

certain impact parameters. The triplet curve (resulting from the *repulsive* triplet interaction) shows no such structure at smaller v ; however it shows a very smooth undulatory behavior at larger v , which must be a reflection of the wiping out of the attraction-repulsion of the singlet-triplet interactions at these energies by the rapidly oscillating momentum factors.

A few remarks are in order about the accuracy of the few results. The exchange potentials (the Coulomb potentials are exact since they are calculated from the analytic expressions of Flannery and Levy¹⁰) are accurate to about three places (see Ref. 1 for a discussion of the accuracy of the ground-state-ground-state curve), except for the $v = 2.0$ curves, which are accurate to about two places. The potentials were so time consuming that their range had to be spanned by only seven or eight points from $R = 0.5$ out, supplemented by points, as needed, to predict the united atom behavior for $R < 0.5$. A four-point Lagrangian inter-

polation was used to compute the potential between the calculated points as called for in the self-choosing step-size technique used to integrate Eq. (2), with a reproducibility of from 1 to 5% at intermediate impact parameters and as high as 10% at small B ($B < 1$). Of course the error in the amplitude is magnified when the probability is computed, so that for small probabilities these results can be no better than semiquantitative and quantitative for larger probabilities, although since the largest amount of error occurs for $B < 1$, the product of $B \times P(B)$ tends to reduce the error in the total cross section. In view of how little is known about these excitation collisions the accuracy of the present results are considered sufficient.

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Total Cross Sections for Inelastic Scattering of Charged Particles by Atoms and Molecules. V. Evaluation to the Next Order beyond the Bethe Asymptote*

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The Bethe procedure to obtain an asymptotic expression for the total cross section for inelastic scattering is extended to include three constants instead of the usual two. Within the first Born approximation, the third constant is essentially related to the total number of electrons in the target. By subtracting the sum of the cross sections for discrete excitations from the total cross section, the ionization cross section can also be given in an asymptotic form with three constants. The Mott formula is used to estimate the correction for electron exchange in the ionization cross section. The resulting cross sections compare favorably with experiments on the ionization of H, He⁺, H⁺, He, and Li⁺ by fast charged particles.

I. INTRODUCTION

The Bethe procedure¹⁻³ provides a convenient

method of expressing the first Born cross sections for individual excitation (or ionization) by charged particles in terms of a few atomic parameters,

which are uniquely determined from the generalized oscillator strengths (GOS). With these parameters, the dependence of the cross sections on the incident velocity can be factored out and a very compact expression is obtained.

Furthermore, sum rules for these parameters enable one to obtain the total inelastic scattering cross section in the form

$$\sigma_{\text{tot}} = A (\ln T) / T + B / T + C / T^2 + O(T^{-3}) , \quad (1)$$

where T is proportional to the square of the incident velocity (see Sec. II for definition), and A , B , and C are constants characteristic of the target atom. As was shown earlier,^{1,3} A can be computed from the ground-state wave function alone, and B requires a knowledge of the oscillator-strength distribution as well. In this paper, we show that the parameter C can be determined from the ground-state wave function alone.

Equation (1) with the first two constants, A and B , is accurate in the limit of fast incident particles. We shall refer to the two-term expression for the cross section as the Bethe asymptote. The usefulness of Eq. (1) is further extended to a lower-velocity region by the inclusion of the third constant. In fact, since other physical effects not included in the first Born approximation, such as electron exchange, target polarization, and distortion of the incident wave may contribute in σ_{tot} to the order of T^{-2} or even slightly larger, we expect that the practical value of the asymptotic expression (1) based on the first Born approximation is more or less exhausted by including the C term. We shall refer to the three-term expression for the cross section as the Born asymptote.

The Born asymptote is expected to be useful down to a region of relatively low velocity when the incident particle is not an electron, there being no exchange contribution to σ_{tot} . Moreover, knowledge of the contribution of the first Born approximation to the T^{-2} order is desirable for further extension of the theory.

Also, the Born asymptote for ionization can be obtained by subtracting the Born asymptote for discrete excitation from that for the total inelastic scattering in the same manner as has been illustrated in Refs. 4 and 5 to obtain the Bethe asymptotes for the ionization of He and Li*.

II. PRELIMINARIES

The GOS for the transition of an atom from state 0 (normally the ground state) to state n is defined by¹

$$f_n(Q) = (E_n/R) |\langle n | \sum_j e^{i\mathbf{K}\cdot\mathbf{r}_j} | 0 \rangle|^2 / Q , \quad (2)$$

where E_n is the excitation energy, R is the Rydberg energy, $\mathbf{K}\hbar$ is the momentum transfer, $Q = (Ka_0)^2$, a_0 is the Bohr radius, and the summation is over

all atomic electrons whose position vectors are \mathbf{r}_j .

The integrated cross section for excitation to the state n by a particle of charge ze and velocity v is then given by¹

$$\sigma_n = 4\pi a_0^2 z^2 R^2 (TE_n)^{-1} \int_{Q_1}^{Q_2} dQ f_n(Q) / Q , \quad (3)$$

where $T = \frac{1}{2}mv^2$, m being the electron mass, and Q_1 and Q_2 are the lower and upper limits of Q , respectively, which depend on both T and E_n .

Our treatment is nonrelativistic throughout. Elementary kinematics leads to

$$Q_1 = E_n^2 (4RT)^{-1} \{2 / [1 + (1-x)^{1/2}]\}^2 \quad (4a)$$

and

$$Q_2 = 4TM^2 (Rm^2)^{-1} \{[1 + (1-x)^{1/2}] / 2\}^2 , \quad (4b)$$

where

$$x = mE_n / MT \quad (5a)$$

and M is the reduced mass of the colliding system. The conservation of energy requires that

$$0 \leq x \leq 1 . \quad (5b)$$

The total cross section is defined as the sum of σ_n over all states n which are accessible energetically:

$$\begin{aligned} \sigma_{\text{tot}} &= \sum_n \sigma_n \\ &= 4\pi a_0^2 z^2 (R/T) D(T) , \end{aligned} \quad (6)$$

where

$$D(T) = \sum_n \int_{Q_1}^{Q_2} dQ g_n(Q) / Q \quad (7a)$$

and

$$g_n(Q) = f_n(Q) R / E_n . \quad (7b)$$

The procedure for the determination of the constant C in Eq. (1) is parallel to that for the so-called inner-shell correction to the stopping power.⁶ We are concerned with $\sum_n \sigma_n$ here instead of $\sum_n E_n \sigma_n$ for the stopping power. We shall denote the sum over energetically accessible states only (including the continua) by \sum_n , that over all states by \sum_{all} , and the difference by $\sum'_n = \sum_{\text{all}} - \sum_n$.

Then, as is shown in Paper I, the Bethe asymptote is given by

$$\sigma_{\text{Bethe}} = 4\pi a_0^2 z^2 (R/T) D_{\text{Bethe}}(T) , \quad (8)$$

where

$$\begin{aligned} D_{\text{Bethe}}(T) &= \sum_{\text{all}} \left(g_n(0) \ln \frac{4RT}{E_n^2} \right. \\ &\quad \left. + \int_0^1 dQ \frac{g_n(Q) - g_n(0)}{Q} + \int_1^\infty dQ \frac{g_n(Q)}{Q} \right) . \end{aligned} \quad (9)$$

The last two integrals in Eq. (9) correspond to $-I_2$

and I_1 , respectively, of Paper I. Our task is, therefore, to find the leading term (in powers of $1/T$) in the difference between $D(T)$ defined by Eq. (7a) and $D_{\text{Bethe}}(T)$ defined above.

For continuum states, the differential GOS, $df(E, Q)/dE$, and the corresponding quantity $dg(E, Q)/dE = (R/E)df(E, Q)/dE$ must be used. We shall also use shorthand notations for the dipole oscillator strengths $f_n = f_n(0)$ and $df/dE = df(E, 0)/dE$.

