

Double closure calculation of the electron-loss cross section for H^- in high-energy collisions with H and He

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An extension of the Bethe theory for the total inelastic cross section in the Born approximation is presented and used to evaluate the total electron-loss cross section for H^- collisions on H and He targets at high energies. Sum rules are used to derive expressions for both the leading and the next leading order contributions to the asymptotic cross section. A comparison with the available experimental data for He targets shows good agreement with the theoretical calculation. In the case of hydrogen the calculated cross section for atomic H targets shows a clear preference for the larger values of the cross section obtained by several groups and disagrees with the conflicting lower experimental data from two other measurements. When corrections for H_2 are included, this conclusion remains true for the conflicting experimental data near 10 MeV, but the calculated cross section in this case favors the lower experimental data near 1 MeV. Results are also presented for the total elastic cross section and the total nondetachment inelastic cross section. The latter is smaller than the total electron-loss cross section at intermediate energies, but exceeds it at sufficiently high energies. However, the convergence of the series generated in the Bethe theory approach for the nonloss cross section appears to be much slower than that of the electron-loss cross section.

I. INTRODUCTION

Attempts to calculate the collisional electron-detachment cross section for negative hydrogen ions incident on hydrogen and helium targets were first carried out by McDowell and Peach,¹ and by Sida,² respectively. Based on the first Born approximation, these efforts were exploratory in concept and only relatively simple models of either the H^- ion or target atoms were examined. Order of magnitude results were correct, but good agreement with experiment was lacking. A free-collision approximation developed by Dmitriev and Nikolaev³ and the quasiclassical impulse approximation given by Bates and Walker⁴ improved the agreement somewhat. However, experimental results by Rose *et al.*⁵ and Berkner *et al.*⁶ above 100-keV incident energy, indicated that the frequently utilized result of the free collision approximation was still about 50% too high in the asymptotic region. Further results obtained by Smythe and Toevs⁷ and also by Dimov and Dudnikov⁸ indicated discrepancies in the experimental data, suggesting that the disagreement with the theory may even be greater. The recent increased interest in neutral beams for the heating of thermonuclear plasmas has revived the work on electron detachment processes and the experimental differences should soon be resolved. However, it seems clear that the theoretical work published to date on the electron-loss cross sections of the negative hydrogen ion will remain unsatisfactory.

Because the negative hydrogen ion has no bound

excited states, the calculation of the total electron-loss cross section is ideally suited to the use of sum-rule techniques, since a sum over all excited final states of the H^- ion will automatically include all detachment states. Bethe's now classic treatment⁹ of the use of sum rules to evaluate the total inelastic cross section of atoms due to structureless charged particle impact first demonstrated the power of this approach. It has been used by many workers since,¹⁰ including the calculation of the H^- detachment cross section due to electron collisions.^{11,12} The work discussed in this paper utilizes an extension of Bethe's theory so that the incident charged particle need not be regarded as structureless. The approach is similar to that used by Levy in evaluating the electron-loss cross sections for neutral hydrogen atoms.¹³ Sum rules applied to the final states of both the incident H^- ion and target H or He atom allow the accurate evaluation of the first Born approximation for collisional detachment at high energies.

Section II A briefly outlines the theoretical framework, Sec. II B calculates the leading order terms of the detachment cross section, and Sec. II C the next leading contributions, still within the context of the first Born amplitude. Section II D derives results for the total elastic and inelastic nondetachment cross sections, in which the target atom, but not the incident ion, may be in an excited final state. That section clearly demonstrates the relationship to the Bethe results for structureless charged particles. A compilation of the available experimental data above 200-keV incident energy

is used in Sec. III to examine the agreement between this theory and experiment. Molecular corrections for H_2 targets are considered in that section. Section IV provides a summary and some discussion of features of the theory not yet established by experiment. Some concluding remarks are presented in the final section.

II. CALCULATION OF THE CROSS SECTIONS

A. Basic formulas and theoretical overview

The differential scattering cross section in the Born approximation for a collision involving a momentum transfer of magnitude K between two atomic systems, initially in their respective ground states, but in final states labeled by n and m , may be written

$$d\sigma_{nm} = 8\pi\alpha_0^2 \frac{\alpha^2}{\beta^2} |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}, \quad (1)$$

when exchange effects are neglected. The incident particle's velocity is contained in the parameter $\beta = v/c$; a_0 and α are the Bohr radius and fine structure constant, respectively. The functions $F_n^{(j)}(K)$ are the atomic form factors for the incident ($j=1$) and target ($j=2$) particles. For the j th atom or ion with nuclear charge $Z_N^{(j)}$ and a total of $Z_e^{(j)}$ electrons, the form factor is given by

$$F_n^{(j)}(K) = {}_j\langle n | [Z_N^{(j)} - \sum_{l=1}^{Z_e^{(j)}} \exp(i\vec{K} \cdot \vec{r}_l^{(j)})] | 0 \rangle_j, \quad (2)$$

where $\vec{r}_l^{(j)}$ is the coordinate vector for the l th electron in the j th atomic system. The matrix element is evaluated for eigenstates, $|n\rangle_j$, of the free Hamiltonian for the j th atom or ion. The nuclear charge term in (2) is omitted by most authors since for the inelastic form factors ($n \neq 0$), the orthogonality of the initial and final states guarantees that its contribution vanish. It is included here so that the elastic form factor ($n=0$) at $K=0$ is the total charge of the atomic system, i.e.,

$$F_0^{(j)}(0) = Z_N^{(j)} - Z_e^{(j)}. \quad (3)$$

(When the nuclear charge term is omitted for the $n=0$ form factor, it is usually referred to as the atomic scattering factor or atomic form factor.) The inelastic atomic form factor is related to the more widely recognized generalized oscillator strength, $f_n^{(j)}(K)$, by

$$f_n^{(j)}(K) = E_n^{(j)} |F_n^{(j)}(K)/a_0 K|^2, \quad (4)$$

where $E_n^{(j)}$ is the excitation energy in rydbergs of the state n . As is customary, the definitions of the form factors and generalized oscillator strengths used in this work include an implied sum over all degenerate final states of energy

$E_n^{(j)}$ (as well as an average over degenerate initial states if appropriate). Such a sum reduces the dependence of these functions on the vector \vec{K} , to a dependence only on the magnitude K of the momentum transfer. The ordinary oscillator strength $f_n^{(j)}$, is defined by the limit of Eq. (4) as K goes to zero.

