (M/m_e)^2 \theta^2$ with a range of integration from 0 to ∞ , we find the following values for the cross section

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

$$\begin{aligned}
\sigma(nh) &= \sigma_{OBK}(nh) \left[1 - \frac{3}{8} Z_2 a^2 + \frac{15}{256} Z_2^2 a^4 \right], \\
\sigma(nd) &= \sigma_{OBK}(nd) \left[1 - 0.4648 Z_2 a^2 + 0.07941 Z_2^2 a^4 \right], \\
\frac{n^3 \sigma_{OBK}(nl)}{\pi a_0^2} &= \frac{2^{6(3+l)} (2l+1)}{5+l} \left[\frac{l!}{(2l+1)!} \right]^2 \frac{Z_1^{5+2l} Z_2^5}{s^{12+2l} a^{10+2l}}, \\
a &= 1 + Z_2^2 s^{-2}, \quad s \gg 1
\end{aligned} \tag{73}$$

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, (71) simplifies and we get the following ratios:

$$\begin{aligned}
\frac{\sigma(ns)}{\sigma_{OBK}(ns)} &\approx 0.811, \quad \frac{\sigma(nh)}{\sigma_{OBK}(nh)} \approx 0.684, \\
\frac{\sigma(nd)}{\sigma_{OBK}(nd)} &\approx 0.615, \quad s \gg 1
\end{aligned} \tag{74}$$

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

Finally, we like to investigate the E^{-3} behavior for capture into the highly excited states. This behavior for capture into the ground state has been investigated by Mapleton³². Applying Eqs. (68) to the $p + H$ case, and noticing that $m_1 = b/\epsilon$, $m_2 = c/\epsilon$, and $m_3 = m_e$, we obtain

$$\frac{n^3 \sigma(n s)}{\pi a_0^2} \approx \frac{32 c Z_1^5 Z_2}{3 \epsilon (E/R)^3}, \quad E/R \gg \epsilon \approx 2.75 \times 10^5 \quad (75)$$

where the validity condition is obtained by considering next to the highest term in (63), which arises from $\lambda = 4$ and C_+^2 limit. Similar expression for $\sigma(n p)$ and $\sigma(n d)$ can be obtained using (68). It should be noted that the validity condition in (75), consistent with the condition given by Mapleton, indicates the $1/E^3$ behavior appear for energies well above 100 MeV. The result given by Mapleton is:

$$\frac{\sigma(1s)}{\pi a_0^2} \approx \frac{1.23 \times 10^3}{(E/R)^3}, \quad E/R \gg \epsilon^{-5/3} \quad (76)$$

By putting $c = Z_1 = Z_2 = 1$ in (75) we see that the coefficient of $(E/R)^{-3}$ in (75) is 15.9 times larger than similar coefficient in (76). This can be taken as an indication that the ground state can not 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}

$$\frac{n^3 \sigma(1s \rightarrow n l)}{\pi a_0^2} \approx \frac{4 Z_1^2}{m_e Z_2^2 E/R} \left[A(1s \rightarrow n l) \ln \frac{m_e E}{4 Z_2^2 R} + B(1s \rightarrow n l) \right],$$

$$A(1s \rightarrow n\ell) = \delta(\ell, 1) \frac{4}{3} |\langle n\ell | Z_2 r / a_0 | 1s \rangle|^2 \quad (77)$$

where $A(1s \rightarrow n\ell)$ and $B(1s \rightarrow n\ell)$ are atomic constants independent of the nuclear charge and μ_1 is the reduced mass of the system. Using the values of these constants⁴², for $Z_1 = Z_2 = 1$, and an incident energy of 100 MeV, we find that

$$\sigma^{Ex}(ms) / \sigma^D(ms) \approx 0.85 \times 10^{-12}, \quad \sigma^{Ex}(nh) / \sigma^D(nh) \approx 0.22 \times 10^{-13}$$

$$\sigma^{Ex}(nd) / \sigma^D(nd) \approx 0.67 \times 10^{-13}$$

However, as Z_1 and Z_2 increase, the exchange effect becomes more important in a complicated way. Using our simple model, from (68) and (76), the first ratio for example increases as $(Z_1 Z_2)^3$.

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 $m_1 = m_2$, also the scattering is 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 can not be separated from each other. However, to get an idea about the relative size of the exchange to the direct amplitudes we use (17) and (68) to get

$$\frac{n^3 \sigma_{OBK}(ns)}{\pi \alpha_0^2} \approx \frac{2^{10} Z_2^5}{(E/R)^6}, \quad \frac{n^3 \sigma(ns)}{\pi \alpha_0^2} \approx \frac{2^8}{3 Z_2 (E/R)^3}, \quad E/R \gg 1 \quad (78)$$

where E/R is the incident energy in rydberg. Then $1/E^3$ behavior becomes valid at much lower energy compared to the $p + H$ case. Expressions similar to (78) can be found for p and d captures.

Comparison of (78) and (77) shows that the ratio of exchange to direct cross section for $e + H$ system increases as Z_2 , the nuclear charge of the H isoelectronic sequence. For 20 rydberg electrons on atomic hydrogen this ratio is 0.115.

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 approximation⁷. Due to 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, and considering capture into the highly excited states. By putting $m_1 = m_2 = m_3 = m_e$, and making use of Eqs. (68) we find that

$$\frac{n^3 \sigma(ns)}{\pi \alpha_0^2} \approx \frac{2^{11}}{81 (E/R)^3}, \quad E/R \gg 1 \quad (79)$$

where E/R is the center of mass energy, equal to the $2/3$ of the incident energy. Similar expressions can be obtained for capture into the $n\ p$ and $n\ d$ states. 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 (79) for $n = 1$ is found to be 1.66, while this coefficient in (79) 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 is an order of magnitude smaller than that of OBK. There are some indications from the measurement⁴⁶ that the first Born cross section is also too large at the threshold of Ps formation.