III. THEORY

In arriving at Eq. (9) from Eq. (7a), we have used essentially two approximations. The first is the replacement of \sum_n by \sum_{all} , thus including energetically inaccessible states. This introduces an error of the order of T^{-2} in σ_{tot} as is shown later. The second is the replacement of Q_1 by its approximate value $E_n^2/4RT$ [Eq. (4a)] and Q_2 by infinity, thus making the limits on both integrals in Eq. (9) independent of T and E_n . As is discussed later, the replacement of Q_1 results in an error of order T^{-2} in σ_{tot} , but that of Q_2 does not.

The exact $D(T)$ defined by Eq. (7a) can be written as

$$D(T) = \sum_n \left(-g_n(0) \ln Q_1 + \int_0^{Q_1} dQ \frac{g_n(Q) - g_n(0)}{Q} + \int_1^\infty dQ \frac{g_n(Q)}{Q} - \int_0^{Q_1} dQ \frac{g_n(Q) - g_n(0)}{Q} - \int_{Q_2}^\infty dQ \frac{g_n(Q)}{Q} \right). \quad (10)$$

The difference between $D(T)$ and $D_{\text{Bethe}}(T)$, therefore, is given by [see Eqs. (4a), (9), and (10)]

$$D(T) - D_{\text{Bethe}}(T) \equiv \Delta(T) = \sum_{j=1}^5 \Delta_j, \quad (11a)$$

where

$$\Delta_1 = -\sum_n' g_n(0) \ln \frac{4RT}{E_n^2}, \quad (11b)$$

$$\Delta_2 = -\sum_n' \left(\int_0^{Q_1} dQ \frac{g_n(Q) - g_n(0)}{Q} + \int_1^\infty dQ \frac{g_n(Q)}{Q} \right), \quad (11c)$$

$$\Delta_3 = -\sum_n g_n(0) \ln \left(\frac{2}{1 + (1-x)^{1/2}} \right)^2, \quad (11d)$$

$$\Delta_4 = -\sum_n \int_0^{Q_1} dQ \frac{g_n(Q) - g_n(0)}{Q}, \quad (11e)$$

and

$$\Delta_5 = -\sum_n \int_{Q_2}^\infty dQ \frac{g_n(Q)}{Q}. \quad (11f)$$

Note that Δ_1 and Δ_2 are well defined although the

sums refer to energetically inaccessible states, always in continua. Hence, the summation in Δ_1 and Δ_2 should actually represent integration of functions such as $Q^{-1} dg(E, Q)/dE$ over the excitation energy E .

A. Evaluation of Δ_1

According to Eq. (11b)

$$\Delta_1 = -\int_{E_m}^\infty dE \frac{df}{dE} \frac{R}{E} \left(\ln \frac{4T}{R} - 2 \ln \frac{E}{R} \right), \quad (12)$$

where E_m is an effective maximum for transferred energy and is of the order of T (see Sec. IIIB for details). Because $df/dE \sim E^{-3.5}$ for sufficiently large E ,⁷ we find that

$$\Delta_1 \sim O(E_m^{-3.5} \ln E_m) \sim O(T^{-3.5} \ln T), \quad (13)$$

which is much smaller than what we are interested in.

B. Evaluation of Δ_2

The integrals in Eq. (11c) can be evaluated exactly only if details of the GOS as a function of E and Q are known. We can evaluate, however, the leading terms only from physical considerations. We first note that, for large E , the GOS is sharply peaked near $Q = E/R$. In fact, in a three-dimensional plot of the GOS as a function of E and Q - we shall call it the Bethe surface⁸ - the peaks along the direction $Q = E/R$ are known as the Bethe ridge. The Bethe ridge, a feature common to all atoms and molecules, occurs because, for a sufficiently large energy transfer, the binding of the atomic electrons is insignificant and the momentum and the energy transferred become correlated as if the electrons were free.

Another important fact to note is the relationship of the Bethe ridge and the limits Q_1 and Q_2 as functions of E and T . As can be seen from Fig. 1, for light incident particles ($m/M \approx 1$), Q_1 and Q_2 are on opposite sides of the Bethe ridge for all accessible excitation energies. On the other hand, for heavy particles ($m/M \ll 1$), the lower limit Q_1 crosses the Bethe ridge (Fig. 2). Thus, for those states for which $4T \leq E \leq MT/m$, the range of integration over Q [see Eq. (3)] excludes the Bethe ridge.

The maximum energy transferred E_m is determined from Eq. (5a) as the energy for which $x = 1$, i. e.,

$$E_m = MT/m. \quad (14a)$$

For a positron $E_m \approx T$ and for heavy particles E_m is extremely large. Furthermore, for an electron, there is an added complication of what E_m should be to "exclude" the exchange effect in the first Born approximation. According to Rudge,⁹ the

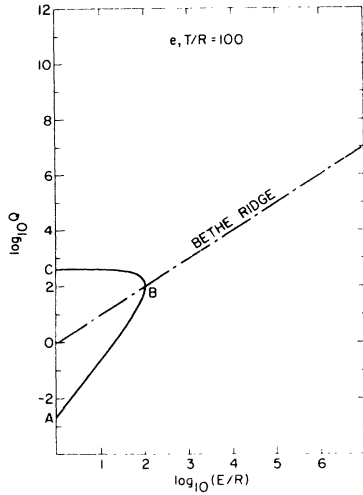


FIG. 1. Minimum (Q_1) and maximum (Q_2) of the square of momentum transfer [Eqs. (4)] as a function of excitation energy E for an incident electron of $T=100R$. (See Sec. II for notations.) The curve AB represents Q_1 and BC represents Q_2 . The Bethe ridge is along the line $Q = E/R$. For larger T , the triangular area ABC extends along the Bethe ridge with the point B ($Q_1 = Q_2$) always on the Bethe ridge.

choice of

$$E_m = I + \frac{1}{2}(T - I) \cong \frac{1}{2}T, \quad (14b)$$

I being the ionization potential, is consistent with "neglecting exchange" when the total spin of the colliding system is not specified. Following Rudge's notation,⁹ we shall refer to Born (a) when $E_m = T$ is used and Born (b) when Eq. (14b) is used.

The transitions to be summed in Eq. (11c) involve large energy transfers ($E > E_m$) in which the Bethe ridge plays a dominant role. Since the electron binding is of secondary importance in the Bethe-ridge region, the free-electron scattering, i. e., the Rutherford scattering, should be the leading contribution there. The Rutherford cross section for N free electrons is given by

$$\frac{d\sigma}{dE} = \frac{4\pi a_0^2 z^2 NR}{T/R E^2},$$

which is merely the continuum notation for σ_n defined by Eq. (3). If we use the Rutherford cross section in the second integral of Eq. (11c) [see Eq. (3) also], we get

$$\sum_n' \int_1^\infty dQ \frac{g_n(Q)}{Q} = \int_{E_m}^\infty dE \frac{NR}{E^2} = \frac{NR}{E_m}. \quad (15)$$

Formally, the same result is obtained by substituting in the left-hand side of Eq. (15) the GOS for free electrons defined as

$$\left. \frac{df(E, Q)}{dE} \right|_{\text{free}} = N\delta(QR - E). \quad (16)$$

The free-electron GOS, however, is only an idealization and in reality it should be replaced with a GOS peaked and concentrated near the Bethe ridge but with a finite width in Q of the order of $(IE)^{1/2}/R$, representing the uncertainty in the momentum transferred.⁸ By expanding Q^{-1} in the first integral of Eq. (15) around $Q = E/R$, one can easily see that the correction due to the binding will modify Eq. (15) by a multiplicative factor of the form $1 + O(I/E_m)$, and Eq. (15) is correct to the order given. For the hydrogen atom, Eq. (15) can be shown to be the correct leading term for the integral.