The total cross section for the excitation of the incident particle to the state n , and of the target particle to the state m , is given by an integral over the momentum transfer,

$$\sigma_{nm} = 8\pi\alpha_0^2 \frac{\alpha^2}{\beta^2} \int_{a_0 K_{\min}}^{a_0 K_{\max}} |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}. \quad (5)$$

The integration limits are determined by the kinematic constraints of the collision. For a collision in which the initial and final relative momentum differ in direction by an angle θ (the center-of-mass scattering angle), the momentum transfer is

$$(a_0 K)^2 = \frac{\alpha^2 M^2 \beta^2}{2} \left\{ 1 - \frac{E_n^{(1)} + E_m^{(2)}}{M\beta^2} - \left[1 - \frac{2(E_n^{(1)} + E_m^{(2)})}{M\beta^2} \right]^{1/2} \cos\theta \right\}, \quad (6)$$

where M is the reduced mass (in rydbergs). The minimum and maximum values of K appearing in (5) correspond to scattering angles of 0 and π , respectively. The integration limits are explicitly state dependent via the excitation energies. However, for large incident velocities, K_{\min} and K_{\max} tend to zero and infinity, respectively [proportional to β^{-2} and β^2 upon expanding (6)]. Together with the known behavior of the form factors at small and large K^2 , this fact allows one to extend the region of integration in (5) to $(0, \infty)$ for all excitations (for $n \neq 0$; however, see Sec. IID). A sum over all final states then permits the use of the completeness of the energy eigenstate basis to evaluate the inelastic cross section in terms of ground-state expectation values only. The application of this procedure to both the incident and target particles constitutes the double-closure approximation.

B. Leading term of the electron loss cross sections

Since the negative hydrogen ion has no bound excited states, a summation over all final states, except the ground state, of the incident H^- ion is

a sum over all states resulting in electron loss. A simultaneous summation over all final states of the target atom (either H or He) yields the total electron-loss cross section. This cross section

$$(\sigma_{-1,0} + \sigma_{-1,1}) = 8\pi a_0^2 \frac{\alpha^2}{\beta^2} \sum_{n \neq 0} \sum_m \int_{a_0 K_{\min}}^{a_0 K_{\max}} |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}, \quad (7)$$

where the summations over the final states labelled by n and m includes an integration over all continuum final states as well. This generalized definition of the summation over discretely labelled states will be used throughout this work. Writing the integrals appearing in Eq. (7) as the sum of three terms,

$$I_{nm} = \int_0^\infty |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}, \quad (8)$$

$$J_{nm}(\beta^2) = \int_0^{a_0 K_{\min}} |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}, \quad (9)$$

$$K_{nm}(\beta^2) = \int_{a_0 K_{\max}}^\infty |F_n^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}, \quad (10)$$

then the total electron-loss cross section becomes $(\sigma_{-1,0} + \sigma_{-1,1})$

$$= 8\pi a_0^2 \frac{\alpha^2}{\beta^2} \sum_{n \neq 0} \sum_m [I_{nm} - J_{nm}(\beta^2) - K_{nm}(\beta^2)]. \quad (11)$$

The integrals defined by (8)–(10) are all well behaved at both small and large K^2 provided that $n \neq 0$, i.e., the final state of the H^- ion is not the ground state. (The case $n=0$ is examined in Sec. II D.) The integral I_{nm} is a constant independent of the incident velocity of the H^- ion and provides the leading contributions to the total electron-loss section. The integrals $J_{nm}(\beta^2)$ and $K_{nm}(\beta^2)$ are velocity dependent. Their contributions are examined in Sec. II C.

Since the integration limits for the evaluation of I_{nm} are independent of the states n and m , the orders of integration and the summation over final states appearing in (11) may be interchanged. The completeness of the energy eigenstate basis may then be used to reduce the matrix element sum to a matrix element involving the ground state only. The result is

$$\sum_{n \neq 0} \sum_m I_{nm} = \int_0^\infty [Z_e^{(1)} S_{\text{inc}}^{(1)}(K)] \times [Z_e^{(2)} S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2] \frac{d(a_0 K)}{(a_0 K)^3}, \quad (12)$$

consists of two terms, one arising from single electron-loss, $\sigma_{-1,0}$, and one arising from double electron-loss, $\sigma_{-1,1}$. These two together are given by

where $S_{\text{inc}}^{(1)}(K)$ is the incoherent scattering function for the H^- ion, $S_{\text{inc}}^{(2)}(K)$ and $F_0^{(2)}(K)$ are the incoherent scattering function and elastic form factor, respectively, of the target hydrogen or helium atom. The incoherent scattering function is expressed in terms of ground-state expectation values by

$$Z_e^{(j)} S_{\text{inc}}^{(j)}(K) = \left\langle 0 \left| \left| Z_N^{(j)} - \sum_{I=1}^{Z_e^{(j)}} \exp(i\vec{K} \cdot \vec{r}_I^{(j)}) \right|^2 \right| 0 \right\rangle_j - |F_0^{(j)}(K)|^2. \quad (13)$$

For the case of a target hydrogen atom, $Z_e^{(2)} S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2$ may be easily evaluated analytically.¹⁴ For the H^- ion, $S_{\text{inc}}^{(1)}(K)$ has been calculated (and the results tabulated) by Inokuti and Kim¹¹ for a 20-term Hylleraas wave function,¹⁵ and by Kim¹⁶ for a 39-term Weiss wave function.¹⁷ The integral in (12) can then be integrated numerically, substitution of the result into (11) yields the leading contribution to the total electron-loss cross section for H^- . For the most accurate H^- wave function,^{16,17} this gives for the case of atomic hydrogen targets

$$(\sigma_{-1,0} + \sigma_{-1,1})(H) = 8\pi a_0^2 (\alpha^2 / \beta^2) (2.42 \pm .01), \quad (14)$$

where the indicated error limits are those associated with the numerical integration.

