High-energy cross sections for H^- ions incident on intermediate and high-Z atoms

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The double-closure Born approximation developed in previous work is used to calculate the asymptotic cross sections for electron loss from H^- ions incident on a variety of atomic targets. Corrections to the closure technique for the next-order terms in heavy-ion–atom cross sections are examined. The corrections for energy conservation are shown to be unimportant, but the Bethe ridge in the inelastic form factors does yield terms which contribute to the next leading order. The total asymptotic electron-loss cross section, and the next-order contribution including the Bethe ridge correction, are calculated using various models for the target atoms obtained from the literature. Comparative results based on Hartree-Fock, configuration-interaction, and relativistic Hartee-Fock wave functions are presented. The results for the electron-loss cross sections for N, O, and Ar target atoms are compared with the available experimental data. Results are also given for parameters which are required for the asymptotic elastic and nondetachment inelastic cross sections. Some comments regarding other applications of these methods are included.

I. INTRODUCTION

Bethe's theory,[1,2] for summed inelastic cross sections in the Born approximation for structureless charged particle impact on atoms, has been extended in recent work so that the structure of the incident ion could be included explicitly.[3] Utilizing sum rules for the final states of both the incident ion and target atom, expressions were derived for the asymptotic (high-energy) cross section, as well as the next leading order contribution (low-energy correction) to the cross section. As an application of the method, the total electron loss cross sections for H^- ions incident on H and He targets were evaluated with a theoretical uncertainty of about 1%. Good agreement was obtained with available experimental data in the asymptotic region. However, sparse data at intermediate energies on those gases permitted very little comparison between theory and experiment down to the lowest energy for which the Born approximation should still be valid. In this paper corrections to the closure approximation and the effect of the Bethe ridge are examined which yield additional terms in the next leading order contribution to the cross section. Cross sections for H^- ions incident on several intermediate and high-Z target atoms are calculated including these terms. Results obtained are then compared with experimental data, which for certain gases is available over a broad energy range including the intermediate region.

II. THEORY

The total electron-loss cross section for H^- ions consists of two contributions, one arising from single electron detachment $\sigma_{-1,0}$ and one arising from double electron detachment $\sigma_{-1,1}$. The sum of these two cross sections was developed in the double-closure Born approximation in previous work[3] and only the results are given here in order to define the parameters calculated in this work. The total electron loss cross section may be expressed as

$$(\sigma_{-1,0}+\sigma_{-1,1}) = 8\pi a_0^2 \frac{\alpha^2}{\beta^2} \sum_{n\neq 0} \sum_{m} [I_{nm} - J_{nm}(\beta^2) - K_{nm}(\beta^2)]. \quad (1)$$

If sums over the final states of the parameter I_{nm} are taken to include all states, energetically accessible or not, the results may be expressed as momentum-transfer integrals over elastic form factors $F_0(K)$ and incoherent scattering functions $S_{\rm inc}(K)$ of the incident ion and target atom. Specifically,

$$\sum_{n\neq 0} I_{n0} = \int_0^\infty Z_e^{(1)} S_{\rm inc}^{(1)}(K) |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)^3}, \quad (2)$$

$$\sum_{n\neq 0}\sum_{m\neq 0} I_{nm} = \int_0^\infty Z_e^{(1)} S_{\rm inc}^{(1)}(K) \times Z_e^{(2)} S_{\rm inc}^{(2)}(K) \frac{d(a_0K)}{(a_0K)^3}. \quad (3)$$

The superscripts 1 and 2 refer to the incident ion and target atom, respectively. These terms are independent of the incident velocity ($\beta = v/c$) and provide the leading order contribution to the cross section at high energy.