For the first integral in Eq. (11c), we first expand the integrand in the Taylor series convergent for $Q < E/R$:

$$\frac{dg(E, Q)}{dE} - \frac{dg(E, 0)}{dE} = \left(\frac{R}{E}\right) \left(\frac{Q}{dE} \frac{df'}{dE} + \frac{Q^2}{2!} \frac{df''}{dE} + \dots \right), \quad (17)$$

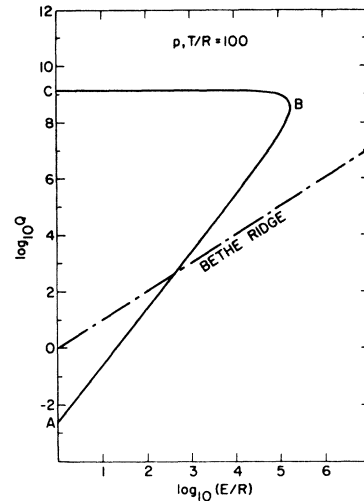


FIG. 2. Minimum and maximum of the square of momentum transfer as a function of excitation energy for an incident proton of $T=100R$. Notations are the same as those in Fig. 1. The Bethe ridge falls below Q_1 for $E \geq 4T$. For larger T , the area ABC expands in the direction of the Bethe ridge, but always in such a way that the curve for Q_1 crosses the Bethe ridge at $E \cong 4T$. Figures 1 and 2 are drawn to the same scale. Areas ABC in both figures represent parts of the Bethe surface contributing to σ_{tot} . The difference in σ_{tot} for incident electrons and protons appears only in the T^{-2} order [Eqs. (39)], mainly because the GOS is concentrated along the Bethe ridge for high E , and for low E in the area bounded by ABC of Fig. 1.

where

$$\frac{df'}{dE} = \frac{d}{dQ} \left. \frac{df(E, Q)}{dE} \right|_{Q=0},$$

and so on. For the hydrogen atom we find¹¹

$$\frac{df'}{dE} = \frac{df}{dE} \left(\frac{9R}{E} - \frac{8R^2}{E^2} \right), \quad (18)$$

$$\frac{df^{(k)}}{dE} \sim \frac{df}{dE} E^{-k} \sim E^{-(k+3.5)} \quad \text{for large } E. \quad (19a)$$

For an arbitrary atom, from Eqs. (1) and (10)-(12) of Ref. 7, it can be shown that, when $E \gg Q$ and $E > I$,

$$\frac{df(Q, E)}{dE} \sim E^{-3.5} F\left(\frac{Q}{E}\right), \quad (19b)$$

where $F(Q/E)$ is an unspecified but well-behaved function of Q/E . We assume that the asymptotic formula (19b) is attained uniformly in Q . Then, Eq. (19a) holds in general.

From Eqs. (17) and (19a) we get

$$\begin{aligned} \sum_n' \int_0^1 dQ \frac{g_n(Q) - g_n(0)}{Q} &= \int_{E_m}^{\infty} dE \int_0^1 dQ \frac{R}{E} \left(\frac{df'}{dE} + \dots \right) \\ &\sim O(T^{-4.5}), \end{aligned} \quad (20)$$

and from Eqs. (11c), (14), (15), and (20) we have

$$\Delta_2 = \begin{cases} -NR/T & \text{for } m/M = 1, \text{ Born (a)} \\ -2NR/T & \text{for } m/M = 1, \text{ Born (b)} \\ -NmR/MT & \text{for } m/M \ll 1 \end{cases} + O(T^{-2}). \quad (21)$$

C. Evaluation of Δ_3

From Eq. (11d) we obtain

$$\Delta_3 = -2 \sum_n g_n(0) \ln y(x), \quad (22)$$

where

$$y(x) = 2/[1 + (1-x)^{1/2}]. \quad (23)$$

For $0 < x \leq 1$, an inequality holds (see Appendix A):

$$\frac{1}{4}x + \frac{3}{32}x^2 < \ln y(x) \leq \frac{1}{4}x + (\ln 2 - \frac{1}{4})x^2. \quad (24)$$

With (24), Eq. (22) can be written as

$$\begin{aligned} \Delta_3 &= -\frac{1}{2} \sum_n g_n(0)x - \lambda \sum_n g_n(0)x^2 \\ &= -mR(2MT)^{-1} \sum_n f_n - \lambda (mR/MT)^2 \\ &\quad \times \sum_n f_n E_n/R, \end{aligned} \quad (25)$$

where

$$\frac{3}{16} < \lambda \leq 2(\ln 2 - \frac{1}{4}). \quad (26)$$

Since f_n is the dipole oscillator strength, we get from the well-known sum rules that^{7,12}

$$\begin{aligned} \sum_n f_n &= \sum_{a11} f_n - \sum_n' f_n \\ &= N + O(T^{-2.5}), \end{aligned} \quad (27)$$

and similarly

$$\sum_n f_n E_n/R = S(1) + O(T^{-1.5}), \quad (28)$$

where

$$S(1) = \sum_{a11} f_n E_n/R. \quad (29)$$

As is well known, the value of $S(1)$ is finite and of the order of the total energy of the atom.¹² From Eqs. (25)-(28) we conclude that

$$\Delta_3 = -NmR/2MT + O(T^{-2}). \quad (30)$$

D. Evaluation of Δ_4

In evaluating Δ_4 we must distinguish the type of incident particles. For light particles ($m/M \cong 1$), $Q_1 \leq E_n/R$ (Fig. 1) and the integrand of Eq. (11e) can be expanded in the Taylor series¹⁰ as is done for the first integral of Δ_2 (Sec. IIIB). Then the contribution Δ_{41} from the region $Q_1 < E_n/R$ is given by

$$\Delta_{41} = -\sum_n (R/E_n) (f_n' Q_1 + \frac{1}{4} f_n'' Q_1^4 + \dots), \quad (31)$$

where

$$f_n' = \left(\frac{d}{dQ} f_n(Q) \right)_{Q=0},$$

and so on. By substituting Eq. (4a) in the above, we have

$$\begin{aligned} \Delta_{41} &= -R(4T)^{-1} \sum_n f_n' E_n [y(x)]^2/R \\ &\quad - R^2(8T)^{-2} \sum_n f_n'' E_n^3 [y(x)]^4/R^3 + O(T^{-3}). \end{aligned} \quad (32)$$

Again we use an inequality (see Appendix A)

$$1 + \frac{1}{2}kx < [y(x)]^{2k} < 1 + (2^{2k} - 1)x, \quad (33)$$

which holds for $0 < x < 1$. We can write

$$[y(x)]^{2k} = 4^k (1/4^k + \mu_k x),$$

where μ_k is a function of x and is less than unity.

Then Eq. (32) becomes

$$\begin{aligned} \Delta_{41} &= -R(4T)^{-1} \sum_{a11} f_n' E_n/R + O(T^{-2}) \\ &= -S'(1)R/4T + O(T^{-2}), \end{aligned} \quad (34)$$

where

$$S'(1) = \sum_{a11} f_n' E_n/R.$$

In Eq. (34), the summation over states has been extended to infinity. But those states with $E_n > T$ do not contribute to the order of T^{-1} [Eq. (19)]. Also note that Eq. (34) applies both to Born (a) and

TABLE I. Values of $S'(1)$ [Eqs. (35) and (B3)].

Atom	H ^a	H ⁻ (1 ¹ S) ^b	He (1 ¹ S) ^c	Li ⁺ (1 ¹ S) ^c
$S'(1)$	1	2.1816	2.0468	2.0243

^aFor any state of any one-electron atom.

^bReference 18.

^cFrom the 53-term correlated wave functions by A. W. Weiss, J. Res. Natl. Bur. Std. U.S. 71A, 163 (1967).

(b) cross sections. As is shown in Appendix B, $S'(1)$ can be evaluated from the ground-state wave function alone, and

$$S'(1) = N + \text{small correction terms.} \quad (35)$$

Accurate values of $S'(1)$ for the ground states of H⁻, He, and Li⁺ are given in Table I.

Because $Q_1 \sim E_n^2/4TR$ [see Eq. (4a)], any attempt to extend the sum rule to terms with higher derivatives in the expansion for Δ_{41} will eventually encounter divergent expressions. For the hydrogen atom, the term with the fourth derivative in Eq. (31) will diverge when summed over all states [see Eq. (19a)]. By definition Δ_{41} is a finite quantity. This divergence, however, puts a limitation on the use of the sum-rule method in extending Eq. (1) to include higher powers of T^{-1} .