By putting $m_1 = m_3 = \text{electron mass}$, $m_2 = \text{proton mass}$, and $Z_1 = 1$ in the general formula (17) and (44) - (46), 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, not much details will be given here. It is of interest, however, that similar to the $p + H$ case, the differential cross section for s captures according to the first Born goes to zero for some scattering angle.

To show this we equate the right hand sides of (17) and (39) in the limit $\zeta(0, C) \rightarrow 1$. This limit is satisfied if $a_0 C_{\min} \gg 1$. From (8) we see that $C^2 = k_1^2 + 1/4 k_2^2 - k_1 k_2 \cos \theta$. Therefore $a_0 C_{\min} \gg 1$ corresponds to $a_0 k_1 \gg 1$. Under this condition and $Z_2 = 1$, the angle at which the zero occurs is given by $C^2 = 2 B \cdot C$. Using (8) we then find that

$$d\sigma(ns)/d\theta \approx 0 \quad \text{for} \quad \theta \approx 29^\circ \quad (80)$$

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.

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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. (44) of the text. Keeping in mind the transformation between the spherical and parabolic hydrogenic wave functions⁴⁷, we can write

$$T(n00, V_{12}) = \sum_{m_1=0}^{n-1} \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & 0 \\ \frac{1}{2}(n_1-m_1) & \frac{1}{2}(n_1-m_2) & 0 \end{pmatrix} \times T(n n_1 0, V_{12}) \quad (\text{A1})$$

where the bracket on the right hand side is the 3-j symbol, and $T(n n_1 0, V_{12})$ is given by Eq. (15) of Ref. 19.

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

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

$$\begin{aligned} T(n n_2 n_1 m, V_{12}) &= T^*(n n_1 n_2 m, V_{12}) \\ &= -T(n n_1 n_2 m, V_{12}) \quad , \quad n_2 \neq n_1 \quad (\text{A2}) \end{aligned}$$

The interchange of the first two columns of the 3j symbol is equivalent to the interchange of n_1 and n_2 . This interchange leaves the 3j symbol invariant. Then the right hand side of (A1) vanishes unless $n_2 = n_1$. It follows that⁴⁸

$$\begin{aligned}
 T(n00, V_{12}) &= \begin{pmatrix} \frac{1}{2}(n-1) & \frac{1}{2}(n-1) & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
 &\quad \times T(n n_1 = n_2 0, V_{12}) \\
 &= (-)^{\frac{1}{2}(n-1)} \frac{32\pi Z_1 Z_2 e^2 d_0^{5/2} \alpha^{3/2}}{d^2 [\alpha_0^2 + (\underline{B} - \underline{C})^2]^2} \quad (A3)
 \end{aligned}$$

where for $T(n n_1 = n_2 0, V_{12})$ Eq. (9) of Ref. 19 has been used. Except for a phase factor, (A3) is the same as (44) 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).

FIGURE CAPTIONS

- Fig. 1. Differential cross section for $p + H(1s) \rightarrow H(n s) + p$, $n^2 \gg 1$. θ is the scattering angle, B and OBK stand for the first Born, and the Oppenheimer, Brinkman, and 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. Notations are the same as in Fig. 1. m_e/M is the ratio of the electron to proton masses.
- Fig. 3. Differential cross section for n p and n d captures, $n^2 \gg 1$, for the first Born approximation. Notations are the same as in Figure 1.
- Fig. 4. Minima in the differential cross section for small scattering angles and n p captures. Notations are the same as in Figure 2.
- Fig. 5. Differential cross section for small scattering angles and n d captures. Notations are the same as in Figure 2.
- Fig. 6. Total cross section for n s, n p, n d, and $n \Sigma \ell$ captures in the OBK approximation as function of the squared 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 n s, n p, n d, and their sum in the Born approximation as a function of the squared of the relative velocity.

Fig. 8. Sum of the capture cross sections for $p + H(1s) \rightarrow H(n, \Sigma \ell) + p$, $n = 13-30$ according to the measurement (Refs. 33 and 34), impact parameter, Refs. 35 and 36, OBK, and the first Born approximations. The sum designated by σ_* is in units of \AA^2 . In the figure the normalized data of Ref. 34, which is slightly lower than Ref. 33, has been used.

Fig. 9. Ratio of the $\sigma(1s \rightarrow n\ell)/\sigma(1s \rightarrow n_0\ell)$, $n^2 \gg 1$, where $n_0 = \ell + 1$. The lower three curves are due to the OBK, and the upper three curves are due to the first Born approximations.