For the case of a helium target atom, the incoherent scattering function and elastic form factor required for the integration in (12) have also been calculated (and tabulated) by Kim and Inokuti,¹⁸ for several different wave functions obtained from the literature. Utilizing the most accurate results given, for a 20-term Hylleraas wave function,¹⁵ the total electron detachment cross section for helium targets is

$$(\sigma_{-1,0} + \sigma_{-1,1})(He) = 8\pi a_0^2 (\alpha^2 / \beta^2) (2.81 \pm .01). \quad (15)$$

Again the possible errors indicated are associated with the uncertainties in the numerical integration.

The dependence of this result on the He wave function was examined by carrying out the same integration utilizing the $S_{\text{inc}}^{(2)}(K)$ and $|F_0(K)|^2$ for a six-term Hylleraas wave function.^{18,19} The results were identical, well within the numerical uncertainties. The integral (12) was also evaluated for the simple product wave function with effective

nuclear screening $Z^* = (2 - \frac{5}{16})$,

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\pi} \left(\frac{Z^*}{a_0} \right)^3 \exp \left[-Z^* \left(\frac{|\vec{r}_1| + |\vec{r}_2|}{a_0} \right) \right]. \quad (16)$$

The function $Z_e^{(2)} S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2$ may be easily evaluated analytically for this case.¹⁴ The resulting cross section (15) was reduced by a little more than 3%. These results indicate that no large uncertainties in the cross section (15) are expected due to the finite accuracy of the He wave function underlying this calculation.

The cross sections are expected to be more sensitive to the H⁻ wave function. The integral in Eq. (12) was also evaluated for the 20-term Hylleraas H⁻ wave function.^{11,15} For H targets, the result is 2.40 ± 0.01 ; for He targets, one gets 2.79 ± 0.01 . This suggests that the error associated with these accurate H⁻ wave functions is only of the order of 1%. For comparison, the Ohmura model²⁰ of H⁻, for which $S_{\text{inc}}^{(1)}(K)$ may be evaluated analytically,¹¹ gives cross sections which are nearly 25% higher than Eqs. (14) and (15).

C. Corrections to the leading term of the electron-loss cross sections

Deviations from the asymptotic forms of the electron-loss cross sections are expected at lower energies due to finite contributions from the terms $J_{nm}(\beta^2)$ and $K_{nm}(\beta^2)$ appearing in (11), as well as from electron exchange effects and higher-

$$\sum_{n \neq 0} \sum_m J_{nm}(\beta^2) \simeq \frac{1}{8} \frac{\alpha^2}{\beta^2} [S^{(1)}(-1)S^{(2)}(1) + 2S^{(1)}(0)S^{(2)}(0) + S^{(1)}(1)S^{(2)}(-1)]. \quad (19)$$

Note that the $m=0$ term does not contribute to the sum since the square of the elastic form factor is proportional to K^4 at low K , consequently, the "ground-state oscillator strength" $f_0^{(2)}$ is zero [or more correctly $f_0^{(2)}/E_0^{(2)}$ as defined by the limit of (4) is zero].

The three moments required for a particular atom or ion are all readily related to ground-state expectation values using well-known sum rules.²¹ $S^{(j)}(0)$ is simply $Z_e^{(j)}$, given by the

order Born amplitudes. The contributions to the next leading term of the first Born cross section arising from $J_{nm}(\beta^2)$ and $K_{nm}(\beta^2)$ may also be calculated in a relatively straightforward manner. These contributions are evaluated in this section. Since it is clear that additional contributions are expected at lower energies, the results for the next leading term developed here must be regarded as only approximate.

For small K^2 the only contributions to $J_{nm}(\beta^2)$ which are of significance arise from optically allowed (dipole) transitions. From Eq. (4) the small- K^2 behavior of these form factors, required to evaluate the integral in (9), is simply related to the ordinary oscillator strengths at $K=0$. Expanding the integration limit, K_{min} , in terms of the parameter $(E_n^{(1)} + E_m^{(2)})/M\beta^2$ (a small parameter implicit within the theoretical framework of the first Born approximation), the following result is obtained:

$$J_{nm}(\beta^2) \simeq \frac{1}{8} f_n^{(1)} f_m^{(2)} \frac{(E_n^{(1)} + E_m^{(2)})^2}{E_n^{(1)} E_m^{(2)}} \frac{\alpha^2}{\beta^2}. \quad (17)$$

The summation over final states appearing in (11) can now be evaluated in terms of the energy moments of the oscillator strength distribution

$$S^{(j)}(\mu) = \sum_{n \neq 0} (E_n^{(j)})^\mu f_n^{(j)}. \quad (18)$$

Specifically,

Thomas-Kuhn-Reiche sum rule. $S^{(j)}(-1)$ is the total dipole matrix element squared, usually referred to as M_{tot}^2 . $S^{(j)}(1)$ is simply related to the ground-state energy and the total momentum matrix element squared. They may be analytically evaluated for atomic hydrogen, and Pekeris^{22,23} has given accurate results for both H⁻ and He. These values are summarized, together with the resulting coefficient of α^2/β^2 appearing in (19), in Table I.