For heavy particles ($m/M \ll 1$), Q_1 crosses the

$$\Delta_4 = \begin{cases} -S'(1)R/4T & \text{for } m/M=1 \\ -[N+S'(1)]R/4T & \text{for } m/M=0 \end{cases} + O(T^{-2}). \quad (37a)$$

$$(37b)$$

E. Evaluation of Δ_5

The upper limit Q_2 in Eq. (7a) for energetically accessible states occurs far out from the Bethe ridge for heavy particles (Fig. 2), and for light particles the significant part of the GOS still occurs for $Q < Q_2$ (Fig. 1). Thus, we may safely use the known asymptotic dependence⁷ of the GOS for large Q :

$$\gamma_{\text{tot}} = T\Delta(T)/R = \begin{cases} -N[\frac{3}{2} + S'(1)/4N] & \text{for } m/M=1, \text{ Born (a),} \\ -N[\frac{5}{2} + S'(1)/4N] & \text{for } m/M=1, \text{ Born (b),} \\ -N[\frac{1}{4} + S'(1)/4N] & \text{for } m/M=0 \end{cases} + O(T^{-1}), \quad (39a)$$

$$(39b)$$

$$(39c)$$

and the Born asymptote for total inelastic scattering is given by

$$\sigma_{\text{tot}} = 4\pi_0^2 z^2 (R/T) [M_{\text{tot}}^2 \ln(4c_{\text{tot}} T/R) + \gamma_{\text{tot}} R/T], \quad (40)$$

Bethe ridge at $E_x \cong 4T$ (Fig. 2). The summation over states in Δ_4 [Eq. (11e)] now must be divided into two parts; the region in which $E_n < E_x$, and that in which $E_x \leq E_n \leq E_m$, E_m being defined by Eq. (14a). For the former region, the integrand is expanded in the Taylor series as is done for the case of light particles and the result is given by Δ_{41} , Eq. (34). For the latter region ($E_x \leq E \leq E_m$), the range of integration over Q includes the Bethe ridge (Fig. 2), and the integrand of Eq. (11e) is replaced by the free-electron result [Eq. (16)]. The contribution from the second region is then given by

$$\Delta_{42} = -\int_{E_x}^{E_m} dE \int_0^{Q_1} dQ \frac{NR\delta(QR-E)}{EQ} = NR \left(\frac{1}{E_m} - \frac{1}{E_x} \right). \quad (36a)$$

Note that the NR/E_m term exactly cancels the contribution from Δ_2 [Eq. (21)], and that $E_x = 4T [1 + O(m/M)]$. For all practical purposes, however, we may set $m/M = 0$. With this approximation

$$\Delta_{42} = -NR/4T + O(T^{-2}) \quad \text{for } m/M=0. \quad (36b)$$

From Eqs. (34) and (36b), we now have

$$f_n(Q) \sim Q^{-k}, \quad k \geq 5$$

to conclude from Eqs. (4b) and (11f) that

$$\Delta_5 \sim O(T^{-5}). \quad (38)$$

IV. BORN ASYMPTOTES

We now have, from Eqs. (11a), (13), (21), (30), (37), and (38),

where constants M_{tot}^2 and c_{tot} are defined in Paper I. When high accuracy is not required, we can simplify Eqs. (39) by setting $S'(1) = N$ [see Eq. (35) and Table I]:

$$\gamma_{\text{tot}} \cong \begin{cases} -7N/4 & \text{for } m/M=1, \text{ Born (a),} & (41a) \\ -11N/4 & \text{for } m/M=1, \text{ Born (b),} & (41b) \\ -N/2 & \text{for } m/M=0. & (41c) \end{cases}$$

From our limited experience on the two-electron atoms (Table I), the correction terms in Eq. (35) amount to less than 10% of N . For most atoms Eqs. (41) may be used unless both M_{tot}^2 and c_{tot} are known accurately.

Once we have the total cross section to the T^{-2} order, we can proceed to evaluate the ionization cross section to the same order by subtracting the sum of the discrete excitation cross sections as we have done for the Bethe asymptote (see Papers III and IV). To this end, the excitation cross section must be evaluated also to the T^{-2} order. It is done simply by summing the terms labeled as γ in Ref. 13, i. e.,

$$\gamma_n = -f_n m/2M - f'_n E_n/4R$$

both for the optically allowed and forbidden transitions. Note that those transitions for which the orbital angular momentum changes by more than two units (such as an $S \rightarrow F$ transition) do not contribute to γ_n because both f_n and f'_n vanish by selection rules [see Eqs. (5) and (6) of Ref. 13]. Hence,

$$\gamma_{\text{ex}} = \sum_{\text{discrete}} \gamma_n = -\frac{S_{\text{ex}}(0)m}{2M} - \frac{S'_{\text{ex}}(1)}{4}, \quad (42a)$$

where

$$S_{\text{ex}}(0) = \sum_{\text{discrete}} f_n \quad (42b)$$

and

$$S'_{\text{ex}}(1) = \sum_{\text{discrete}} \frac{f'_n E_n}{R}. \quad (42c)$$

Equation (42a) is valid for an arbitrary mass unlike Eqs. (39) and (41).

In the notations used previously,^{4,5} the Born asymptotes for excitation and ionization are given, respectively, by

$$\sigma_{\text{ex}} = 4\pi a_0^2 z^2 (R/T) [M_{\text{ex}}^2 \ln(4c_{\text{ex}} T/R) + \gamma_{\text{ex}} R/T], \quad (43a)$$

$$\sigma_i = 4\pi a_0^2 z^2 (R/T) [M_i^2 \ln(4c_i T/R) + \gamma_i R/T], \quad (43b)$$

where

$$M_i^2 = M_{\text{tot}}^2 - M_{\text{ex}}^2, \quad (44a)$$

$$M_i^2 \ln c_i = M_{\text{tot}}^2 \ln c_{\text{tot}} - M_{\text{ex}}^2 \ln c_{\text{ex}}, \quad (44b)$$

and

$$\gamma_i = \gamma_{\text{tot}} - \gamma_{\text{ex}}. \quad (44c)$$

V. APPLICATIONS

A. Application to H(1s)

For the hydrogen atom in the ground state, Bethe¹ has shown that $M_{\text{tot}}^2 = 1$, $\ln c_{\text{tot}} = 0.4495$, and, from Table I, $S'(1) = 1$. By substituting these values in Eqs. (39) and (40), we get

$$\sigma_{\text{tot}} = 4\pi a_0^2 z^2 (R/T) [\ln(T/R) + 1.836 + \gamma_{\text{tot}} R/T], \quad (45a)$$

with

$$\gamma_{\text{tot}} = \begin{cases} -\frac{7}{4} & \text{for } m/M=1, \text{ Born (a),} & (45b) \\ -\frac{11}{4} & \text{for } m/M=1, \text{ Born (b),} & (45c) \\ -\frac{1}{2} & \text{for } m/M=0. & (45d) \end{cases}$$

All but one constant for the Born asymptote for excitation are known: $M_{\text{ex}}^2 = 0.7166$, $\ln c_{\text{ex}} = -0.5780$, and $S_{\text{ex}}(0) = 0.5650$. The value of $S'_{\text{ex}}(1)$ can be readily calculated from Eq. (18) and the data in Ref. 14:

$$\begin{aligned} S'_{\text{ex}}(1) &= 9S_{\text{ex}}(0) - 8S_{\text{ex}}(-1) \\ &= -0.6477, \end{aligned}$$

where

$$S_{\text{ex}}(-1) = \sum_{\text{discrete}} \frac{f_n R}{E_n}.$$

By substituting these values in Eq. (42a), we get¹⁴

$$\begin{aligned} \sigma_{\text{ex}} &= 4\pi a_0^2 z^2 (R/T) [0.7166 \ln(T/R) + 0.5792 \\ &\quad - 0.1206 R/T] \quad \text{for } m/M=1 \\ &= 4\pi a_0^2 z^2 (R/T) [0.7166 \ln(T/R) + 0.5792 \\ &\quad + 0.1619 R/T] \quad \text{for } m/M=0. \end{aligned} \quad (46)$$

By subtracting Eq. (46) from Eqs. (45), we find

$$\sigma_i = 4\pi a_0^2 z^2 (R/T) [0.2834 \ln(T/R) + 1.2566 + \gamma_i R/T], \quad (47a)$$

with

$$\gamma_i = \begin{cases} -1.6294 & \text{for } m/M=1, \text{ Born (a),} & (47b) \\ -2.6294 & \text{for } m/M=1, \text{ Born (b),} & (47c) \\ -0.6619 & \text{for } m/M=0. & (47d) \end{cases}$$

To verify the usefulness of the Born asymptote, we compare in Fig. 3 the ionization cross section by electron impact. We find that Eq. (47b) reproduces the exact Born (a) cross section¹⁵ (calculated directly from the ground-state and continuum wave functions) within 1% when $T \geq 15R$, whereas the Bethe asymptote alone reproduces the exact cross section to a similar precision only when $T \geq 60R$.