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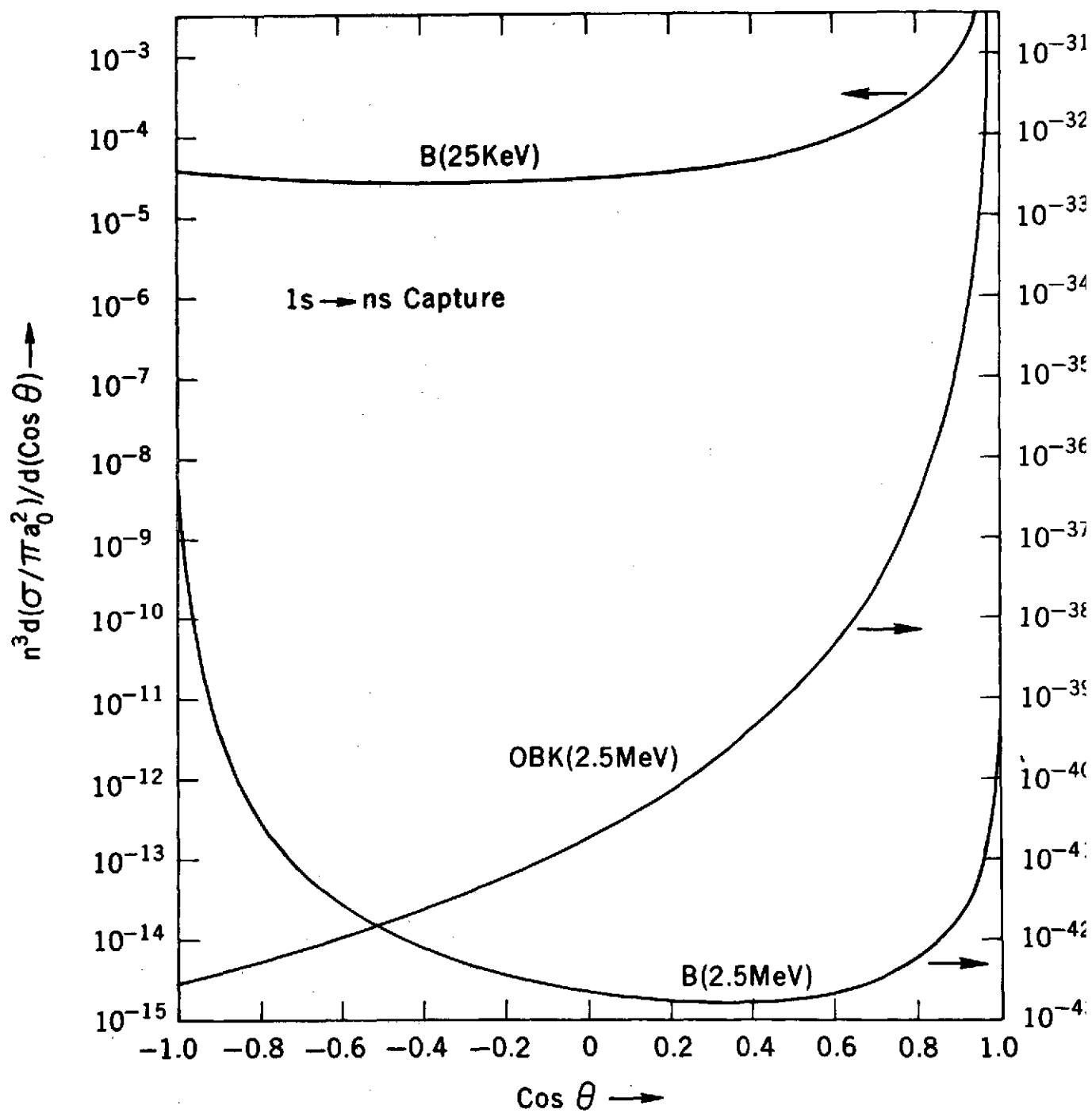