TABLE I. Values of $S^{(j)}(\mu)$ for $\mu = -1, 0, 1$, and the resulting sum $(\beta^2/\alpha^2) \sum_{n \neq 0} \sum_{m=0} J_{nm}(\beta^2)$ for small α^2/β^2 . The uncertainties in these numbers are less than one unit in the last significant figure.

Atomic system	$S^{(j)}(-1)$ (M_{tot}^2)	$S^{(j)}(0)$ ($Z_e^{(j)}$)	$S^{(j)}(1)$	$\frac{\beta^2}{\alpha^2} \sum_{n \neq 0} \sum_{m=0} J_{nm}(\beta^2)$
H ⁻ ($j=1$)	7.484 ^a	2	1.495 ^a	...
H ($j=2$)	1	1	$\frac{4}{3}$	1.934
He ($j=2$)	0.7525 ^a	2	8.167 ^a	8.781

^aThese values are from Pekeris, H⁻ data from Ref. 22, He data from Ref. 23.

Contributions to the next leading term of the electron-loss cross section arising from $K_{nm}(\beta^2)$ may also be calculated by using the closure approximation. Utilizing the same expansion parameter, $(E_n^{(1)} + E_m^{(2)})/M\beta^2$, the integration limit $a_0 K_{\max}$ is simply $\alpha M\beta$ to first order, independent of the state n and m . Consequently, the orders of summation and integration may also be interchanged for these terms and the contributions to the cross section evaluated by using the same closure approximation as used for the leading term. Only the large K^2 behavior of the incoherent scattering functions and elastic form factors is now required. These are readily established, namely,

$$\lim_{K \rightarrow \infty} Z_e^{(j)} S_{\text{inc}}^{(j)}(K) = Z_e^{(j)} \quad (20)$$

and

$$\lim_{K \rightarrow \infty} F_0^{(j)}(K) = Z_N^{(j)}. \quad (21)$$

The resulting contributions of the $K_{nm}(\beta^2)$ terms are then

$$\sum_{n \neq 0} \sum_m K_{nm}(\beta^2) \approx \frac{1}{2} Z_e^{(1)} [Z_e^{(2)} + (Z_N^{(2)})^2] \frac{1}{\alpha^2 M^2 \beta^2}. \quad (22)$$

Recalling that M is the reduced mass in Rydbergs, it is obvious that this contribution is down by a factor of the square of the electron to proton mass ratio, compared to the $J_{nm}(\beta^2)$ contribution, and is consequently negligible compared to that term.

Combining the results of this section with the leading terms of the electron-loss cross sections, the cross sections may be written

$$(\sigma_{-1,0} + \sigma_{-1,1})(\text{H}) = 8\pi a_0^2 (\alpha^2/\beta^2) [2.42 - 1.93(\alpha^2/\beta^2)], \quad (23)$$

$$(\sigma_{-1,0} + \sigma_{-1,1})(\text{He}) = 8\pi a_0^2 (\alpha^2/\beta^2) [2.81 - 8.78(\alpha^2/\beta^2)]. \quad (24)$$

D. Elastic and nondetachment inelastic cross sections

The total elastic cross section for H^- scattering on H and He in Born approximation may be cal-

culated in a straightforward manner since the elastic form factors are available. Using the H^- form factor also given by Inokuti and Kim¹¹ and the H and He form factors already discussed, the asymptotic elastic cross sections are

$$\sigma_{\text{el}}(\text{H}) = 8\pi a_0^2 (\alpha^2/\beta^2) (0.125 \pm 0.003), \quad (25)$$

$$\sigma_{\text{el}}(\text{He}) = 8\pi a_0^2 (\alpha^2/\beta^2) (0.262 \pm 0.005). \quad (26)$$

These terms arise, of course, only from the I_{00} integral given by (8). Within the context of the first Born approximation, the next leading terms to these cross sections are negligibly small. $J_{00}(\beta^2)$ is identically zero and $K_{00}(\beta^2)$ is of the same form as the electron-loss sum in (22), only with the Z terms replaced by $(Z_N^{(1)} Z_N^{(2)})^2$, according to (21). [Consequently, the first significant corrections at low energies to (25) and (26) are expected to arise from the second Born amplitude, which is beyond the scope of this work.]

The total nondetachment inelastic cross section provides a direct comparison with the Bethe theory. The difference between this theory and the total inelastic cross section due to charged-particle impact in the Bethe theory is the inclusion here of the structure of the incident charged particle via the form factor $F_0^{(1)}(K)$. The total non-loss, inelastic cross section is given by

$$\sigma_{\text{nonloss,inel}} = 8\pi a_0^2 (\alpha^2/\beta^2) \sum_{m \neq 0} [I_{0m} - J_{0m}(\beta^2) - K_{0m}(\beta^2)]. \quad (27)$$

The leading-order contributions to this cross section come from I_{0m} and $J_{0m}(\beta^2)$ given by (8) and (9). Neither of these is well defined separately since the lower limit in the K integral is logarithmically divergent. The combination $I_{0m} - J_{0m}(\beta^2)$ appearing in (27) is well defined. Consequently, this combination will be treated together, defined by

$$[I_{0m} - J_{0m}(\beta^2)] = \int_{a_0 K_{\min}}^{\infty} |F_0^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3}. \quad (28)$$

For optically allowed transitions, the lower limit in (28) may be evaluated by examining the small- K^2 behavior of the form factors, as given by (3) and (4). This gives

$$\begin{aligned} [I_{0m} - J_{0m}(\beta^2)] &= \int_{\lambda}^{\infty} |F_0^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \frac{d(a_0 K)}{(a_0 K)^3} \\ &- \int_{a_0 K_{\min}}^{\lambda} \left(|F_0^{(1)}(0)|^2 \frac{f_m^{(2)}}{E_m^{(2)}} (a_0 K)^2 - |F_0^{(1)}(K)|^2 |F_m^{(2)}(K)|^2 \right) \frac{d(a_0 K)}{(a_0 K)^3} \\ &- |F_0^{(1)}(0)|^2 \frac{f_m^{(2)}}{E_m^{(2)}} \left[\ln \left(\frac{a_0 K_{\min}}{\lambda} \right) \right]. \end{aligned} \quad (29)$$