For a hydrogenic ion of nuclear charge Ze , the

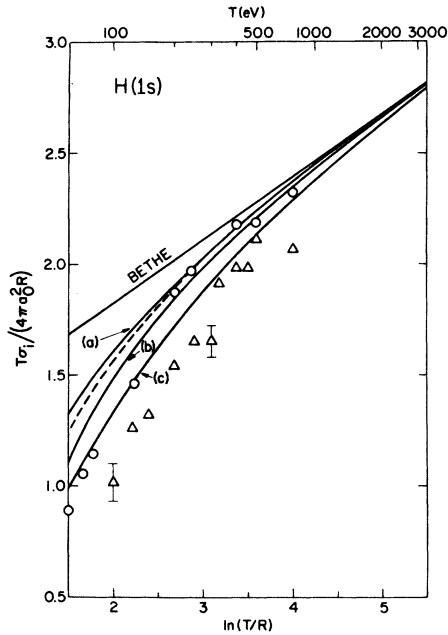


FIG. 3. Cross sections for the ionization of H (1s) by electron. For electrons, T is the incident energy. The solid line labeled BETHE represents the Bethe asymptote, and the solid curves labeled (a), (b), and (c) corresponds to the Born (a), Born (b), and Born plus free-electron exchange cross sections, respectively. The dotted curve represents the exact Born (a) cross section calculated directly from the ground state and the continuum wave functions by Omidvar (Ref. 15). The circles are the experimental data by Fite and Brackmann (Ref. 33), and the triangles are those by Rothe *et al.* (Ref. 34), both of which were normalized to the absolute measurement of the ionization cross section of H_2 by Tate and Smith [Phys. Rev. **39**, 270 (1932)]. The error limits quoted are random errors.

constants for the Bethe cross section [see Eqs. (40) and (43)] M^2 and $\ln c$ become M^2/Z^2 and $\ln(c/Z^2)$ respectively.¹⁵ The γ terms, however, are invariant, as is evident from the discussions in Sec. III.

Comparison of the Born ionization cross section with experiment has been thoroughly discussed in the literature already.⁹ We defer our comments until Sec. VE.

B. Application to $H^-(1^1S)$

Since the publication of Ref. 16, more accurate theoretical data have become available on the Bethe cross section of H^- . Rotenberg and Stein¹⁷ gave the value $I_1 - I_2 = -10.665$ [see Eq. (9)] evaluated from a correlated wave function with proper asymptotic behavior. We also obtained $I_1 - I_2 = -10.598$ from a 39-term correlated wave function by Weiss.¹⁸ The former value is likely to be more accurate, and the uncertainty in the value of B in Eq. (1) is reduced by a factor of $\frac{1}{3}$ from that given in Paper II. With the new data and the value of $S'(1)$ from

Table I, the Born asymptote for H^- becomes

$$\sigma_{\text{tot}} = 4\pi a_0^2 z^2 (R/T) [7.484 \ln(T/R) + 25.11 + \gamma_{\text{tot}} R/T], \quad (48a)$$

with

$$\gamma_{\text{tot}} = \begin{cases} -3.545 & \text{for } m/M=1, \text{ Born (a), (48b)} \\ -5.545 & \text{for } m/M=1, \text{ Born (b), (48c)} \\ -1.045 & \text{for } m/M=0. \quad (48d) \end{cases}$$

In Fig. 4, we compare the Born (b) cross section with the electron-impact data by Dance, Harrison, and Rundel,¹⁹ by Tisone and Branscomb,²⁰ and also those by Peart, Walton, and Dolder.²¹ As is stated in Paper II, our cross section includes the double detachment $e + H^- \rightarrow H^+ + 3e$ and is an upper limit to the experimental single-detachment cross section. As we also have noted in Paper II, the experimental data by Tisone and Branscomb²⁰ do not exhibit proper asymptotic behavior, but they agree well with those by Dance, Harrison, and Rundel¹⁹ in the low-energy region ($T \leq 60$ eV). If we extrapolate the experience on the hydrogen atom (Sec. VA), we ex-

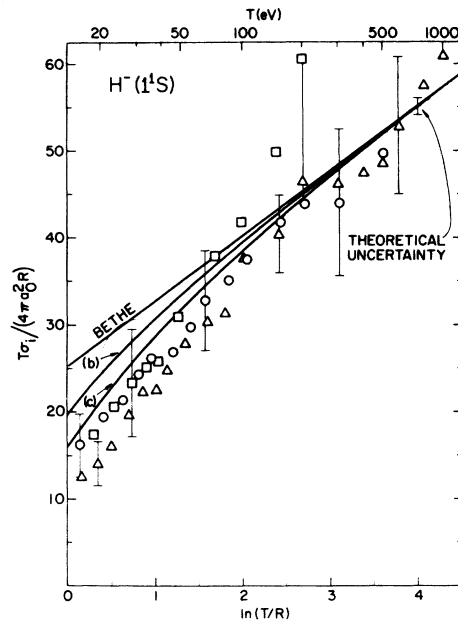


FIG. 4. Cross sections for the electron detachment of $H^-(1^1S)$ by electron. The labels on the solid curves are the same as those in Fig. 3. The circles represent the experimental data by Dance, Harrison, and Rundel (Ref. 19), the squares those by Tisone and Branscomb (Ref. 20), and the triangles those by Peart, Walton, and Dolder (Ref. 21). All experiments measured the single-detachment cross section, and the theory corresponds to the simple sum of the single- and double-detachment cross sections. Experimental errors quoted are the sum of random and systematic errors.

pect Eqs. (48) to represent the exact Born cross sections for $T \geq 20$ eV. It is evident from Fig. 4, therefore, that the first Born approximation alone is not sufficient to explain the experimental cross section for $T \leq 100$ eV.

C. Application to He (1^1S)

With the values of the Bethe cross sections in Papers I and III and that of $S'(1)$ from Table I, the Born asymptote for the total inelastic scattering by He becomes

$$\sigma_{\text{tot}} = 4\pi a_0^2 z^2 (R/T) [0.7525 \ln(T/R) + 0.6628 + \gamma_{\text{tot}} R/T], \quad (49a)$$

with

$$\gamma_{\text{tot}} = \begin{cases} -3.512 & \text{for } m/M=1, \text{ Born (a),} & (49b) \\ -5.512 & \text{for } m/M=1, \text{ Born (b),} & (49c) \\ -1.012 & \text{for } m/M=0. & (49d) \end{cases}$$

The values of γ_n for most important discrete excitations are given in Refs. 13 and 22. For higher excitations we have adopted extrapolation formulas for γ_n as functions of effective quantum numbers (Table II). The sum of the limiting values of γ_n as $n \rightarrow \infty$ in Table II matches very well with the sum deduced from the measured GOS at the ionization threshold,²³ providing a strong support for our extrapolation procedure. The Born asymptote for the sum of discrete excitations thus obtained is

$$\sigma_{\text{ex}} = 4\pi a_0^2 z^2 (R/T) [0.2633 \ln(T/R) - 0.0514 + \gamma_{\text{ex}} R/T], \quad (50a)$$

with

$$\gamma_{\text{ex}} = \begin{cases} 0.007 & \text{for } m/M=1, & (50b) \\ 0.197 & \text{for } m/M=0. & (50c) \end{cases}$$

TABLE II. Adopted values of γ_n for He.^{a,b}

Excited states	$\gamma_n^{(e)}$	1P	1S	1D
		$\gamma_n^{(\infty)}$	γ_n	γ_n
$n=2$	0.0376	0.1755	-0.0317	
3	0.0255	0.0392	-0.0072	-0.0041
4	0.0002	0.0152	-0.0027	For $n \geq 4$,
≥ 5	$-0.029(n^*)^{-3}$ $+0.63(n^*)^{-5}$	$0.886(n^*)^{-3}$ $+1.64(n^*)^{-5}$	$-0.152(n^*)^{-3}$ $-0.0575(n^*)^{-5}$ $-0.625(n^*)^{-7}$	$-0.1683(n^*)^{-3}$ $-0.499(n^*)^{-5}$
Σ_n	0.0630	0.2524	-0.0456	-0.0101

^aNotations: $\gamma_n^{(e)} = \gamma_n$ for $m/M=1$, $\gamma_n^{(\infty)} = \gamma_n$ for $m/M=0$, $n^* = n + \delta$, where $\delta = 0.0121$, -0.140 , and -0.00209 for the 1P , 1S , and 1D states, respectively.