Figure 1

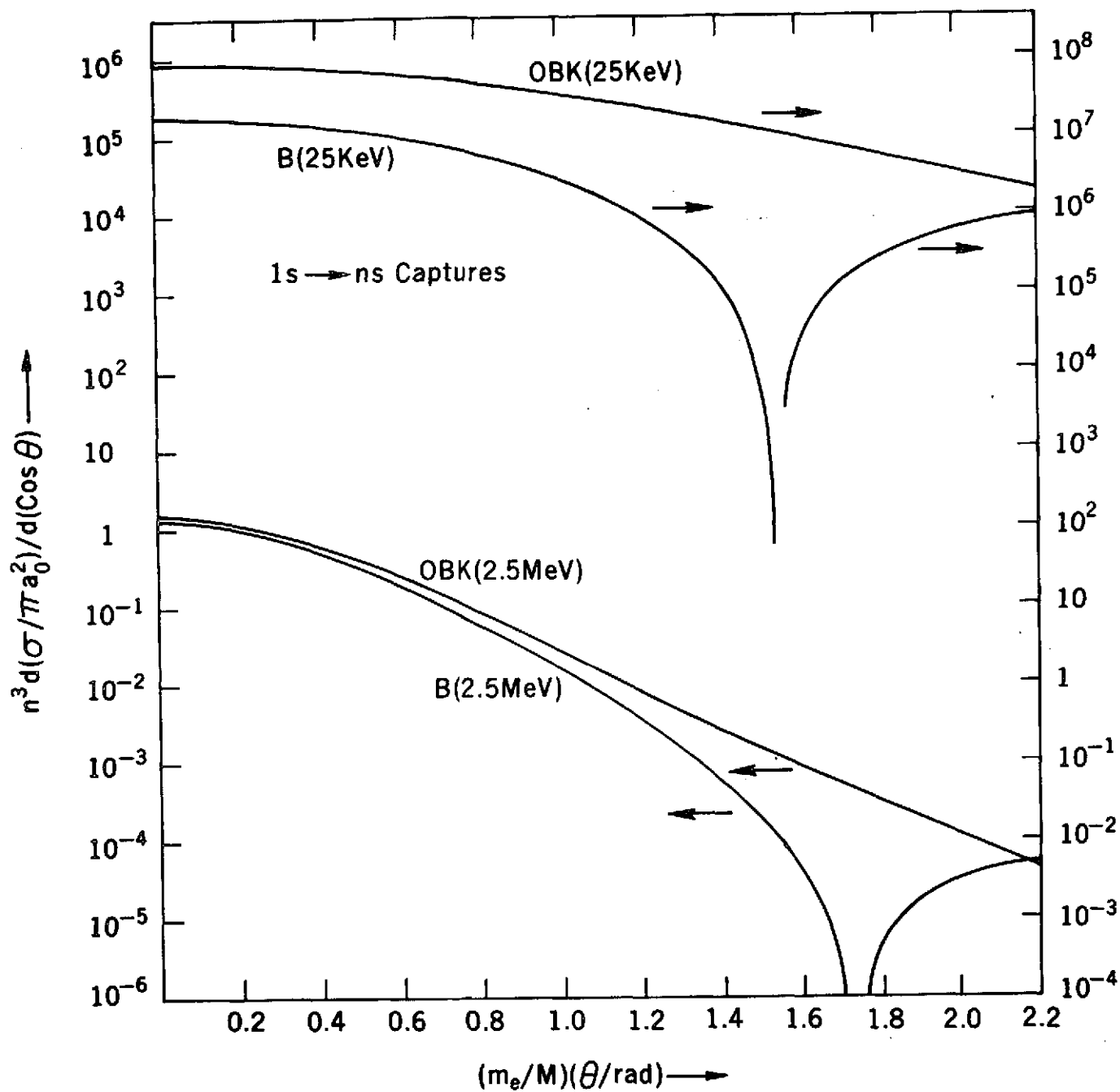


Figure 2

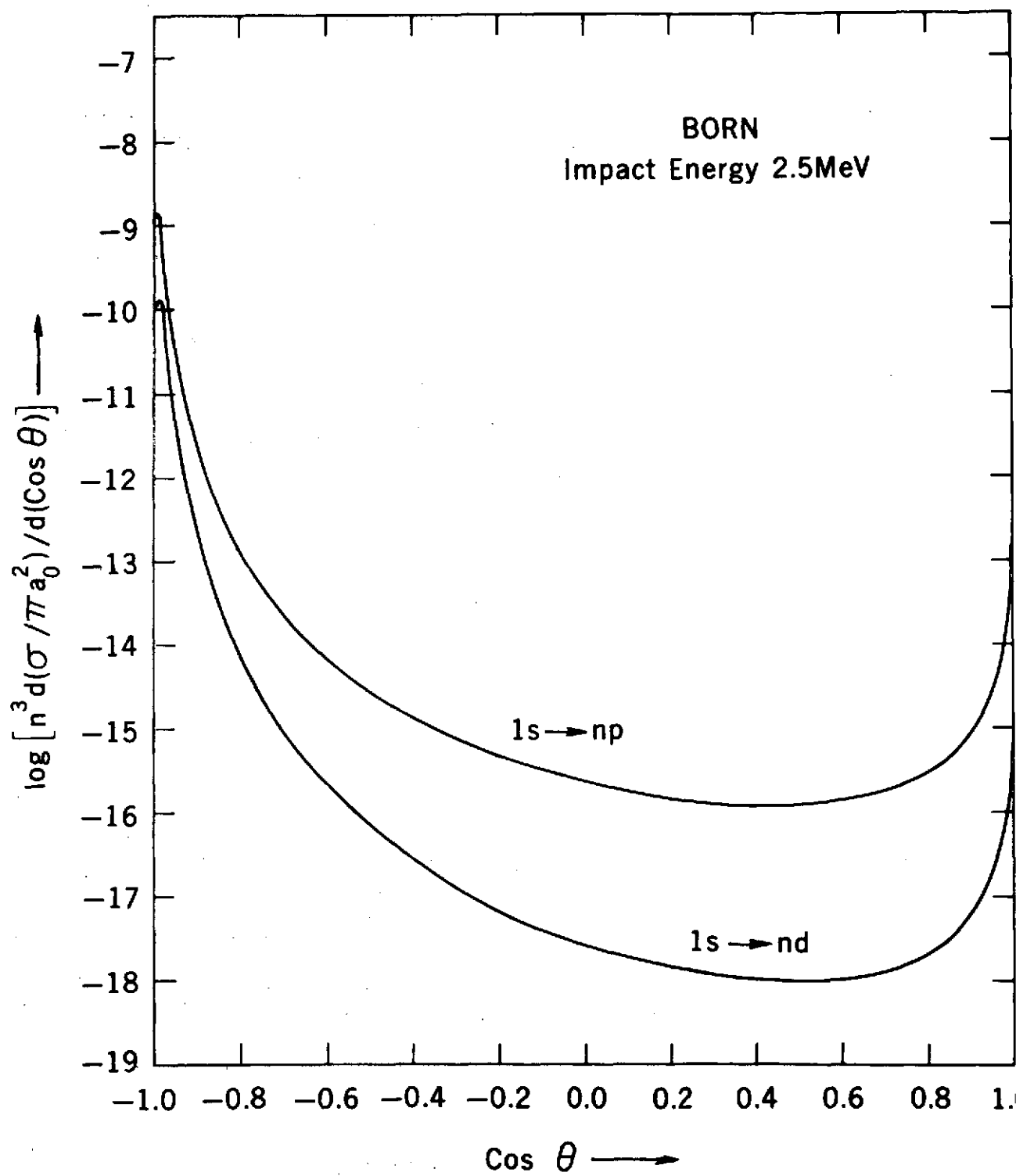


Figure 3