Within the context of the Born approximation, the next order contributions to the cross section were given by Eq. (19) of Ref. 3. That correction for low energies is approximate and it includes only the contributions arising from the lower limits of the momentum-transfer integrals, under the assumption that

they are small. Kim and Inokuti[4] have examined the effects of electron exchange, closure, and the contribution of the Bethe ridge[2,4] for the case of structureless charged-particle impact on light ions and atoms. Corrections for the closure approximation arise because the sums over the final states appearing in Eqs. (1)–(3) have been extended to all states, although in an exact calculation they should be restricted to only those states with excitation energies which are less than or equal to those permitted by the conservation of energy. In the case of heavy ions (as opposed to electrons) further corrections arise because the kinematical lower limit of the momentum transfer integral is no longer small for highly excited states, and can exceed the value where the inelastic form factors reach their maximum value. This correction will be referred to as the Bethe-ridge correction.[5]

The closure and Bethe-ridge corrections require, in principle, a detailed knowledge of the inelastic form factors (i.e., the generalized oscillator strengths) in order to calculate their effects precisely. However, using techniques similar to those developed by Kim and Inokuti, the next leading order contributions to the cross sections for these corrections may be evaluated approximately using known properties of the form factors together with simple physical arguments.

As an example, consider corrections which arise to the asymptotic sum rule contributions given by Eq. (2). The exact contributions to the electron detachment cross section, which arise from a collision in which the target atom remains in the ground state, may be written

$$\sum_{n\neq 0}^{n_{\max}} [I_{n0} - J_{n0}(\beta^2) - K_{n0}(\beta^2)] = \sum_{n\neq 0}^{n_{\max}} \int_{a_0K_{\min}}^{a_0K_{\max}} |F_n^{(1)}(K)|^2 |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)^3} . \tag{4}$$

The upper limit $n_{\max}$ on the summation is obtained from conservation of energy. Taking the difference between this and the asymptotic form given by (2) yields a low-energy correction which will be written as the sum of three contributions:

$$\sum_{n\neq 0}^{n_{\max}} [I_{n0} - J_{n0}(\beta^2) - K_{n0}(\beta^2)] - \sum_{n\neq 0}^{\infty} I_{n0} = -\left(\sum_{n\neq 0}^{n_{\max}} J_{n0}(\beta^2) + \sum_{n\neq 0}^{n_{\max}} K_{n0}(\beta^2) + \sum_{n_{\max}}^{\infty} I_{n0}\right) . \tag{5}$$

The summations in Eq. (5) may all be expressed as integrals over the excitation energy of the incident ion, since all excitations of the H^- ion are in the continuum. The inelastic form factors may be written in terms of the continuum generalized oscillator strengths $df^{(1)}(K,E)/dE$ as

$$|F_n^{(1)}(K)|^2 = \frac{(a_0K)^2}{E} \frac{df^{(1)}(K,E)}{dE} , \tag{6}$$

in analogy with Eq. (4) of Ref. 3. The excitation energy of the ion ($E_n^{(1)}$ in Ref. 3) is now simply given as E. In this notation the terms on the right-hand side of Eq. (5) may be expressed as

$$\sum_{n\neq 0}^{n_{\max}} J_{n0}(\beta^2) = \int_{E_B^{(1)}}^{E_{\max}^{(1)}} \frac{dE}{E} \int_0^{a_0K_{\min}} \frac{df^{(1)}(K,E)}{dE} \times |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)} , \tag{7}$$

$$\sum_{n\neq 0}^{n_{\max}} K_{n0}(\beta^2) = \int_{E_B^{(1)}}^{E_{\max}^{(1)}} \frac{dE}{E} \int_{a_0K_{\max}}^{\infty} \frac{df^{(1)}(K,E)}{dE} \times |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)} , \tag{8}$$

$$\sum_{n_{\max}}^{\infty} I_{n0} = \int_{E_{\max}^{(1)}}^{\infty} \frac{dE}{E} \int_0^{\infty} \frac{df^{(1)}(K,E)}{dE} \times |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)} . \tag{9}$$

The minimum and maximum excitation energies appearing in (7)–(9) are the binding energy of the incident H^- ion, $E_B^{(1)}$, and $E_{\max}^{(1)}$ determined from conservation of energy,

$$E_{\max}^{(1)} = \tfrac{1}{2}M\beta^2 . \tag{10}$$

As in Ref. 3, M is the reduced mass, and all masses and energies are assumed to be in rydbergs.