^bSources Refs. 13 and 22; W. J. B. Oldham, Jr., Phys. Rev. **174**, 145 (1968); **181**, 463 (1969); Ref. 7 of Paper III.

By subtracting Eqs. (50) from Eqs. (49), we get the Born asymptote for the ionization of He:

$$\sigma_i = 4\pi a_0^2 z^2 (R/T) [0.489 \ln(T/R) + 0.714 + \gamma_i R/T], \quad (51a)$$

with

$$\gamma_i = \begin{cases} -3.519 & \text{for } m/M=1, \text{ Born (a),} & (51b) \\ -5.519 & \text{for } m/M=1, \text{ Born (b),} & (51c) \\ -1.209 & \text{for } m/M=0. & (51d) \end{cases}$$

The ionization cross section given by Eqs. (51) is in very close agreement down to $T \geq 150$ eV with the Born cross sections calculated directly from continuum wave functions by Bell and Kingston,²⁴ and also by Economides and McDowell.²⁵ Equations (51), however, are more accurate in the high-energy region $T \geq 700$ eV. In our method, the γ_i term and higher orders not included in the Born asymptote become less significant as T is increased, whereas in the partial-wave method used in Refs. 24 and 25, the difficulty increases as higher partial waves contribute substantially. Some typical experimental data²⁶⁻²⁸ are compared with our results in Fig. 5. By virtue of sum rules, our σ_i is a simple sum of the single- and double-ionization cross sections and should represent an upper limit to the experimental data on single-ionization events. Some experiments measure the current of ejected electrons and hence count the double ionization with twice the weight given to the single ionization. For He, however, the single ionization is by far the dominant process and the double ionization can safely be neglected in the comparison with experiment. Among many electron-impact experiments, the Born (b) cross section supports the high-energy dependence apparent in the data by Smith,²⁶ confirming the conclusion drawn in Paper III.

D. Application to Li (1^1S)

From the value of $S'(1)$ in Table I and the Bethe asymptote in Paper IV, we get for the total inelastic scattering

$$\sigma_{\text{tot}} = 4\pi a_0^2 z^2 (R/T) [0.2860 \ln(T/R) - 0.031 + \gamma_{\text{tot}} R/T], \quad (52a)$$

with

$$\gamma_{\text{tot}} = \begin{cases} -3.506 & \text{for } m/M=1, \text{ Born (a),} & (52b) \\ -5.506 & \text{for } m/M=1, \text{ Born (b),} & (52c) \\ -1.006 & \text{for } m/M=0. & (52d) \end{cases}$$

For the discrete excitation, we have from Paper IV and Table III

$$\sigma_{\text{ex}} = 4\pi a_0^2 z^2 (R/T) [0.1415 \ln(T/R)$$

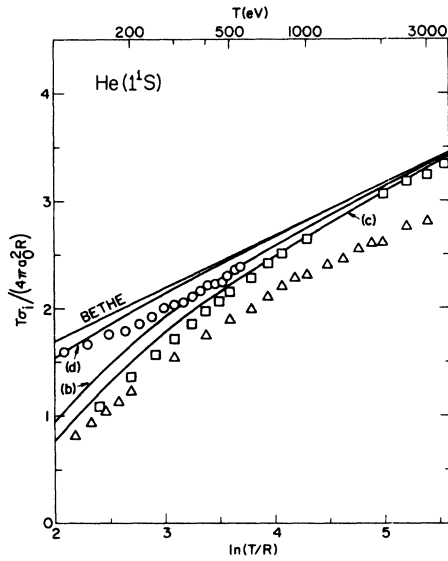


FIG. 5. Cross sections for the ionization of He (1^1S). The curve labeled (d) shows the cross section for ionization by heavy particle ($M=\infty$) and other labels are the same as those in Fig. 3. The circles represent the proton-impact experiment by Hooper *et al.* (Ref. 28), the squares represent the electron-impact experiment by Smith (Ref. 26), and the triangles that by Schram *et al.* (Ref. 27).

$$-0.168 + \gamma_{\bullet x} R/T], \quad (53a)$$

with

$$\gamma_{\bullet x} = \begin{cases} -0.067 & \text{for } m/M=1, \\ -0.270 & \text{for } m/M=0; \end{cases} \quad (53b)$$

$$-0.270 & \text{for } m/M=0; \quad (53c)$$

and thus for the ionization

$$\sigma_i = 4\pi a_0^2 z^2 (R/T) [0.1445 \ln(T/R) + 0.137 + \gamma_i R/T], \quad (54a)$$

with

$$\gamma_i = \begin{cases} -3.439 & \text{for } m/M=1, \text{ Born (a),} \\ -5.439 & \text{for } m/M=1, \text{ Born (b),} \\ -1.276 & \text{for } m/M=0. \end{cases} \quad (54b)$$

$$-5.439 & \text{for } m/M=1, \text{ Born (b),} \quad (54c)$$

$$-1.276 & \text{for } m/M=0. \quad (54d)$$

The Born (b) cross section [Eqs. (54a) and (54c)] agrees very well with the "length" form of the Born cross section calculated by Economides and McDowell²⁵ down to $T \approx 300$ eV. Comparison with the electron-impact data of Peart *et al.*²⁹ (Fig. 6) indicates that the Born approximation overestimates the ionization cross section for $T \lesssim 3$ keV. (As in the case of He, the double ionization can be neglected in the comparison with experiment.)

TABLE III. Adopted values of γ_n for Li^+ .^{a, b}

Excited states	Li^+			
	1P	1S	1D	
$n=2$	$\gamma_n^{(e)}$	$\gamma_n^{(\infty)}$	γ_n	
$n=3$	0.0392	0.2674	-0.0447	
$n=4$	-0.0066	0.0486	-0.0099	-0.0095
$n \geq 4$	$-0.412(n^*)^{-3}$	$0.880(n^*)^{-3}$	$-0.2035(n^*)^{-3}$	$-0.3634(n^*)^{-3}$
	$+2.05(n^*)^{-5}$	$+3.90(n^*)^{-5}$	$-0.360(n^*)^{-5}$	$+0.852(n^*)^{-5}$
	$+1.48(n^*)^{-7}$			
Σ_n	0.0195	0.3570	-0.0637	-0.0227

^aNotations: See Ref. a of Table II for $\gamma_n^{(e)}$ and $\gamma_n^{(\infty)}$; and $n^* = n + \delta$, where $\delta = 0.0136$, -0.074 , and -0.0012 for the 1P , 1S , and 1D states, respectively.

^bSource: Paper IV.