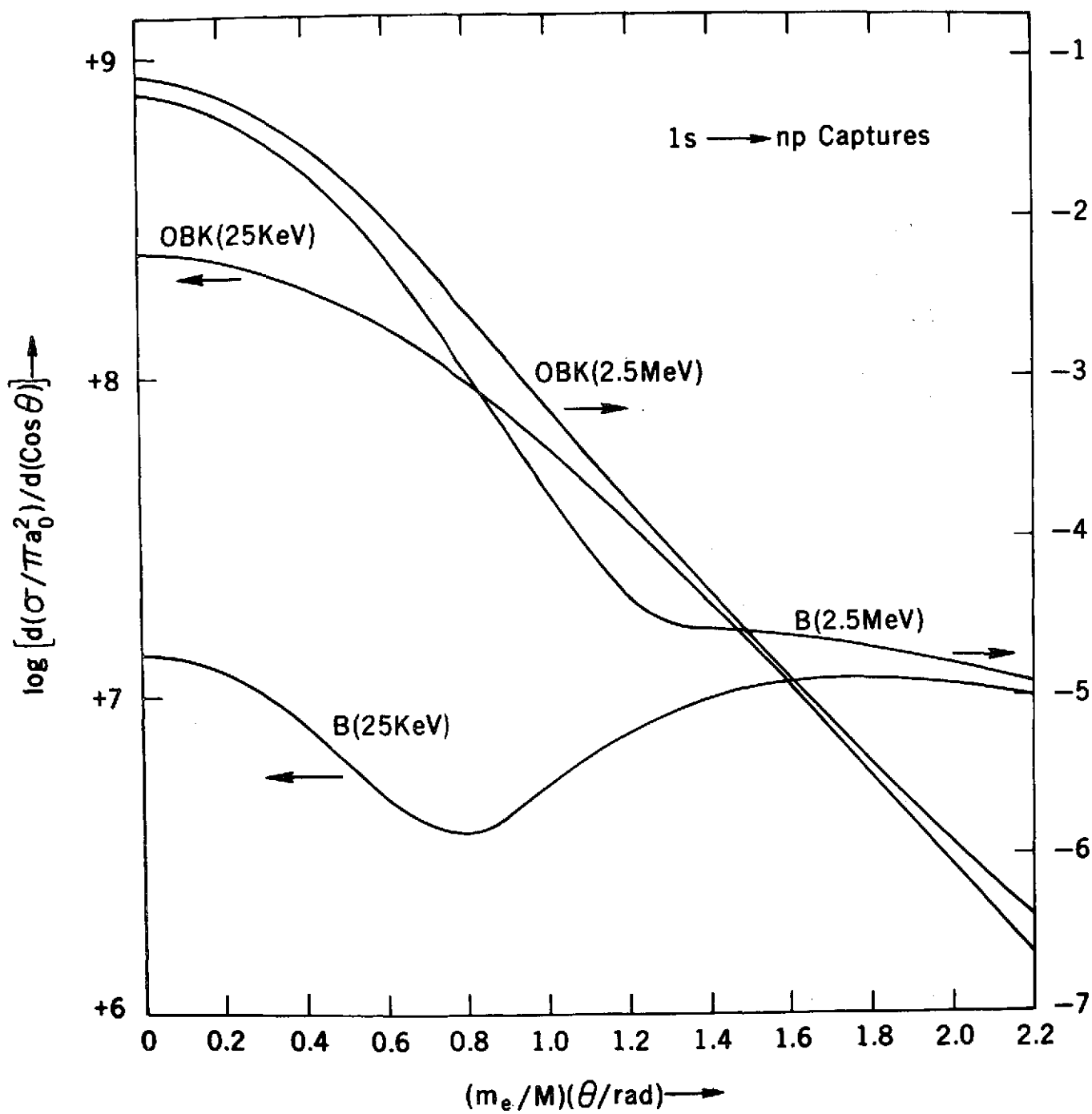


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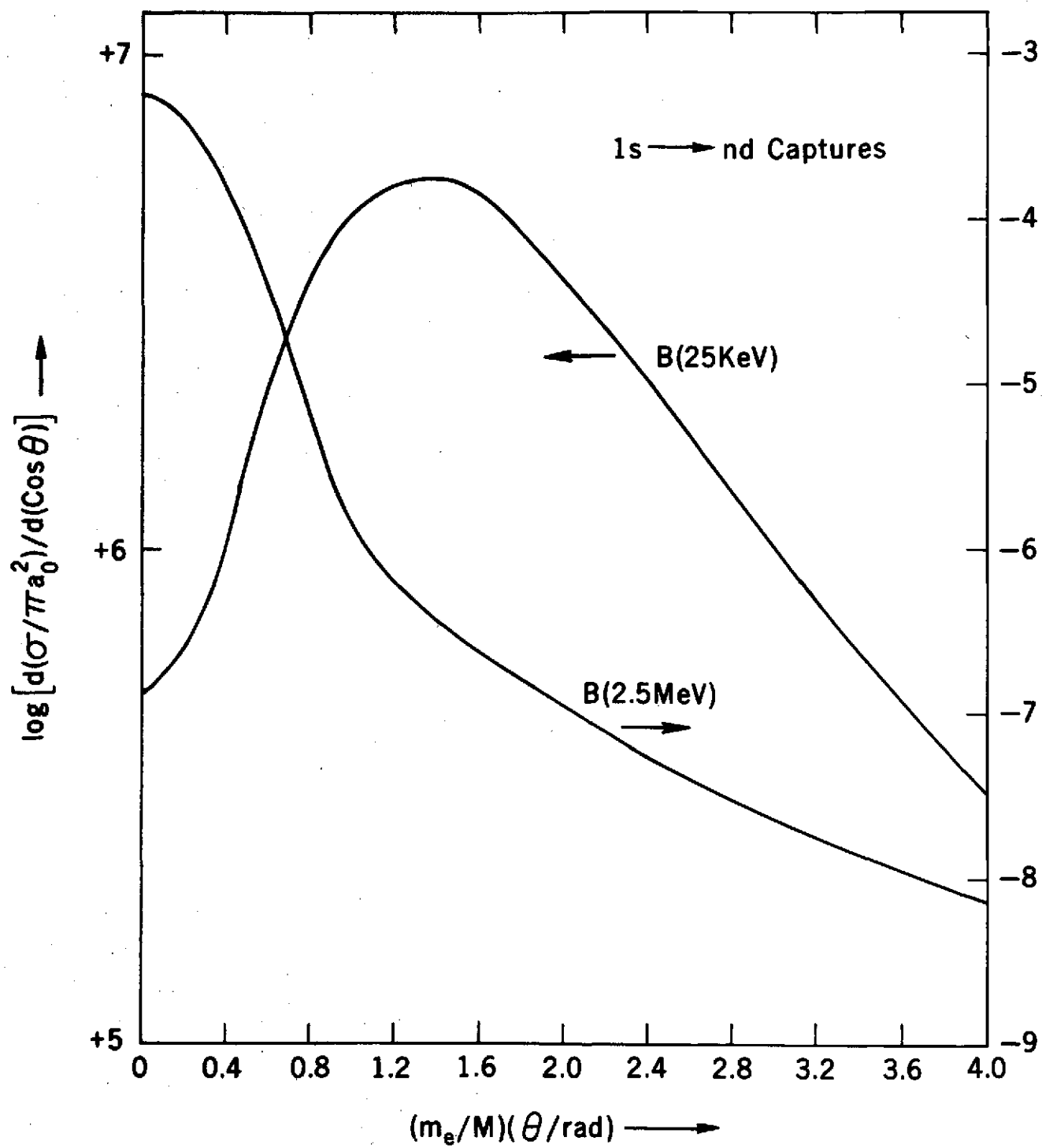