The approximate evaluation of Eqs. (7)–(9), valid for large β, only requires the use of sum rules and a few properties of the generalized oscillator strengths. Rau and Fano[6] derived results for the asymptotic form of $df^{(1)}(K,E)/dE$ for either large K or large E. Their results for the case under consideration may be expressed as

$$\frac{df^{(1)}(K,E)}{dE} \propto \begin{cases} (a_0K)^{-2(L+5)}, & a_0K \gg E^{1/2}; \\ (a_0K/E^{1/2})^{2(L-1)}(E)^{-7/2}, & E^{1/2} \gg a_0K , \end{cases} \tag{11}$$

and L is an integer ≥ 0. The asymptotic behavior given in (11) is modified for the case where $E \sim (a_0K)^2 \gg E_B^{(1)}$. The generalized oscillator strength has a maximum in this region, frequently referred to as the Bethe ridge. Following the arguments given by Kim and Inokuti, a free-electron approximation should be adequate for the leading order, i.e.,

$$\frac{df^{(1)}(K,E)}{dE} \simeq Z_e^{(1)}\delta[(a_0K)^2 - E]\,,$$
$$a_0K \sim E^{1/2} \gg (E_B^{(1)})^{1/2}\,. \quad (12)$$

The contributions given by (7) may be evaluated by dividing the integral over excitation energy into two parts,

$$\sum_{n\neq 0}^{n_{\max}} J_{n0}(\beta^2) = \int_{E_B^{(1)}}^{\bar{E}^{(1)}} \frac{dE}{E} \int_0^{a_0K_{\min}} \frac{df^{(1)}(K,E)}{dE} \times |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)} + \int_{\bar{E}^{(1)}}^{E_{\max}^{(1)}} \frac{dE}{E} \int_0^{a_0K_{\min}} \frac{df^{(1)}(K,E)}{dE} \times |F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)}\,. \quad (13)$$

The parameter $\bar{E}^{(1)}$ represents a mean excitation energy of the H^- ion. The precise value will be unimportant provided it is much greater than $E_B^{(1)}$, serving to define the region of applicability of Eq. (11) and (12). The first term in (13) may be evaluated by expanding $df^{(1)}(K,E)/dE$ and $F_0^{(2)}(K)$ for small K and integrating. The second term gives no significant contributions for small K due to the large-E behavior of (11). However, $K_{\min}$ can, in fact, become large enough so that the conditions in (12) are satisfied. Consequently,

$$\sum_{n\neq 0}^{n_{\max}} J_{n0}(\beta^2) \simeq \frac{|F_0'^{(2)}(0)|^2}{4} \times \int_{E_B^{(1)}}^{\bar{E}^{(1)}} \frac{df^{(1)}(0,E)}{dE}(a_0K_{\min})^4 \frac{dE}{E} + \frac{Z_e^{(1)}}{2} \int_{\bar{E}^{(1)}}^{E_{\max}^{(1)}} \Theta[(a_0K_{\min})^2 - E] \times \left|F_0^{(2)}\left(\frac{E^{1/2}}{a_0}\right)\right|^2 \frac{dE}{E^2}\,. \quad (14)$$

Examination of the step function in the second integral of (14) shows that it in effect replaces the lower integration limit by $(1+m_e/M)^{-2}4\beta^2/\alpha^2$. To lowest order in an expansion in β^{-2}, $K_{\min}$ is given by

$$(a_0K_{\min})^2 \simeq \tfrac{1}{4}(\alpha^2/\beta^2)E^2\,. \quad (15)$$

To this same order, the first integral in (15) gives no contribution and the second yields

$$\sum_{n\neq 0}^{n_{\max}} J_{n0}(\beta^2) \simeq \frac{Z_e^{(1)}|Z_N^{(2)}|^2}{2} \times \left[\frac{1}{4}\left(1+\frac{m_e}{M}\right)^2 - \frac{m_e}{M}\right]\frac{\alpha^2}{\beta^2}\,, \quad (16)$$

utilizing the asymptotic behavior of $F_0^{(2)}(E^{1/2}/a_0)$ from Eq. (21) of Ref. 3. The first term in (16) is a consequence of the Bethe ridge; the second comes from the finite value of the maximum excitation energy allowed by energy conservation.

