Born cross sections for ion-atom collisions

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Selected total cross sections are calculated in the closure-Born approximation for the ions Li^+, Cs^+, and Au^+ incident on several gas constituents. Targets included are H, H_2, He, C, N, and O. Four general types of cross sections are considered depending on whether the incident ion or target atom is scattered elastically or inelastically. Expressions are given for the Born cross sections to the first two orders in an expansion in β^{-2}, where $\beta = v/c$ and v is the relative velocity. The atomic form factors and incoherent-scattering functions for the ions Cs^+ and Au^+, which are required in order to evaluate the leading-order cross-section parameters, are calculated from the relativistic and nonrelativistic Hartree-Fock wave functions. Results are also given for some of the energy moments of the dipole-oscillator-strength distributions for Cs^+ and Au^+, as determined from the ground-state wave functions. These parameters, together with atomic properties taken from the literature for Li^+ and the various targets considered are then used to evaluate the cross sections to the first two orders in the expansion.

I. INTRODUCTION

The use of sum rules in calculating Born-approximation cross sections for atomic collisions involving both complex ions and atoms has recently been examined in some detail.[1,2] The techniques developed, which are valid for collisions at large relative velocities, are applicable to certain classes of total cross sections in which only sums over all possible final states, or all final states except the initial state, are required. The method is particularly simple to apply, since the closure property of the energy eigenstates permits the evaluation of all but one of the required atomic properties in terms of initial-state expectation values.

For all neutral atoms the ground-state properties are available already or they may be evaluated from other known atomic data. However, application of these methods to a number of problems of current interest is presently limited by the unavailability of suitable ground-state properties for all but a few ions. In this paper we present results for these properties for the ions Cs^+ and Au^+, and together with available data for Li^+,[3] calculate the various cross-section parameters for these ions incident on a variety of atoms characteristically associated with background gases in accelerators. Some of the results for Li^+ are compared with available experimental data on the electron-loss cross sections $\sigma_{1,2}$. The cross sections for Cs^+ and Au^+ are of interest since they may be used to establish vacuum requirements for accelerators or storage rings using these ions. Heavy ions with closed-shell configurations are considered potential candidates for projectiles to be used in the pellet fusion scheme by heavy ions.[4]

Although we used a nonrelativistic formulation of the collision process, both relativistic and nonrelativisitic wave functions were used for the form factors and other atomic properties to account for the relativistic change in electron distributions of the Cs^+ and Au^+ ions.

II. THEORY OF THE CROSS SECTIONS

Cross sections for collisions between two atomic particles, either ions or atoms, may be broadly categorized according to whether or not the final electronic states differ from the initial states. If both of the colliding particles have atomic structure, i.e., are not electrons or fully stripped ions, then there are four distinct types of such cross sections: For each atomic system, either the final electronic state is the same as the initial state (elastic), or it is a different state (inelastic). In the context of the Born approximation, neglecting exchange, the cross sections, differential in momentum transfer, may be written in terms of the form factors connecting specific initial and final states. Total cross sections for collision processes in which either (or both) of the particles are scattered inelastically are obtained by summing over final states and integrating over the momentum transfer. Kinematical constraints on the momentum transfer, and conservation of energy constraints on the possible final states, place restrictions on the integration and summation which make the exact evaluation of this type of cross section impractical for complex ions or atoms. Consequently an expansion

of the Born cross section in terms of β^{-2} ($\beta = v/c$, where v is the relative velocity) has been developed in recent work[1,2] which permits a precise evaluation of these cross sections to the first two orders in the expansion. This technique is based on a generalization of the Bethe theory for the total inelastic cross section for structureless charged-particle impact on atoms, and closely follows the development of that theory given by Kim and Inokuti.[5]

Various aspects of the theory have been derived in the previous work,[1] but a comprehensive summary of the results is still lacking. In this section we review some of the important aspects of the theory and provide a complete description of the first two orders for the cross sections. Following the previous work,[1] superscripts (1) and (2) are used to label parameters or functions associated with the incident particle and target particle, respectively. We also adopt a notation for the different cross-section types which uses ordered subscripts to indicate whether the incident particle (1), first subscript, or the target particle (2), second subscript, are scattered elastically (el) or inelastically (in). There are four possible types of cross sections and for the case in which the incident particle is an ion and the target particle is a neutral atom or molecule, the first two orders to the Born cross sections may be written (nonrelativistically)

$$\sigma_{\mathrm{el,el}} = 8\pi a_0^2(\alpha^2/\beta^2)[I_{\mathrm{el,el}} + (\alpha^2/\beta^2)\gamma_{\mathrm{el,el}}], \tag{1}$$