E. Exchange Correction

In Figs. 3–6, for $T \lesssim 40I$, we see a systematic departure of the electron-impact experimental data from the Born (b) cross sections. It is very likely that the exchange effect is one of the major causes for the departure. Unfortunately, no theory for the exchange effect is as widely applicable as the first Born approximation for the direct process. The exchange effect is important when the energy transfer is large, and thus the binding energy of the atomic electrons involved is expected to play a secondary role. To gain some insight on the energy dependence of the electron-exchange correction, we have used the Mott formula for the scattering of

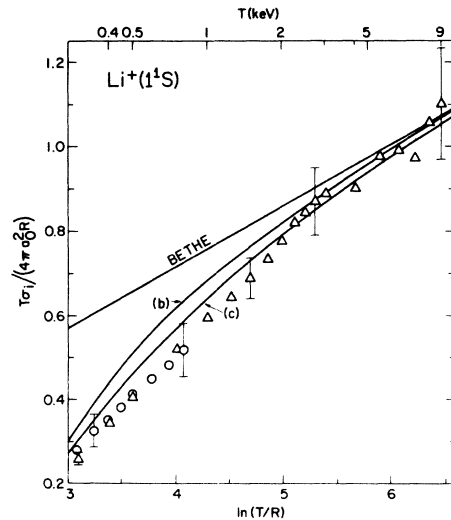


FIG. 6. Cross sections for the ionization of Li^+ (1^1S) by electron. The labels are the same as those used in Fig. 3. The circles represent the experiment by Lineberger, Hooper, and McDaniel [Phys. Rev. **141**, 151 (1966)], and the triangles that by Peart, Walton, and Dolder (Ref. 29). The error limits quoted are the sum of random and systematic errors.

two electrons.³⁰

According to the Mott formula, the cross section corresponding to Eq. (3), but including the exchange, is given by³⁰

$$d\sigma_{\epsilon} = 4\pi a_0^2 NR^2 [\epsilon^{-2} - \epsilon^{-1}(T - \epsilon)^{-1} + (T - \epsilon)^{-2}] d\epsilon/T, \quad (55)$$

where ϵ is the energy of the slower electron after the collision. The first term in the brackets of Eq. (55) is the direct term [same as Eq. (3)], the second is the interference term, and the last is the exchange term. Equation (55) can also be derived from the Ochkur approximation by using the free-electron GOS, Eq. (16).³¹ Since the direct term is already accounted for in the Born cross section, the integral over ϵ of the last two terms in Eq. (55) gives the necessary correction for exchange³²:

$$\begin{aligned} \sigma_{\text{exch}} &= 4\pi a_0^2 NR^2 T^{-1} \int_I^{(T+I)/2} d\epsilon \left(\frac{1}{\epsilon(T-\epsilon)} + \frac{1}{(T-\epsilon)^2} \right) \\ &\cong 4\pi a_0^2 N(R/T)^2 [\ln(I/T) + 1] \end{aligned} \quad (56)$$

when $I/T \ll 1$. The lower limit I of the integral in Eq. (56) need not be exactly an ionization potential, but in the following applications it is taken as the first ionization potential of the atom.

It is also worthwhile to note that the contribution of the exchange term alone, in Eq. (56), is the same as the difference between the Born (a) and (b) cross sections $4\pi a_0^2 N(R/T)^2$, in support of the argument presented by Rudge.⁹ We conclude, therefore, that Eq. (56) should be used in conjunction with the Born (b) cross sections. Alternatively, only the logarithmic term in Eq. (56) should be used with the Born (a) cross sections. The resulting ionization cross sections with the free-electron exchange correction are presented along with the Born (b) cross sections in Figs. 3–6. Although the agreement with experiment is improved in all cases, the success must be accepted with caution.

We expect that the exchange correction based on a free-electron model is appropriate only when I/T is small. The model is justifiable only in the part of the Bethe surface where the Bethe ridge is dominant, and we should expect such a theory to work better for H^- than for Li^+ , for instance. The comparison with experiment, however, does not bear this expectation out. In fact, the exchange correction when combined with the Born asymptotes seems to work equally well in all the cases discussed below. The most useful lesson to learn from the asymptotic Mott formula is the dependence of σ_{exch} on T .

The experimental data^{33,34} on H presented in Fig. 3 have been normalized to an absolute measurement on H_2 . The theory is in better agreement with the

high-energy data ($T \geq 300$ eV) by Rothe, Marino, Naynaber, and Trujillo,³⁴ according to which the theory becomes poor for $T \leq 25R$. Other electron-impact data³⁵ on H have been normalized to the Born cross sections at various energies near or below 500 eV. As can be seen from Fig. 3, the exchange correction at $T = 500$ eV amounts to almost 5%. It may be necessary to renormalize the experimental data if a better accuracy is desired. The ionization cross section obtained from Eqs. (47) and (56) is in excellent agreement for $T \geq 80$ eV with that calculated by Ochkur³¹ using the exact GOS of H.

For H^- , the exchange correction again brings the theoretical cross section closer to the experimental data in Fig. 4. We see, however, a small systematic departure at $T \leq 100$ eV. Certainly the difference partially comes from the polarization and distortion, but it is difficult at present, because of the large experimental uncertainties, to speculate on the magnitudes of such effects and also on the region of T in which they are significant.

On He, after the exchange correction, the theory is in excellent agreement with the experiment by Smith²⁶ for $T \geq 500$ eV (see Fig. 5). For Li^+ , the theory departs from experiment only below $T \leq 2$ keV (Fig. 6).

For a hydrogenic ion of nuclear charge Ze , $I = Z^2R$, and the ionization cross section with the exchange correction is given by [Eqs. (47) and (56)]

$$\begin{aligned} \sigma_i &= 4\pi a_0^2 (R/T) \{ (0.2834/Z^2) \ln(84.241 T/Z^2R) \\ &\quad - (R/T) [1.6294 - \ln Z^2 + \ln(T/R)] \} . \end{aligned} \quad (57)$$

In Fig. 7, Eq. (57) is compared with the experiment on He^+ by Peart, Walton, and Dolder.²⁹ Again, the inclusion of the exchange correction improves the agreement between theory and experiment. The excellent agreement for $T \leq 1$ keV, however, may be fortuitous because the experimental values for $2 \text{ keV} \leq T \leq 5 \text{ keV}$ hint that they may be too large by $\sim 5\%$ or more. If all the experimental data are reduced by $\sim 5\%$, then the departure between the theory and experiment follows the general pattern as those we have seen in Figs. 3–6.

VI. CONCLUDING REMARKS

Although we must distinguish the type of incident particle to evaluate the constant C in Eq. (1), the numerical procedure is far simpler than that required in evaluating the second constant B . In fact, Eqs. (41) are very simple to use and will provide reliable values particularly when only crude values of the first two constants in Eq. (1) are available. The comparisons with the exact Born cross section of the hydrogen atom and other theoretical data for He and Li^+ amply demonstrate that our method can represent the Born cross section with high precision down to rather low values of T , much lower than the

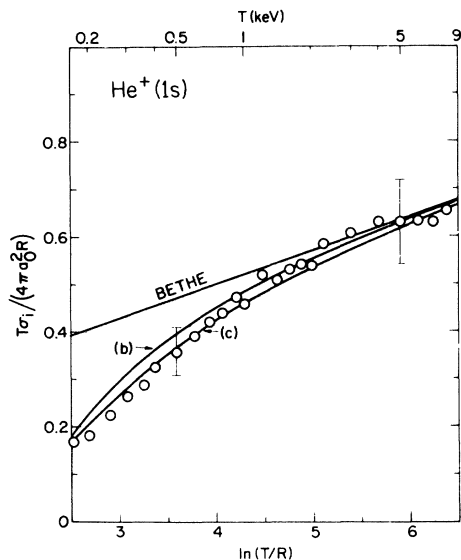


FIG. 7. Cross sections for the ionization of He^+ (1s) by electrons. The labels are the same as those used in Fig. 3. The circles represent the experiment by Peart, Walton, and Dolder (Ref. 29). The error limits quoted are the sum of random and systematic errors.

region where the first Born approximation by itself provides realistic cross section. We find that the modification proposed by Rudge⁹ to exclude the exchange contribution from the first Born approximation [Born (b)] requires only a simple change as indicated in Sec. III B. We also find, for the ionization cross sections of all cases presented here, that the distinction between cases (a) and (b) in Rudge's notation becomes significant only in the low-incident-energy region where the electron-exchange effect contributes substantially also.