The contributions to lowest order in α^2/β^2 arising from (9) in the limit where $E_{\max}^{(1)}$ is taken to infinity (i.e., in the closure approximation) were derived previously and shown to be small [second term of Eq. (22) in Ref. 3]. However, when a finite value for $E_{\max}^{(1)}$ is used, these terms in fact give no contribution to this order owing to the asymptotic form of the generalized oscillator strength given by the first line in (11). (The small, finite result obtained in the closure approximation when $K_{\max}$ is expanded to lowest order arose because the Bethe ridge in that approximation is inadvertently included in the region of integration.)

Equation (10) yields a correction for closure arising from the finite value of $E_{\max}^{(1)}$. From (11), it is clear that no contribution to lowest order occurs either for very small, or very large momentum transfer. Only the Bethe-ridge region of the integral gives any significant contribution. Substituting in the approximation (12) yields

$$\sum_{n_{\max}}^{\infty} I_{n0} \simeq \frac{Z_e^{(1)}|Z_N^{(2)}|^2}{2}\frac{m_e}{M}\frac{\alpha^2}{\beta^2}\,, \quad (17)$$

which cancels the second term of Eq. (16). This cancellation assures that no effect on the closure approximation from the constraints of energy conservation appear to order α^4/β^4 in these contributions to the cross section. In contrast to problems involving electron collisions, where energy conservation does play a role at the velocities of interest, there is ample energy available in the case of heavy ions at these same velocities to permit excitation to a much larger number of final states. However, the dynamical structure of the atom, in particular the Bethe ridge, coupled with the kinematical constraint on the minimum momentum transfer allowed, does have an impact on corrections to order α^4/β^4.

The leading low-energy corrections to (3) may also be evaluated in a similar manner, although the larger number of terms which must be considered complicates the analysis somewhat. Within the context of the closure approximation, and the assumption of small values of $K_{\min}$, the leading contributions were given previously [Eq. (19) of Ref. 3]. When closure corrections are included it can be shown that the limits imposed on the summations in (3) by the conservation of energy give no contributions to lowest order, whereas the Bethe ridge introduces an additional contribution to lowest order which may be expressed as

$$\sum_{n\neq 0}\sum_{m\neq 0} J_{nm}(\beta^2)\Big|_{\substack{\text{Bethe}\\ \text{ridge}}} \simeq \tfrac{1}{8}Z_e^{(1)}Z_e^{(2)}\left(1+\frac{m_e}{M}\right)^2\frac{\alpha^2}{\beta^2}\,. \quad (18)$$

When closure corrections are included, no contributions to this order arise from $K_{\max}$.

In summary, the corrections to the asymptotic total electron-loss cross section when closure and Bethe-ridge corrections have been included, are given by

$$\sum_{n\neq 0}\sum_{m} J_{nm}(\beta^2) \simeq \frac{1}{8}\left(\frac{\alpha^2}{\beta^2}\right)[S^{(1)}(-1)S^{(2)}(1) + 3S^{(1)}(0)S^{(2)}(0) + S^{(1)}(1)S^{(2)}(-1) + Z_e^{(1)}|Z_N^{(2)}|^2], \quad (19)$$

where terms of order m_e/M have been neglected, and the Thomas-Kuhn-Reiche sum rule has been used. This result should replace that of Eq. (19) in Ref. 3.

III. CALCULATION OF THE CROSS SECTIONS AND COMPARISON WITH EXPERIMENT

The leading order contributions to the total electron-loss cross sections for H^- ions have been calculated for the target atoms C, N, and O as well as for all the noble gases (except He which was calculated in Ref. 3). The integrals given by Eq. (2) and (3) have been evaluated using the $F_0^{(2)}(K)$ and $Z_e^{(2)}S_{\rm inc}^{(2)}(K)$ given by Hubbell *et al.*[7] For atoms with Z greater than 6, these are based on Hartree-Fock values due to Cromer and Mann.[8] For C the Hubbell *et al.* tables are based on a configuration interaction wave function from Brown.[9] Integrals (2) and (3) were also evaluated using the form factors and incoherent scattering functions given by Tanaka and Sasaki[10] for N, O, and Ne and by Naon *et al.*[11] for Ar, all obtained from configuration-interaction wave functions. The impact of relativistic effects on the elastic form factors has been examined by Doyle and Turner[12]; the integral in (2) has been evaluated using their form factors for the heavier noble gases. The results of these calculations are given in Table I. In each case the incoherent scattering function of H^- due to Kim[13] has been used.