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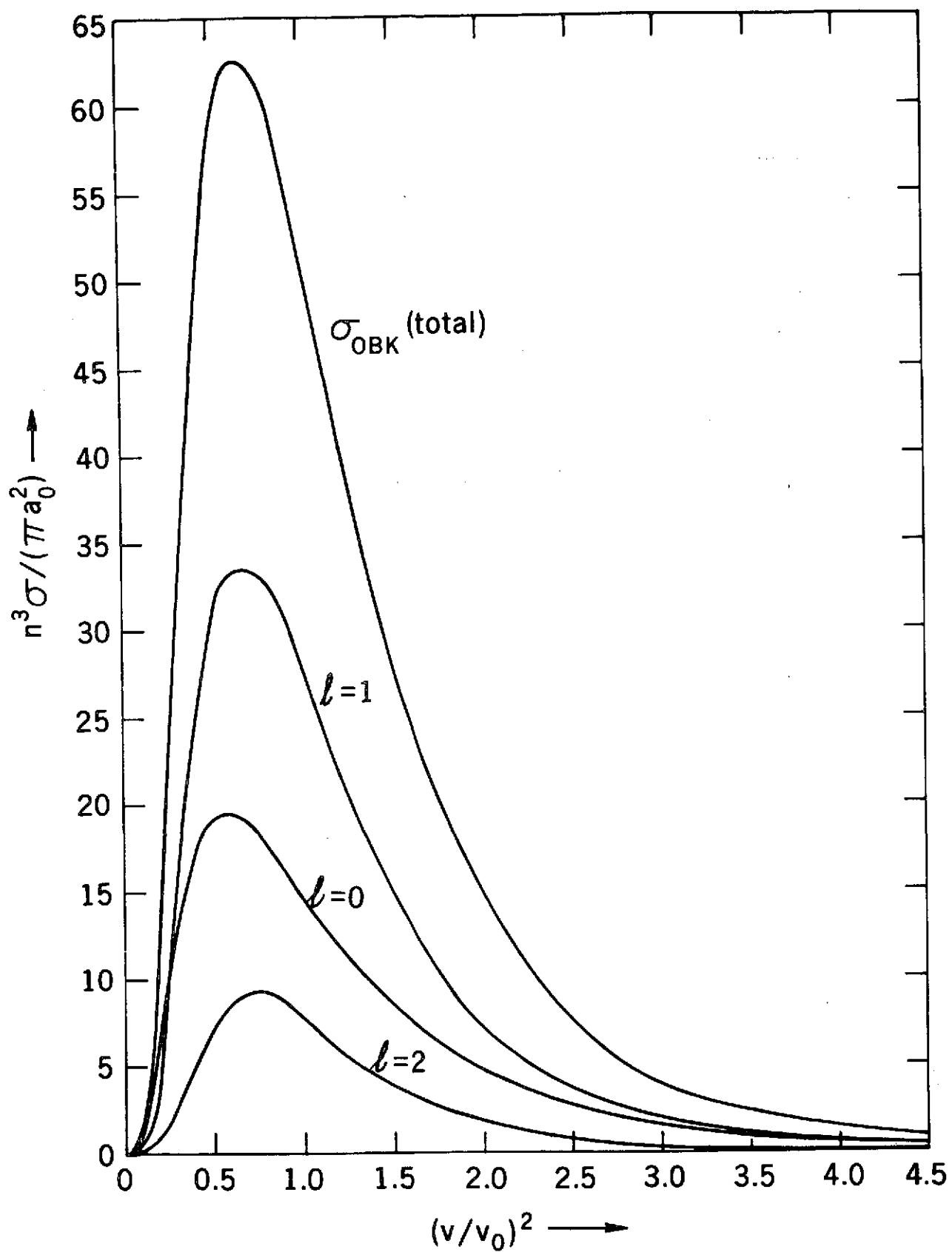