Expanding the lower integration limit, $a_0 K_{\min}$, then yields the leading terms to the cross section. Summing over all excited final states of the target atom yields [note that Eq. (29) is valid for optically unallowed transitions as well, simply setting $f_m^{(2)}/E_m^{(2)} = 0$]

$$\sum_{m \neq 0} [I_{om} - J_{om}(\beta^2)] \simeq |F_0^{(1)}(0)|^2 [S^{(2)}(-1) \ln(2\beta/\alpha) - L^{(2)}(-1)] + \frac{1}{2}(\mathcal{G}_1 - \mathcal{G}_2), \quad (30)$$

where

$$\mathcal{G}_1 = 2 \int_{\lambda}^{\infty} |F_0^{(1)}(K)|^2 Z_e^{(2)} S_{\text{inc}}^{(2)}(K) \frac{d(a_0 K)}{(a_0 K)^3}, \quad (31)$$

$$\mathcal{G}_2 = 2 \int_0^{\lambda} [|F_0^{(1)}(0)|^2 S^{(2)}(-1)(a_0 K)^2 - |F_0^{(1)}(K)|^2 Z_e^{(2)} S_{\text{inc}}^{(2)}(K)] \frac{d(a_0 K)}{(a_0 K)^3} - 2 |F_0^{(1)}(0)|^2 S^{(2)}(-1) \ln(\lambda), \quad (32)$$

and $L^{(2)}(-1)$ is defined by

$$L^{(j)}(\mu) = \sum_{n \neq 0} (E_n^{(j)})^{\mu} \ln(E_n^{(j)}) f_n^{(j)}. \quad (33)$$

The integrals \mathcal{G}_1 and \mathcal{G}_2 are generalizations of those used for structureless ions^{10,24} to include the structure of the ion in terms of the elastic form factor. They may be evaluated numerically using the H^- elastic form factor and the incoherent scattering functions previously utilized. The integrand in \mathcal{G}_2 is well defined as $K \rightarrow 0$ since $Z_e^{(2)} S_{\text{inc}}^{(2)}(K)$ approaches $S^{(2)}(-1)(a_0 K)^2$ for small K . The combination $\mathcal{G}_1 - \mathcal{G}_2$ should be independent of λ , for λ of the order of unity. It is usually set to 1 by most authors; however, because of the limited number of tabulated points for the integrands near $a_0 K = 1$, the integrals \mathcal{G}_1 and \mathcal{G}_2 were evaluated for several values of λ . $L^{(2)}(-1)$ is not directly related to a simple ground-state expectation value in the same way that $S^{(2)}(\mu)$ is simply given by sum rules for several integer values of μ . However, reliable values of $L^{(2)}(-1)$ for both H and He atoms are available.²⁴ The parameters $L^{(2)}(-1)$, \mathcal{G}_1 and \mathcal{G}_2 , as well as the combination

$$\ln c_{\text{tot}}^{(2)} = - \frac{2L^{(2)}(-1) |F_0^{(1)}(0)|^2 - (\mathcal{G}_1 - \mathcal{G}_2)}{|F_0^{(1)}(0)|^2 S^{(2)}(-1)}, \quad (34)$$

for both H and He targets are given in Table II. The values of the integrals \mathcal{G}_1 and \mathcal{G}_2 are those obtained for the 39-term Weiss H^- wave functions and the 20-term Hylleraas He wave function; representative results are given for $\lambda = 1$ and $\lambda = 3$. The resulting cross sections are given by precisely the same form as the Bethe asymptotic cross-section formula, i.e.,

$$\sigma_{\text{nonloss,inel}} = 4\pi a_0^2 \frac{\alpha^2}{\beta^2} |F_0^{(1)}(0)|^2 \times S^{(2)}(-1) \ln \left(4c_{\text{tot}}^{(2)} \frac{\beta^2}{\alpha^2} \right), \quad (35)$$

The dependence of the integrals \mathcal{G}_1 and \mathcal{G}_2 on the wave functions was examined in the same manner as for the leading contribution to the electron-loss cross section. Again the results showed negligible differences between the six-term and 20-term Hylleraas He wave functions. However, for the simple He wave function given by (16), the combination $\mathcal{G}_1 - \mathcal{G}_2$ was reduced in magnitude by nearly 10% from the accurate values given in Table II. The values of $\mathcal{G}_1 - \mathcal{G}_2$ for the 20-term Hylleraas H^- wave functions were reduced in magnitude by about 3% from those values given in Table II, but the integration uncertainties associated with this case

TABLE II. Parameters required for the evaluation of the nondetachment inelastic cross section; and the combination, $\ln c_{\text{tot}}^{(2)}$, defined by Eq. (34). The values for \mathcal{G}_1 and \mathcal{G}_2 are based on the 39-term Weiss H^- function (Refs. 16 and 17), and on the 20-term Hylleraas He wave function (Refs. 15 and 18). The limits on \mathcal{G}_1 and \mathcal{G}_2 are associated only with the uncertainties in the numerical integration.