$$\sigma_{\mathrm{in,el}} = 8\pi a_0^2(\alpha^2/\beta^2)[I_{\mathrm{in,el}} + (\alpha^2/\beta^2)\gamma_{\mathrm{in,el}}], \tag{2}$$

$$\sigma_{\mathrm{in,in}} = 8\pi a_0^2(\alpha^2/\beta^2)[I_{\mathrm{in,in}} + (\alpha^2/\beta^2)\gamma_{\mathrm{in,in}}], \tag{3}$$

$$\sigma_{\mathrm{el,in}} = 4\pi a_0^2(\alpha^2/\beta^2)\{S^{(2)}(-1)\,|F_0^{(1)}(0)|^2 \times \ln[4c_{\mathrm{el,in}}(\beta^2/\alpha^2)] + (\alpha^2/\beta^2)\gamma_{\mathrm{el,in}}\}. \tag{4}$$

The parameters a_0 and α are the Bohr radius and fine-structure constant, and as previously indicated β is the relative velocity divided by the speed of light. The terms in brackets may be regarded as a measure of the collision strength to the first two orders in β^{-2}.

These results for the forms of the asymptotic (leading-order) Born cross sections are generally well known. The elastic cross section, Eq. (1), is valid as long as one of the colliding particles is neutral. If both particles are ions, the total elastic (Coulomb) cross section diverges. The cross section given by Eq. (4), describing inelastic collisions of the (neutral) target atom while the incident ion is scattered elastically, is the same form as the Bethe asymptotic cross section for total inelastic scattering due to structureless charged-particle impact. For the collision between two neutrals, $\sigma_{\mathrm{el,in}}$ changes to the form of Eq. (2) with labels for the incident and target particles interchanged. Inelastic scattering of an incident ion, without excitation of the neutral target, is described by Eq. (2). The doubly inelastic cross section $\sigma_{\mathrm{in,in}}$ is valid for any combination of charged and neutral particles. (Of course, $\sigma_{\mathrm{in,el}}$ and $\sigma_{\mathrm{in,in}}$ vanish for incident structureless charged particles since their electronic states cannot change.)

Expressions for the leading term in each of the first three cross sections, Eqs. (1)–(3), may be written as integrals over momentum transfer K. Restricting our attention to the case where initially both the incident ion and target atom are in their respective ground states, then the integrands consist either of elastic form factors, $F_0^{(j)}(K)$, or with the aid of a sum rule, incoherent scattering functions $S_{\mathrm{inc}}^{(j)}(K)$, or a combination of both. Specifically

$$I_{\mathrm{el,el}} = I_{00} = \int_0^\infty |F_0^{(1)}(K)|^2\,|F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)^3}, \tag{5}$$

$$I_{\mathrm{in,el}} = \sum_{n\neq 0} I_{no} = \int_0^\infty Z_e^{(1)} S_{\mathrm{inc}}^{(1)}(K)\,|F_0^{(2)}(K)|^2 \frac{d(a_0K)}{(a_0K)^3}, \tag{6}$$

$$I_{\mathrm{in,in}} = \sum_{n\neq 0}\sum_{m\neq 0} I_{nm} = \int_0^\infty Z_e^{(1)} S_{\mathrm{inc}}^{(1)}(K) Z_e^{(2)} S_{\mathrm{inc}}^{(2)}(K) \frac{d(a_0K)}{(a_0K)^3}, \tag{7}$$

where $Z_e^{(j)}$ is the number of electrons in the jth particle. The functions $F_0^{(j)}(K)$ and $S_{\mathrm{inc}}^{(j)}(K)$ are defined by

$$F_0^{(j)}(K) = Z_N^{(j)} - {}_j\langle 0 | \sum_{l=1}^{Z_e^{(j)}} \exp(i\vec{K}\cdot\vec{r}_l^{(j)})\,|0\rangle_j, \tag{8}$$

and

$$Z_e^{(j)} S_{\mathrm{inc}}^{(j)}(K) = {}_j\langle 0 | \left| Z_N^{(j)} - \sum_{l=1}^{Z_e^{(j)}} \exp(i\vec{K}\cdot\vec{r}_l^{(j)}) \right|^2 |0\rangle_j - |F_0^{(j)}(K)|^2 \tag{9}$$

where ${}_j\langle 0|\cdots|0\rangle_j$ denotes the expectation value in the ground state (of the jth particle) and $Z_N^{(j)}$ is the nuclear charge of the jth particle. The intermediate equalities in Eqs. (5)–(7) are given in order to relate the notation of this work to that given in previous papers.[1]