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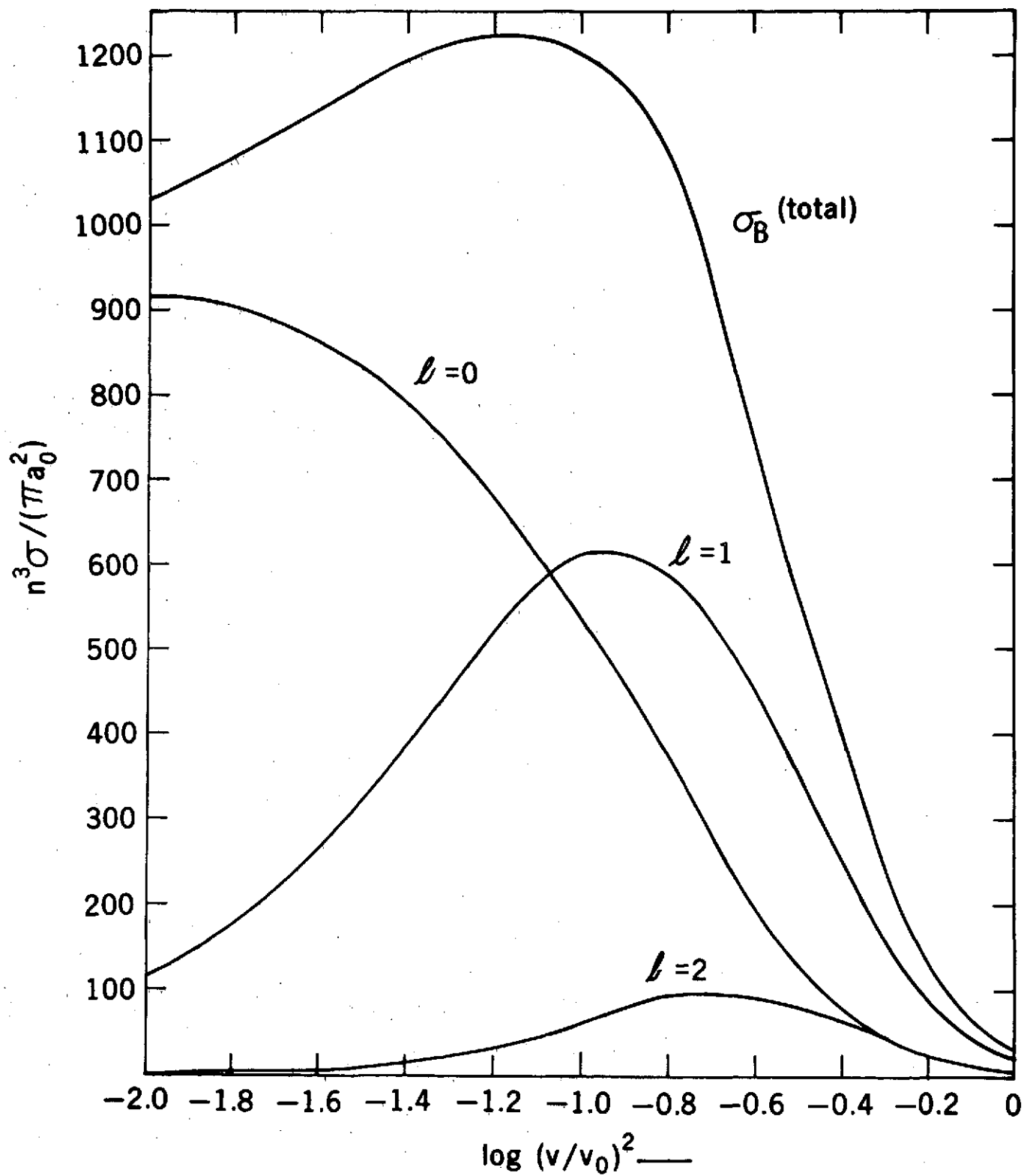