Atomic system	$L^{(2)}(-1)$	λ	$\frac{1}{2}\mathcal{G}_1$	$\frac{1}{2}\mathcal{G}_2$	$\frac{1}{2}(\mathcal{G}_1 - \mathcal{G}_2)$	$\ln c_{\text{tot}}^{(2)}$
H	-0.073 25 ^a	1	0.167 ± 0.001	1.356 ± 0.009	-1.189 ± 0.008	
		3	0.0517 ± 0.0001	1.240 ± 0.008	-1.188 ± 0.008	-2.23 ± 0.02
He	+0.638 ± 0.002 ^a	1	0.259 ± 0.001	1.003 ± 0.006	-0.744 ± 0.006	
		3	0.0992 ± 0.0001	0.843 ± 0.006	-0.743 ± 0.006	-3.67 ± 0.02

^aThese values are from Ref. 24. [The value of $L^{(2)}(-1)$ for H was not calculated in this reference explicitly, but appears in footnote 9 of Ref. 24.]

were considerably larger and could account for this difference.

The next-order contributions to the nondetachment inelastic cross section may be obtained by retaining the second leading terms in the expansion of K_{\min} in Eq. (29). [Again, the contributions arising from $K_{om}(\beta^2)$ are negligible, being of the same form as (22) with the Z factor now replaced by $Z_e^{(2)}(Z_N^{(1)})^2$.] The nonloss inelastic cross section may then be written

$$\sigma_{\text{nonloss,inel}} = 4\pi a_0^2 \frac{\alpha^2}{\beta^2} \times \left[|F_0^{(1)}(0)|^2 S^{(2)}(-1) \ln \left(4c_{\text{tot}}^{(2)} \frac{\beta^2}{\alpha^2} \right) + \gamma \frac{\alpha^2}{\beta^2} \right], \quad (36)$$

where γ is given by

$$\gamma = -\frac{1}{4} |F_0^{(1)}(0)|^2 S'^{(2)}(1) - \frac{1}{2} F_0^{(1)}(0) F_0'^{(1)}(0) S^{(2)}(1) - \frac{1}{2} (m_e/M) |F_0^{(1)}(0)|^2 S^{(2)}(0), \quad (37)$$

and m_e is the electron mass. The first and third terms contributing to γ in (37) are the same as those for the next-order corrections in the Bethe theory,¹⁰ since $|F_1^{(1)}(0)|^2$ is just the square of the net charge of the incident ion. The second term is an additional contribution arising from the structure of the H^- ion. Two additional parameters not appearing in the previous results are required, both are derivatives with respect to $(a_0 K)^2$ at $K=0$. They are defined by

$$S'^{(j)}(\mu) = \lim_{K \rightarrow 0} \frac{\partial}{\partial (a_0 K)^2} \sum_{n \neq 0} (E_n)^\mu f_n^{(j)}(K) \quad (38)$$

and

$$F_0'^{(j)}(0) = \lim_{K \rightarrow 0} \frac{\partial}{\partial (a_0 K)^2} F_0^{(j)}(K). \quad (39)$$

Both of these parameters may be related to ground state properties. $F_0^{(1)}(0)$ is simply the expectation value of $\frac{1}{3} |\vec{r}_1^{(1)}|^2$, and Pekeris has calculated an accurate value of $\frac{1}{3}(11.914)$ for the H^- ion.²² The evaluation of $S'^{(2)}(1)$ requires a more complicated expectation value.^{10,12} However, for H targets¹⁰ it is simply 1, and for He targets the value given by Kim and Inokuti¹² is 2.047. These parameter values, together with those previously given, yields the following correction factors for H and He targets:

$$\gamma(H) = 2.40, \quad (40)$$

$$\gamma(He) = 15.6. \quad (41)$$

It should be noted that these are strongly dominated by the second term in (37) due to the large expectation value of the square of the electron orbit radius for the loosely bound H^- ion. [The first term in (37) is only about 10% of (40) and about

3.2% of (41); the third term in (37) is negligible. Note that the first term is of the opposite sign as the dominant second term.]

III. COMPARISON WITH EXPERIMENT

The Born approximation for atomic scattering cross sections is expected to be valid if the incident velocities are sufficiently large compared to typical atomic electron orbital velocities, i.e., if $\alpha^2/\beta^2 \ll 1$. This is the effective expansion parameter appearing in the results given in this work.²⁵ Requiring $\beta^2 \geq 10\alpha^2$ implies that the cross sections calculated here should be valid for H^- laboratory energies greater than about 200 keV. There are no direct measurements of H^- detachment cross sections on atomic H targets in this energy region. However, there is data on molecular H_2 and atomic He targets over a wide energy range.

The data above 200 keV are summarized in Fig. 1, together with the theoretical results of this work. The cross sections for H are presented in units of cm^2/atom , i.e., one half the H_2 cross sec-

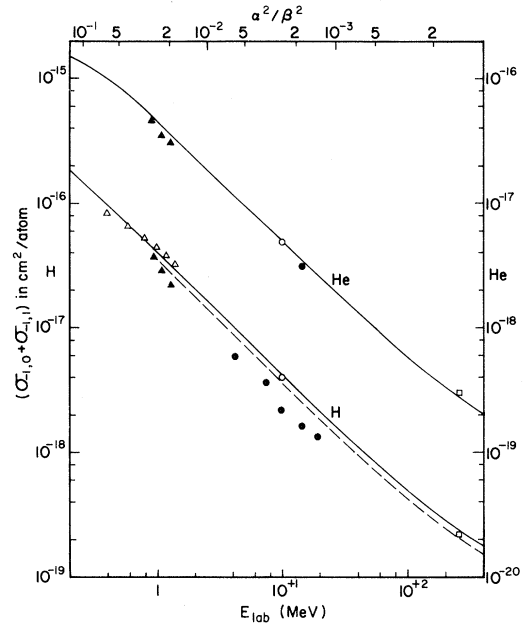


FIG. 1. Total electron detachment cross section ($\sigma_{-1,0} + \sigma_{-1,1}$) for H^- collisions on H and He targets as a function of energy. Solid curves, theoretical results of this work for atomic H and He targets. Broken line, results of this work for the asymptotic cross section for H_2 targets. Open triangles (Δ), data of Rose *et al.* (Ref. 5, $\sigma_{-1,0}$ only); solid triangles (\blacktriangle), Dimov and Dudnikov (Ref. 8, $\sigma_{-1,0}$ only for H_2 targets at 1.3 MeV); open circles (\circ), Berkner *et al.* (Ref. 6, 20 MeV D^-); solid circles (\bullet), Smythe and Toevs, (Ref. 7); open squares (\square), Hayward and Tesmer (Ref. 26). The upper scale gives the parameter $\alpha^2/\beta^2 = \alpha^2(1+\kappa)^2/(1+2\kappa)$, where $\kappa = M_p c^2/E_{\text{lab}}$, M_p being the proton rest mass.