It should be noted that in cases where the published tables did not extend into the asymptotic regions of large momentum transfer, a "tail" was included using the tables from Hubbell *et al.* In addition, for a_0K less than 0.1, the elastic form factors and incoherent scattering functions were constrained to be given by

$$F_0^{(j)}(K) \simeq F_0^{(j)}(0) + F_0'^{(j)}(0)(a_0K)^2, \quad a_0K \ll 1; \quad (20)$$

$$Z_e^{(j)}S_{\rm inc}^{(j)}(K) \simeq S^{(j)}(-1)(a_0K)^2, \quad a_0K \ll 1. \quad (21)$$

The values for these parameters used in carrying out the integrations in Eqs. (2) and (3) are also given in Table I. They have been estimated in most cases from the low momentum-transfer behavior of the results given by Hubbell *et al.* The values of $S^{(2)}(-1)$ determined in this way for the noble gases are in generally good agreement with other direct calculations using Hartree-Fock wave functions such as those of Bell and Dalgarno.[14,15] Other parameter values for N, O, and Ne have been estimated from the tables of Tanaka and Sasaki, and for Ar from the direct calculation by Naon

TABLE I. Results of the numerical evaluation of the integrals given by Eqs. (2) and (3) for the case of H^- ions incident on various target atoms. In all cases the H^- incoherent scattering function of Kim for a 39-term Wiess wave function has been used (Ref. 13). For the target atoms, the models examined include Hartree-Fock (HF), configuration-interaction (CI), and relativistic-Hartree-Fock (RHF), as described in Refs. 7–12. Also given are the atomic parameters which fix the low-momentum-transfer region of the elastic form factors and incoherent scattering functions according to Eqs. (20) and (21). Representative errors associated with the numerical integrations are given for certain cases.

Atom	Model (Ref.)	$S^{(2)}(-1)$	$F_0'^{(2)}(0)$	$\sum_{n\neq 0} I_{n0}$	$\sum_{n\neq 0}\sum_{m\neq 0} I_{nm}$
C	CI(7,9)	2.94	2.30	10.4	6.45
N	HF(7,8)	2.92	2.08	11.7	6.88
	CI(10)	2.6	2.0	11.6	6.16
O	HF(7,8)	2.53	1.87	12.8	6.58
	CI(10)	2.3	1.9	12.7 ± 0.1	6.05 ± 0.01
Ne	HF(7,8)	2.02	1.56	14.3	6.00
	CI(10)	1.9	1.6	14.3 ± 0.1	5.60 ± 0.01
Ar	HF(7,8)	5.42	4.31	52.6	12.6
	CI(11)	4.27	4.12	51.7 ± 0.3	10.7 ± 0.1
Kr	HF(7,8)	7.79	6.55	135	17.8
Xe	HF(7,8)	11.6	10.4	290	25.0
	RHF(12)	...	10.4	284	...
Rn	HF(7,8)	14.4	13.4	537	30.8
	RHF(12)	...	13.4	513	...

TABLE II. Values of $S^{(2)}(\mu)$ for $\mu=-1$, 0, 1 and the resulting sum of Eq. (19) times (β^2/α^2), for small α^2/β^2, including the Bethe-ridge correction.

Atomic system [a]	$S^{(2)}(-1)$ $(M^2_{\rm tot})$	$S^{(2)}(0)$ $(Z_e^{(2)})$	$S^{(2)}(1)$	$\frac{\beta^2}{\alpha^2}\sum_{n\neq 0}\sum_m J_{nm}(\beta^2)$
H	1	1	$\frac{4}{3}$	2.434
H_2(17)	1.55	2	3.34	2×2.71
He(16)	0.7525	2	8.167	10.28
C	2.9	6	1.0×10^2	1.1×10^2
N	2.6	7	1.5×10^2	1.6×10^2
O	2.3	8	2.0×10^2	2.1×10^2
Ne(14)	2.02	10	3.03×10^2	3.16×10^2
Ar(14)	5.502	18	1.149×10^3	1.170×10^3
(18)	4.409	18	1.115×10^3	1.138×10^3
Kr(14)	7.86	36	5.34×10^3	5.35×10^3
Xe(14)	10.3	54	1.32×10^4	1.31×10^4
Rn(14,15)	14.4	86	3.63×10^4	3.59×10^4

[a] Values of $S^{(2)}(-1)$ and $S^{(2)}(1)$ are from the references indicated in parentheses.

et al.