Figure 7

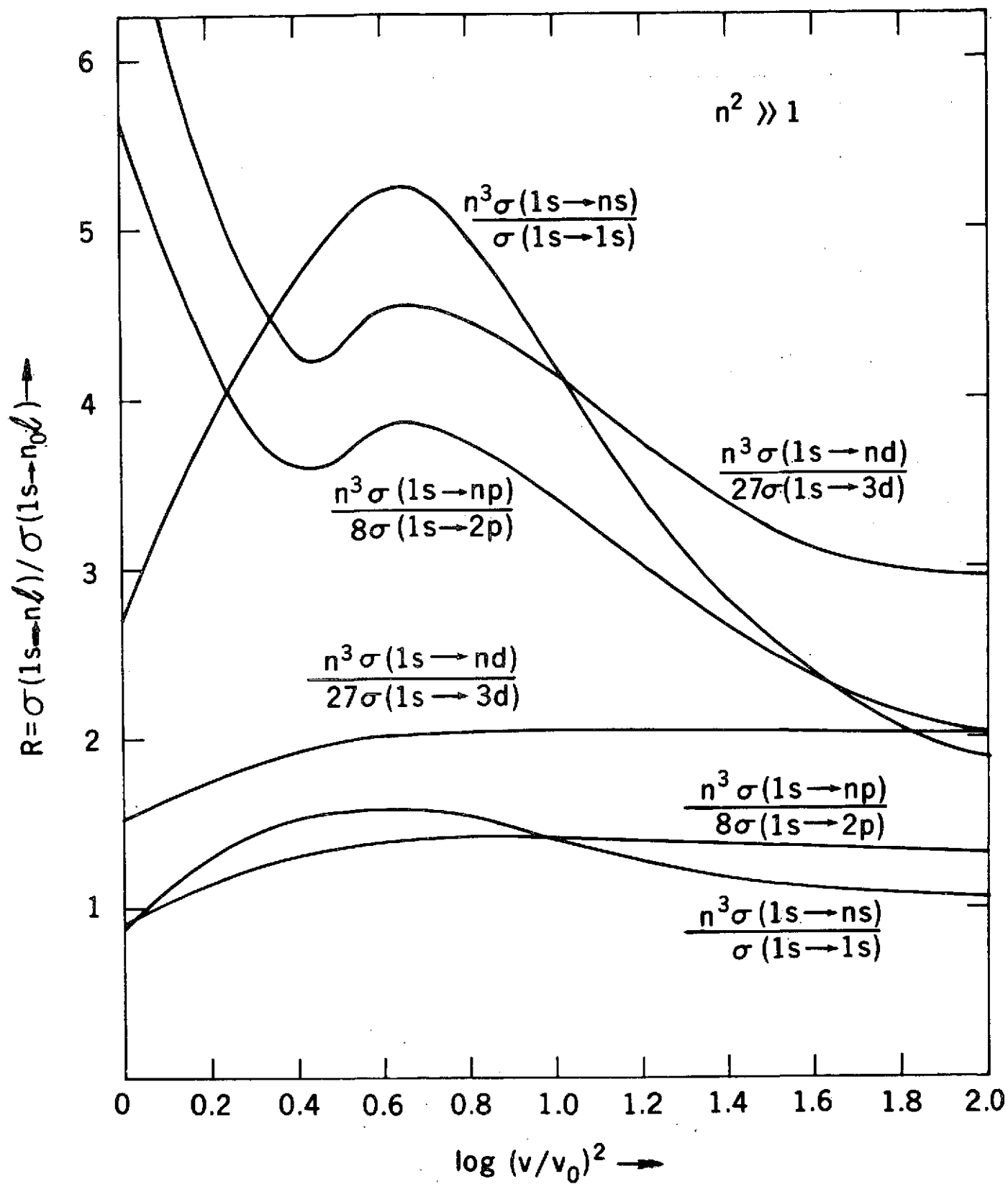


Figure 8

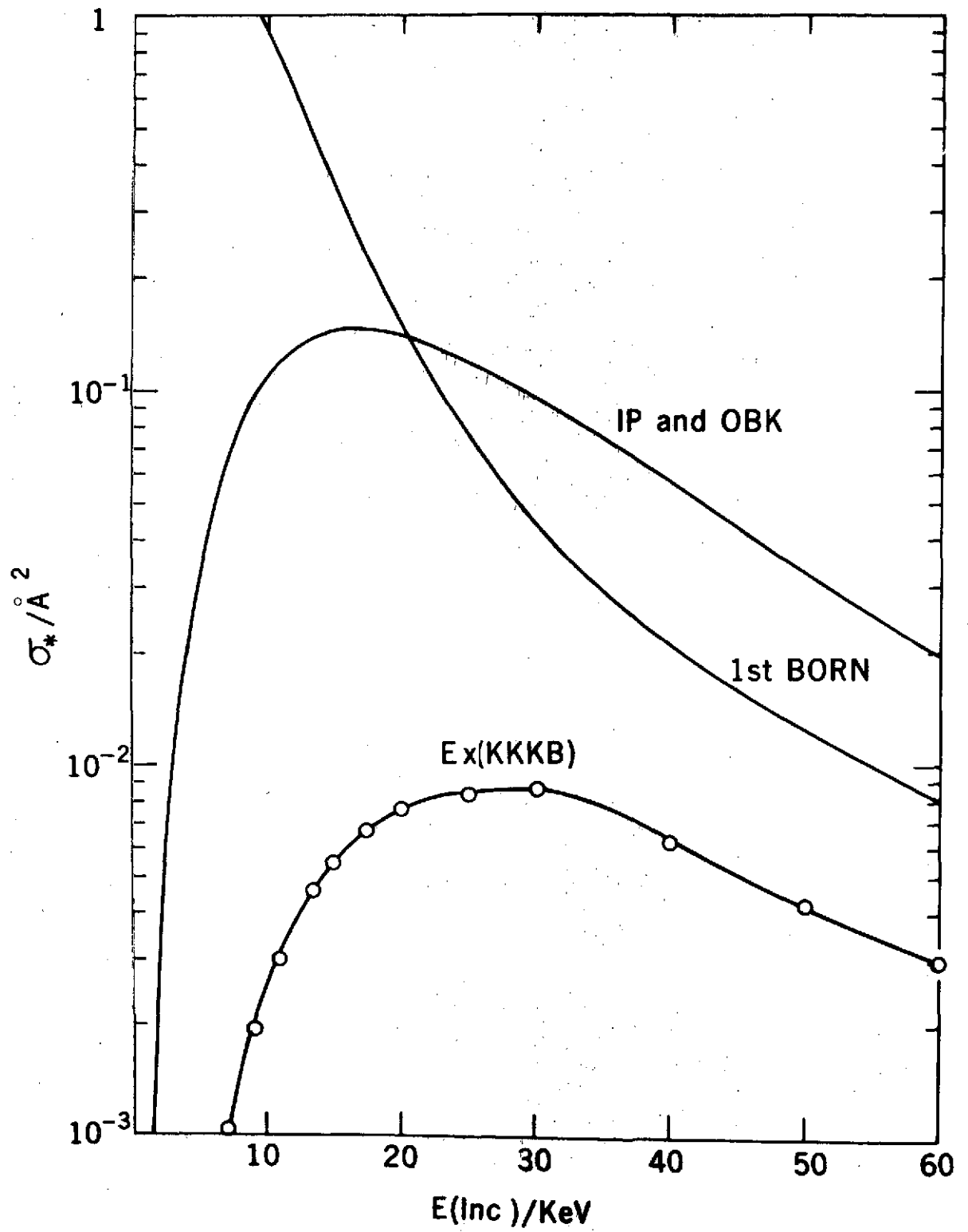


Figure 9