The leading term of the Bethe-type cross section Eq. (4) involves not only an integral over momentum transfer with these functions, but also requires two kinds of energy moments of the dipole

oscillator strengths of the target atom. The parameter $c_{\mathrm{el,in}}$ is given by[6]

$$\ln c_{\mathrm{el,in}} = \frac{\mathcal{I}_1 - \mathcal{I}_2 - 2|F_0^{(1)}(0)|^2 L^{(2)}(-1)}{|F_0^{(1)}(0)|^2 S^{(2)}(-1)}, \tag{10}$$

where $\mathcal{I}_1$ and $\mathcal{I}_2$ are the momentum transfer integrals given by

$$\mathcal{I}_1 = 2\int_\lambda^\infty |F_0^{(1)}(K)|^2 Z_e^{(2)} S_{\mathrm{inc}}^{(2)}(K) \frac{d(a_0K)}{(a_0K)^3}, \tag{11}$$

$$\mathcal{I}_2 = 2\int_0^\lambda \left[|F_0^{(1)}(0)|^2 S^{(2)}(-1)(a_0K)^2 - |F_0^{(1)}(K)|^2 Z_e^{(2)} S_{\mathrm{inc}}^{(2)}(K)\right] \frac{d(a_0K)}{(a_0K)^3}$$

$$-2|F_0^{(1)}(0)|^2 S^{(2)}(-1)\ln(\lambda). \tag{12}$$

These are generalizations of the corresponding integrals for structureless ions; the structure of the incident ion is included via the elastic form factor, $F_0^{(1)}(K)$. Note that the combination $\mathcal{I}_1 - \mathcal{I}_2$ appearing in Eq. (10) is independent of λ.[1] The energy moments of the dipole oscillator strengths, $S^{(2)}(-1)$ and $L^{(2)}(-1)$, may be obtained from the general definitions

$$S^{(j)}(\mu) = \sum_{n\neq 0} [E_n^{(j)}]^\mu f_n^{(j)}, \tag{13}$$

$$L^{(j)}(\mu) = \sum_{n\neq 0} [E_n^{(j)}]^\mu \ln[E_n^{(j)}] f_n^{(j)}, \tag{14}$$

where $E_n^{(j)}$ is the excitation energy (in rydbergs) and $f_n^{(j)}$ is the corresponding dipole oscillator strength of the nth state of the jth particle.

The next-order contributions to the cross sections defined in Eqs. (1)–(4) have also been examined in recent work.[1,2] The first-order effects due to kinematical constraints (including the Bethe ridge correction[1]) and energy conservation have been included, but electron exchange between the incident ion and target atom is not included. In the Born approximation, neglecting exchange, the results may be expressed as

$$\gamma_{\mathrm{el,el}} = -\tfrac{1}{8}[Z_N^{(1)} Z_N^{(2)}(m_e/M)]^2, \tag{15}$$

$$\gamma_{\mathrm{in,el}} = -\tfrac{1}{8} Z_e^{(1)}(Z_N^{(2)})^2, \tag{16}$$

$$\gamma_{\mathrm{in,in}} = -\tfrac{1}{8}[S^{(1)}(-1)S^{(2)}(1) + 3Z_e^{(1)}Z_e^{(2)} + S^{(1)}(1)S^{(2)}(-1)], \tag{17}$$

$$\gamma_{\mathrm{el,in}} = -\tfrac{1}{4}[|F_0^{(1)}(0)|^2 S'^{(2)}(1) + 2F_0^{(1)}(0)F_0'^{(1)}(0)S^{(2)}(1) + (Z_N^{(1)})^2 Z_e^{(2)}], \tag{18}$$

where in Eqs. (16)–(18) we have neglected terms of order m_e/M (ratio of the electron mass to the reduced mass of the colliding particles). By definition, Eq. (8), $F_0^{(1)}(0)$ is simply the net charge of the incident ion. In order to evaluate these expressions, one requires the electronic and nuclear charges of the colliding particles, the +1 and −1 energy moments of the oscillator strengths given by (13), and two other properties which are given by derivatives with respect to momentum transfer:

$$F_0'^{(j)}(0) = \lim_{(a_0K)\to 0}\left(\frac{\partial}{\partial(a_0K)^2} F_0^{(j)}(K)\right), \tag{19}$$

$$S'^{(j)}(\mu) = \lim_{(a_0K)\to 0}\left(\frac{\partial}{\partial(a_0K)^2}\sum_{n\neq 0}[E_n^{(j)}]^\mu f_n^{(j)}(K)\right). \tag{20}$$

Here, $f_n^{(j)}(K)$ is the generalized oscillator strength for the nth state of the jth atom or ion. (The dipole oscillator strength is obtained at $K=0$.)