As can be seen from the results given in Table I the asymptotic total electron-loss cross section, for H^- incident on the target atoms considered here, is dominated by collisions in which the target atom remains in the ground state $(\sum_{n\neq 0} I_{n0})$. Within the context of the Hartree-Fock (HF) model of the target atoms,[7,8] this contribution accounts for nearly 63% of the cross section for N, and increases monotonically with $Z_N^{(2)}$ to nearly 95% for H^- incident on Rn. (This percentage was only about 20%, 22%, and 28% for the cases of H, H_2, and He targets considered in Ref. 3.) The results are similar when configuration interactions (CI) are included in the wave functions as described in Ref. 10 and 11. As noted by several authors,[7-11] the role of electron correlations is important in accurately describing the incoherent scattering function of a many electron atom. This is reflected by significant differences in $S^{(2)}_{\rm inc}(K)$ obtained from HF and CI models of the atoms.[7-11] The contributions to the total electron-loss cross section arising from this function $(\sum_{n\neq 0}\sum_{m\neq 0} I_{nm})$ are reduced from the HF values, when CI models are used. The reduction in this contribution is about 10% for N and increases to about 15% for the case of Ar targets. However, the elastic form factors are not significantly affected by the inclusion of configuration interactions in the wave functions.[7-11] Since this gives the dominant contribution to the total electron-loss cross section for these atomic targets, the resulting difference in this cross section for the HF and CI models considered is only of the order of (2-4)%. Relativistic-Hartree-Fock (RHF) calculations of the elastic form factors have indicated differences from HF values.[12] The impact on the electron-loss cross sections is a reduction of about 2% and 4% for the heaviest targets considered, Xe and Rn, respectively. This examination of the influence of different models of the target atoms, suggests that the theoretical uncertainties in the leading (asymptotic) term of the total electron-loss cross section for H^- may be of the order of 5%.

The next order terms for these cross sections, from Eq. (19), are given in Table II, together with the parameters used. The H^- parameters required are those of Pekeris,[16] also given in Table I of Ref. 3. For comparison the results for atomic H and He have been restated, but now include the contribution of the Bethe ridge to this order, and results for H_2 are given based on the energy moments of the oscillator strengths of Gerhart.[17] The parameter values $S^{(2)}(-1)$ and $S^{(2)}(1)$ for He are also from Pekeris, and for the other noble gases from Bell and Dalgarno. For comparison, the more recent Ar values of Eggarter[18] are also given. For C, N, and O, the values of $S^{(2)}(-1)$ are the same as those determined for Table I; the values of $S^{(2)}(1)$ were estimated from the total energy of the atoms.[19] The Bethe-ridge contribution to the total low-energy correction given by (19) varies between 20% for H to about 5% for Rn. In all cases, this order in the expansion of the cross section is dominated by the first term in Eq. (19).

For completeness the parameters I_{00} and $g_1 - g_2$, required for evaluating the elastic and nondetachment inelastic cross sections, have been calculated and are summarized in Table III. The asymptotic elastic cross section is completely determined by I_{00}, but the nonloss inelastic cross section requires $L^{(2)}(-1)$ as well as $g_1 - g_2$ (see Sec. IID of Ref. 3). While $L^{(2)}(-1)$ can, in principle, be determined from the ordinary oscillator

TABLE III. Values of the parameters I_{00} and $\mathcal{J}_1 - \mathcal{J}_2$ which are required to evaluate the total elastic and nondetachment inelastic cross sections. The low momentum-transfer region of the elastic form factors and incoherent scattering functions was fixed according to Eqs. (20) and (21) using the same parameters as given in Table I. Representative numerical integration errors are indicated.