Among the many theoretical detachment cross sections of H^- quoted in Paper II, our result agrees best with that of McDowell and Williams.³⁶ By comparing our detachment cross section with available experimental data, we conclude that the first Born approximation overestimates the detachment cross section for incident electron energies below 100 eV. For H, He^+ , He, and Li^+ , our results confirm the Born cross sections calculated directly from continuum wave functions, and therefore support the general experience that the Born approximation is reliable when $T \gtrsim 40I$ for these cases.

Our treatment here has been nonrelativistic. It is very likely that for relativistic incident velocities, the Bethe asymptote should be sufficient, and the third term [C in Eq. (1)] would be required only in the nonrelativistic region. A naive replacement of v in the third term by the relativistic counterpart βc would lead to a constant bias of the Bethe cross section in the limit $\beta \rightarrow 1$, which contradicts

the excellent performance of the Bethe cross sections of fast electrons and positrons scattered by He reported in Paper I.

The present theory is not restricted to the target atoms in the ground state. All discussions are applicable to any initial state.³⁷ The theory should also be applicable to molecules as well, with appropriate modifications to account for the additional degrees of freedom.

The inclusion of the asymptotic Mott formula for the exchange scattering improves the agreement of theory and experiment in all cases presented. The theory leads to $(\ln T)/T^2$ dependence for the direct-exchange interference term in the cross section, and T^{-2} dependence for the exchange term alone. With the exchange correction (56), the Born asymptotes are expected, in general, to produce reliable ionization cross sections for incident electron energies of about 20–30 times the first ionization potential, and higher. Our ionization cross sections for H, He^+ , and He may serve as alternative standards to which high-energy electron-impact experiments can be normalized.

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APPENDIX A: PROOF OF INEQUALITIES (24) AND (33)

Let [see Eq. (23)]

$$Y(x) = \ln y(x) = \ln \{2/[1 + (1-x)^{1/2}]\}. \quad (\text{A1})$$

By expanding dY/dx in power series and integrating term by term, we get

$$Y(x) = \sum_{k=1}^{\infty} x^k \frac{(2k-1)!!}{2k(2k)!!} \quad \text{for } 0 \leq x \leq 1, \quad (\text{A2})$$

where $(2k)!! = 2 \times 4 \times 6 \times \dots \times (2k)$ and $(2k-1)!! = 1 \times 3 \times 5 \times \dots \times (2k-1)$. Define $W(x)$ by

$$W(x) \equiv [Y(x) - \frac{1}{4}x]/x^2. \quad (\text{A3})$$

Then it follows from Eq. (A2) that $dW/dx > 0$ for $0 < x \leq 1$ and therefore $W(x)$ is monotonically increasing in that interval. In other words, $W(0) < W(x) \leq W(1)$, which is equivalent to inequality (24).

The first half of inequality (33) is readily seen by expanding $y(x)$ in power series for $0 \leq x \leq 1$:

$$y(x) = 1 + \frac{1}{4}x + \frac{1}{8}x^2 + \dots \geq 1 + \frac{1}{4}x. \quad (\text{A4})$$

For the second half of inequality (33), we note that $[y(x)]^{2k}$ is a convex function for $0 \leq x < 1$ because $d^2y/dx^2 > 0$ in the interval.³⁸ Therefore,

$$[y(x)]^{2k} \leq \lim_{\epsilon \rightarrow 0} \{ (1-x)[y(\epsilon)]^{2k} + x[y(1-\epsilon)]^{2k} \}.$$

APPENDIX B. DERIVATION OF EQ. (35)

Sum rules for the derivative with respect to Q of the GOS can be computed either by (a) summing the expression for each derivative over states, or by (b) summing first the GOS over the states and then differentiating with respect to Q . Formally, methods (a) and (b) are equivalent as long as the summation and the differentiation are interchangeable.

To follow method (b), we define $S(1, K)$ by

$$S(1, K) = \sum_{a11} \frac{E_n}{R} f_n(K).$$

We replace E_n by the commutator of the Hamiltonian operator and get

$$S(1, K) = - (QR^2)^{-1} \sum_{a11} \langle 0 | [H, \sum_k e^{-iK \cdot r_k}] | n \rangle \times \langle n | [H, \sum_j e^{iK \cdot r_j}] | 0 \rangle, \quad (B1)$$

with

$$H = - (\hbar^2/2m) \sum_j \nabla_j^2 + V,$$

V standing for the Coulomb potential terms. We take the direction of \vec{K} as the z axis for brevity.

After some manipulation, Eq. (B1) reduces to

$$S(1, K) = \frac{4}{3R} \langle 0 | \mathcal{K} | 0 \rangle + Q \left(N + \sum_{j, k \neq j} \langle 0 | e^{iK \cdot (r_j - r_k)} | 0 \rangle \right) - 4a_0^2 \sum_{j, k \neq j} \left\langle 0 \left| e^{iK \cdot (r_j - r_k)} \frac{\partial^2}{\partial z_j \partial z_k} \right| 0 \right\rangle. \quad (B2)$$

where \mathcal{K} is the kinetic-energy operator. Equation (B2) leads to the well-known expression for the corresponding sum rule of the dipole-oscillator strengths¹² when $K \rightarrow 0$. Note that

$$S(1, K) \rightarrow NQ \text{ as } K \rightarrow \infty.$$

For large momentum transfers, the binding of atomic electrons becomes insignificant and Eq. (B2) is expected to reduce to the free-electron result $S(1, K) = NQ$ [see Eq. (14)].

The first derivative $S'(1)$ is then given by

$$S'(1) = \frac{d}{dQ} [S(1, K)] \Big|_{Q=0}$$

$$= N^2 + 2 \sum_j \sum_{k \neq j} \left\langle 0 \left| (z_j - z_k)^2 \frac{\partial^2}{\partial z_j \partial z_k} \right| 0 \right\rangle. \quad (B3)$$

It is obvious from Eq. (B3) that $S'(1) = 1$ for a one-electron atom regardless of the state and nuclear charge. Further simplification occurs when a single-determinant wave function is used in evaluating the cross-term integrals in Eq. (B3). Let

$$I_{jk} \equiv \left\langle 0 \left| (z_j - z_k)^2 \frac{\partial^2}{\partial z_j \partial z_k} \right| 0 \right\rangle.$$

Then, from the odd parity of the operator

$$\left(z_j^2 \frac{\partial^2}{\partial z_j \partial z_k} \right)_{j \neq k}$$

and the well-known rules for the Slater determinant,³⁹ we have

$$\sum_{j, k \neq j} I_{jk} = -2 \sum_a \sum_{b \neq a} \left(\left\langle a \left| z \frac{\partial}{\partial z} \right| a \right\rangle \left\langle b \left| z \frac{\partial}{\partial z} \right| b \right\rangle - \left| \left\langle a \left| z \frac{\partial}{\partial z} \right| b \right\rangle \right|^2 \right), \quad (B4)$$

where a and b refer to orbitals in the determinant. Equation (B4) is further simplified by partial integration to read

$$\sum_{j, k \neq j} I_{jk} = -\frac{N(N-1)}{2} + 2 \sum_a \sum_{b \neq a} \left| \left\langle a \left| z \frac{\partial}{\partial z} \right| b \right\rangle \right|^2$$

and we finally have

$$[S'(1)]_{\text{single determinant}} = N + 4 \sum_a \sum_{b \neq a} \left| \left\langle a \left| z \frac{\partial}{\partial z} \right| b \right\rangle \right|^2. \quad (B5)$$

For the Hartree wave functions, the exchange integrals in Eq. (B5) do not occur. For correlated wave functions, Eq. (B4) does not hold, and Eq. (B3) must be computed directly. In view of Eq. (B5), we expect, in general,

$$S'(1) = N + \text{correction terms}, \quad (B6)$$

where the correction terms may be positive or negative.

As can be seen from the examples given in Table I, the correction terms in Eq. (B6) depend on the electron correlation and amount to 10% or less of N . Equation (B6) has been used also in the theory of the stopping power.⁶ The same result is obtained by summing the expression for the first derivative of the GOS [see Eq. (5) of Ref. 13] over all states.

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