tions. In all cases $(\sigma_{-1,0} + \sigma_{-1,1})$ has been plotted except for the noted exceptions for which only $\sigma_{-1,0}$ was available. However, experimentally $\sigma_{-1,1}$ is only about 4% of $\sigma_{-1,0}$. Since the experimental uncertainties for the absolute cross sections are 10–20%, whether or not $\sigma_{-1,1}$ is included in the data is largely academic.

The theory agrees well with the experimental data for He targets. The theoretical cross section for H targets clearly favors the experimental results of Rose *et al.*, Berkner *et al.*, and Hayward and Tesmer,²⁶ over the lower data given by Dimov and Dudnikov, and Smythe and Toevs. The theoretical curve is expected to be lowered somewhat by considering H_2 rather than atomic H targets. This correction was estimated for the leading term of the electron-loss cross section by using the H_2 incoherent scattering function calculated by Liu²⁷ for a five-term configuration interaction wave function, and the square of the H_2 elastic form factor given by Liu and Smith²⁸ for the Davidson-Jones wave function.²⁹ The value of the integral (12), which appears as the numerical factor in the cross section (14), is 1.98 ± 0.01 per H atom in this case, a reduction of about 18%. This cross section is shown in the figure as a broken line. With this lower value of the cross section, the theory is still close to the higher-lying values of the experimental data at the higher energies, but is now closer to the results of Dimov and Dudnikov near 1 MeV. The trend of the lower-energy data of Rose *et al.*, suggests that the low-energy corrections for H derived in Sec. II C may not be adequate. This is not surprising since contributions in this region due to the second Born amplitude may be important. (In addition, consideration of H_2 may make a larger correction at lower energies than in the asymptotic region.)

IV. DISCUSSION

The relationship between the total electron-loss cross section in this work and the free collision approximation given by Dmitriev and Nikolaev, can be understood in terms of the derivation presented in Sec. II. The leading term to the detachment cross section arises from the integral given by Eq. (12). Besides the photon propagator and density of final states, the integrand consists of two factors describing the structures of the incident and target atomic systems. A simple examination of these factors, $Z_e^{(1)}S_{\text{inc}}^{(1)}(K)$ and $Z_e^{(2)}S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2$, shows that they decrease rapidly from their maximum (large K) values as K becomes increasingly smaller than the typical electron orbital momentum; i.e., for K smaller than $[2m_e E_B^{(j)}]^{1/2}$, where $E_B^{(j)}$ is the binding energy of j th atomic sys-

tem. The low- K region of the integral in Eq. (2) is then primarily cutoff by the structure factor associated with the more tightly bound system, that is, by the target atom. As the target atom's structure factor begins to cutoff the low K region of integration, the incoherent scattering function of the H^- ion is still a large fraction of its maximum value. As K becomes increasingly smaller, so that it is less than the typical momentum of the loosely bound H^- ion, the contribution to the integral becomes virtually negligible. This suggests that the incoherent scattering function of the incident ion may be given, as a first approximation, by its limiting values.

$$Z_e^{(1)}S_{\text{inc}}^{(1)}(K) \simeq \begin{cases} 0 & \text{for } K < [2m_e E_B^{(1)}]^{1/2}, \\ Z_e^{(1)} & \text{for } K \geq [2m_e E_B^{(1)}]^{1/2}. \end{cases} \quad (42)$$

Utilization of this approximation for the incoherent scattering function in Eq. (12), together with the analytic forms for the H and He factors given in footnote 14, gives the free collision results of Dmitriev and Nikolaev at high energies. The numerical factors of Dmitriev and Nikolaev, which appear in the expression for the leading term to the electron-loss cross sections given by (14) and (15), obtained in this way are 3.78 and 3.79, respectively. These are not particularly bad estimates, acknowledging the simplicity of their model. The results presented in the previous section do indicate that the factors derived in this work are in much better agreement with the experimental data.

There are no published experimental data on the elastic or nondetachment inelastic cross sections at high energies. However, there are a few features of the Born approximation for these cross sections which should be mentioned and may be accessible to experimental tests in the future. For any negative ion, the elastic form factor has a zero at a certain value of the momentum transfer, K_0 . This is clear since the small and large K^2 limits of $F_0^{(1)}(K)$ given by (3) and (21) are of the opposite sign. For the case of H^- , the zero occurs at $a_0 K_0 \simeq 0.78$. As a result, there will be a zero in the (angular) differential elastic cross section³⁰ at a fixed scattering angle, θ_0 . This angle depends only on the incident energy, the particle masses and the zero of the incident-ion's elastic form factor. From (6),

$$\cos \theta_0 = 1 - 2(a_0 K_0)^2 / \alpha^2 M^2 \beta^2. \quad (43)$$

It is entirely independent of the structure of the target particle. However, the percentage of the total elastic cross section which lies inside of this

angle depends strongly on the target particle. For H targets it is about 11%, for He it drops to around 3.6%. For increasingly higher $Z_N^{(2)}$ targets, this percentage can be expected to decrease rapidly as the bulk of the integral I_{00} is determined by increasingly larger values of K . Nevertheless, this zero in the elastic differential cross section for negative loss represents a rather unique prediction of the Born approximation which may be experimentally accessible.