Atom	Model (Ref.)	$\mathcal{J}_1 - \mathcal{J}_2$	I_{00}
C	CI(7, 9)	−6.51	2.80
N	HF(7, 8)	−6.24	3.40
	CI(10)	−5.52	3.37
O	HF(7, 8)	−5.06	3.95
	CI(10)	−4.51 ± 0.01	3.95 ± 0.03
Ne	HF(7, 8)	−3.57	4.90
	CI(10)	−3.35 ± 0.01	4.91 ± 0.04
Ar	HF(7, 8)	−11.5	15.7
	CI(11)	−8.60 ± 0.01	15.6 ± 0.1
Kr	HF(7, 8)	−16.5	43.7
Xe	HF(7, 8)	−19.5	92.4
	RHF(12)	...	90.0
Rn	HF(7, 8)	−31.4	180
	RHF(12)	...	171

strength distribution, it is only known for a few atomic systems. Among the target atoms examined in this work, a reasonably accurate value of 2.84 has been given by Eggarter[18] for Ar. The parameter $\ln c_{\text{tot}}^{(2)}$ which appears in the expression for the nonloss inelastic cross section, comes out to be

$$\ln c_{\text{tot}}^{(2)}(\text{Ar}) = \begin{cases} -2.23 & (\text{HF}), \\ -2.15 & (\text{CI}). \end{cases}$$

Note that $\mathcal{J}_1 - \mathcal{J}_2$ is quite sensitive to the value of $S^{(2)}(-1)$, but the ratio $(\mathcal{J}_1 - \mathcal{J}_2)/S^{(2)}(-1)$ giving the dominant contribution to $\ln c_{\text{tot}}^{(2)}$ is much less sensitive to this parameter. Unfortunately, the actual cross section $\sigma_{\text{nonloss,inel}}$ is proportional to $S^{(2)}(-1)$ $\ln c_{\text{tot}}^{(2)}$, and is consequently very sensitive to $S^{(2)}(-1)$. Because of the theoretical uncertainties in these parameters, and the lack of experimental data with which to compare results, no further discussion of this cross section will be undertaken.[20]

Figure 1 summarizes the available experimental data for the total electron-loss sections for H^- ions incident on N_2, O_2, and Ar,[21-26] and shows the theoretical results for the cross sections on N, O, and Ar obtained in this work. For comparison, the results of this work for a heavier noble gas Xe are also shown. Fremlin and Spiers[27] and Verba *et al.*[28] have determined the effective electron-loss cross section per air atom in the regions 1.5–5.5 MeV and 14–45 MeV, respectively, by observing H^- beam loss in a cyclotron and assuming an inverse energy dependence for the cross sections. Their results are shown by broken lines in Fig. 1.

The theoretical cross sections shown are based on the configuration interaction wave functions for N, O, and Ar; the Xe results use the relativistic-Hartree-Fock elastic form factor. In each case the low-energy corrections have been included from Table II, but the plots only extend down in energy until the maximum value of the cross section has been attained. For the case of N and O targets in the asymptotic region, the agreement with the experimental data is satisfactory, with the possible exception of the data of Fremlin and Spiers.[27] At intermediate energies, the experimental data appear to drop slightly below the asymptotic form of the cross section before the low energy corrections given in Table II become significant. However, the two term expansion for the cross section does correctly indicate the energy below which a significant departure from the asymptotic cross section occurs.

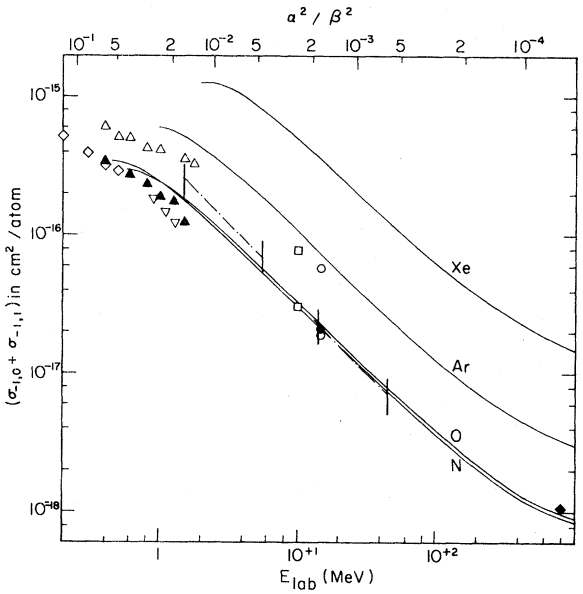

FIG. 1. Total electron-loss cross section $(\sigma_{-1,0} + \sigma_{-1,1})$ for H^- incident on N, O, Ar, and Xe targets as a function of energy. Solid curves are the theoretical results of this work. Open symbols are data on N_2 and Ar; solid symbols are data on O_2: △ ▲, from Rose *et al.* (Ref. 21, $\sigma_{-1,0}$ only); ◇, from Kovács (Ref. 22); ▽, from Dimov and Dudnikov (Ref. 23); □, from Berkner *et al.* (Ref. 24, 20-MeV D^-); ○ ●, from Symthe and Toevs (Ref. 25); ◆, from Hayward and Tesmer (Ref. 26). Broken lines give data on air from Fremlin and Spiers (Ref. 27), 1.5–5.5 MeV; and from Verba *et al.* (Ref. 28), 14–45 MeV. The upper scale gives the expansion 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 mass.

For the case of Ar targets, the experimental data lie significantly below the theoretical results of this work at all energies. Based on the discussion given in comparing the results of various target atom models, it does not appear that the theoretical uncertainties in the asymptotic cross section would be sufficient to explain this discrepancy, although this possibility cannot be entirely ruled out. It may be that the total electron-loss cross section for H^- on Ar has not yet reached its asymptotic value at 14.6 MeV, the highest-energy data available. In connection with this, it should be mentioned that the inclusion of the second Born amplitude in the scattering matrix would in principle yield a contribution to order α^3/β^3 in the expansion for the cross section. This is between the asymptotic order (α^2/β^2), and the low-energy correction (α^4/β^4) to the cross sections given here, and could conceivably explain a slower approach to the asymptotic value. However, without further analysis this must be regarded as only a speculative explanation at present. (Earlier theoretical estimates of the electron-loss cross sections for H^- on N_2, O_2, and Ar due to Wright[29] using the free collision approximation, give asymptotic values which are more than 50% above those calculated in this work. However, only very simple models of the targets, as well as of H^-, were used in those estimates.)

IV. CONCLUSIONS

The results of this work indicate that the asymptotic total electron-loss cross section for H^- ions incident on atoms of arbitrary Z can be calculated with high theoretical accuracy, utilizing existing tables for the required atomic properties. The next leading order contributions to the cross section appear to give at the least a reasonable prediction of where significant departures from the asymptotic form of the cross sections can be expected. Based on the comparison with experiments on Ar, the heaviest target for which data is available, the approach to the asymptotic cross section appears to be slower than that predicted by the next leading term. An examination of the second Born amplitude could shed considerable light on this. Additional experimental data at very high velocities and on heavier targets would also be very useful in this respect.

In a broader context, the double closure Born approximation, based on a generalization of the Bethe theory for the total inelastic cross section, provides a simple method for calculating selected high-energy cross sections in ion-atom scattering. Utilizing only ground-state properties and energy moments of the ordinary oscillator strength distribution, all but one of which $[L^{(2)}(-1)]$ may also be related to ground-state expectation values, both the asymptotic and next leading order contribution to the Born cross sections may be obtained. The methods developed can be applied to a wide class of problems of current interest. Very recently, Inokuti[30] has also examined these techniques with a view toward more general applications, and has calculated explicit results for the case of collisions between one-electron ions. Currently, this approach is being utilized to obtain total excitation plus ionization cross sections for low charge-state heavy ions[31] utilizing atomic properties for these ions calculated by Kim.[32] Based on the results of this and previous work, these methods can be expected to provide accurate cross sections with a relatively small investment of effort.

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[20]Corrections for energy conservation and the Bethe ridge do not occur for the elastic cross section and the next leading order contribution to that cross section as given in Ref. 3 is unaltered. The Bethe ridge does contribute to the next leading order of $\sigma_{\text{nonloss, incl}}$. An additional term of $-\frac{1}{4}|Z_N^{(1)}|^2 Z_e^{(2)}$ should be added to the expression for γ in Eq. (37) of Ref. 3, to include this effect. While this alters the numerical results somewhat, the general discussion of this cross section in Ref. 3 is unaffected.
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