The nondetachment inelastic cross section, if excitation to a specific final excited state of the target particle is considered, also displays a zero in the differential cross section. In this case, however, the location of the zero angle θ_0 depends on the excitation energy of the final state. Again, this feature is characteristic of nondetachment scattering of all negative ions if only a single final state of the target particle is considered (or a sum over degenerate substates), and in principle could be examined experimentally. (Of course, the angular distribution of the cross section need not be measured specifically, measurements at a fixed angle near the zero, with the incident energy varied appropriately would also display a zero according to the Born approximation.)

The most interesting feature of the inelastic cross section derived in Sec. IID is the predictions of the Bethe theory for the nondetachment cross section. At low energies the leading term of the total nondetachment cross section, $\sigma_{-1,-1}$, ($\sigma_{-1,-1} \equiv \sigma_{e1} + \sigma_{\text{nonloss,inel}}$) is lower than the total detachment cross section. Because of the logarithmic factor in the incident velocity, the leading term of the nondetachment cross section eventually exceeds the total electron-loss cross section at sufficiently high energy. The energy where this crossover occurs, that is, where $\sigma_{-1,-1}$ is equal to $\sigma_{-1,0} + \sigma_{-1,1}$, is a little above 10 MeV for atomic H targets and slightly more than 300 MeV for He. This says in effect that as the energy increases beyond these values, the loosely bound H⁻ ion has a higher probability of exciting the more tightly bound target atom than it does of exciting itself. The next leading terms for the detachment and nondetachment cross sections are of the opposite sign. Consequently, as the energy is decreased, the nonloss cross section again eventually exceeds the total detachment cross section if only the two terms calculated in this work are retained for each case. However, the basic expansion implicit in the Bethe theory approach for the nonloss inelastic cross section is almost certainly no longer converging in this energy region.

In the case of the total electron-detachment cross sections (23) and (24), the second-order term is of the same magnitude as the leading contribution

at approximately 20 and 80 keV, respectively, for H and He targets. At higher energies, the second-order term rapidly becomes a small correction to the leading term so that in the region where the Born approximation is expected to be valid, above 200 keV or so, the series generated by this approach (of which only the first two terms have been calculated here) appears to rapidly converge, presumably to the exact Born cross section. This is of major importance in the success of the Bethe theory for summed inelastic cross sections, that the implicit expansion converges rapidly to the complete Born cross section in an energy region which is the same as that for the validity of the Born approximation itself. For the case of the nondetachment inelastic cross section of H⁻ examined in this work, the second-order term in (36) is of the same order as the leading term at significantly higher energies than in the case of the electron-loss cross section. This occurs near 100 keV for H-target atoms and near 400 keV in the case of He. This suggests that the series generated by this approach to the total nonloss cross section converges in a region which is significantly smaller than that for the corresponding total detachment cross section, and that it most likely does not converge in the full region of the applicability of the Born approximation.

Examination of the "low-energy correction factor" γ , given by (37) shows that the large values of this term are due to the contributions arising from the structure of the incident ion. The effective expansion parameter in the Bethe theory, as presented here for the cross section $\sigma_{\text{nonloss,inel}}$, contains a factor which is essentially the expectation value of $|\hat{r}_1^{(1)}|^2$. For negative ions this is not a small parameter. Clearly the problem is only associated with the structure of the negative ion; indeed, the Bethe asymptotic cross section for structureless charged particle impact on these same target atoms gives reasonable results.^{12,24}

The results of this work are insufficient to determine conclusively the regions of convergence of the series expansions for the various Born cross sections. It should be noted, however, that if this region is very small for the nonloss cross section, a summation or rearrangement of the series may be required (i.e., a more "exact" evaluation of the Born cross section) which could lead to an alteration of the results concerning the relative sizes of $\sigma_{-1,-1}$ and $\sigma_{-1,0} + \sigma_{-1,1}$.³¹

V. CONCLUSIONS

The extension of the Bethe theory, for the asymptotic cross section for charged-particle impact, to the case where the structure of the charged

particle is treated explicitly, provides a means for the accurate calculation of the total electron-loss cross section for the H^- ion at high energies. The method applied to the specific examples of H and He targets gives results which are in good agreement with experiment. The nonleading corrections, which are important at lower energies, appear to be inadequate based on the very limited data available in that energy region. This tentatively suggests that contributions from the second Born amplitude are required to accurately describe the cross section there. Similar conclusions have been reached by Kim and Inokuti for the case of the detachment cross section for H^- due to electron impact.¹²

The leading contribution to the total elastic cross section calculated in this paper gives results which are physically reasonable, but as yet no experimental data on this cross section have been published in the asymptotic region. The total nonde-

tachment inelastic cross section, as calculated in the modified Bethe theory, gives results which are suspect. An examination of this cross section within a different theoretical framework, or an experimental determination of the ratio $\sigma_{-1,-1}/(\sigma_{-1,0} + \sigma_{-1,1})$ at various energies is suggested for some future work.

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$$S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2 = 2\{1 - [1 + (a_0 K/2)^2]^{-2}\}.$$

For the helium wave function (16) one gets

$$2S_{\text{inc}}^{(2)}(K) + |F_0^{(2)}(K)|^2 = 2\{2 - [1 + (a_0 K/2Z^*)^2]^{-2}\} - 2.$$

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complete to order α^4/β^4 for nonrelativistic energies, but additional corrections may be involved at relativistic energies. However, these terms, give negligible contributions in the asymptotic region (see, however, Ref. 12). Of course, for higher $Z_N^{(2)}$ targets, one expects an effective expansion parameter more like $[Z_N^{(2)}(\alpha/\beta)]^2$. The significantly larger coefficient of the nonleading terms for He than for H is already suggestive of this.

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