The +1 and −1 energy moments of the dipole oscillator strengths required in Eqs. (17) and (18), as well as the additional two parameters given by Eqs. (19) and (20), may all be expressed in terms of ground-state expectation values. Specifically

$$S^{(j)}(-1) = \tfrac{1}{3}\left[{}_j\langle 0|\left(\sum_k \vec{r}_k^{(j)}\right)^2|0\rangle_j\right], \tag{21}$$

$$S^{(j)}(1) = \tfrac{4}{3}\left[{}_j\langle 0|\left(\sum_k \vec{p}_k^{(j)}\right)^2|0\rangle_j\right], \tag{22}$$

$$S'^{(j)}(1) = Z_e^{(j)} - \tfrac{4}{3}\left[{}_j\langle 0|\sum_k\sum_{l\neq k}(\vec{r}_k^{(j)}\cdot\vec{p}_k^{(j)}) \times (\vec{r}_l^{(j)}\cdot\vec{p}_l^{(j)})|0\rangle_j\right], \tag{23}$$

$$F_0'^{(j)}(0) = \tfrac{1}{6}\left[{}_j\langle 0|\sum_k(\vec{r}_k^{(j)})^2|0\rangle_j\right], \tag{24}$$

where $\vec{p}_k^{(j)}$ and $\vec{r}_k^{(j)}$ represent the momentum and the position vectors of the kth electron of the jth particle.[7] Experience on small atoms[5] shows that the value of $S'^{(j)}(1)$ defined by Eq. (23) is closely approximated by

$$S'^{(j)}(1) \approx Z_e^{(j)}. \tag{25}$$

Finally, we note that the factors of $(Z_N^{(2)})^2$ appearing in Eqs. (15) and (16) arise from the large momentum transfer behavior of the square of the elastic form factor. For atoms, this approaches the square of the nuclear charge as $a_0K\to\infty$, but for molecules the elastic form factor squared goes to the sum of the squares of the nuclear charges of the atoms which comprise the molecule. Consequently, $(Z_N^{(2)})^2$ as it appears in Eqs. (15) and (16) should be interpreted as the sum of the squares of the atomic numbers of the various constituents of a molecular target.

III. ATOMIC FORM FACTORS AND INCOHERENT SCATTERING FUNCTIONS OF Cs^+ AND Au^+

We used both relativisitc and nonrelativistic numerical Hartree-Fock wave functions[8] for Cs^+ and Au^+ to compute elastic form factors and incoherent scattering functions defined by Eqs. (8) and (9). The second term on the right-hand side of Eq. (8) is better known as the atomic form factor $F(K)$,

$$F(K) = \langle 0 | \sum_{l=1}^{Z_e} \exp(i\vec{K}\cdot\vec{r}_l) | 0 \rangle , \tag{26}$$

where we omitted the particle label (j) for simplicity.

In addition to the well-known applications to the coherent and incoherent scattering of x rays, $F(K)$ may be considered as a measure of the screening of the nucleus by atomic electrons, and $S_{\rm inc}(K)$ as the effective number of electrons participating in all inelastic collisions caused by a fast-charged projectile.[9]

The values of $F(K)$ and $S_{\rm inc}(K)$ are presented in Tables I and II. The differences between the relativistic and nonrelativistic data are readily understood from the known differences in the charge distributions. For large K, the relativistic $F(K)$ values diminish slower than the nonrelativistic ones reflecting a higher relativistic charge density near the nuclues. On the other hand, the relativistic $S_{\rm inc}(K)$ of Au^+ for small K rises faster than the nonrelativistic values reflecting a larger value of $S(-1)$ from the relativistic charge distribution. (The trend for Cs^+ is opposite.) For small K, both $F(K)$ and $S_{\rm inc}(K)$ can be expanded in a power series:

$$F(K) = Z_e - F_0'(0)(a_0K)^2 + \cdots ,$$

$$Z_e S_{\rm inc}(K) = S(-1)(a_0K)^2 - \cdots ,$$

where $F_0'(0)$ is defined by Eqs. (19) and (24), and $S(-1)$ by Eq. (21). The values of $F_0'(0)$ and $S(-1)$ in Table III show that for Au^+, $S(-1)$ is affected more by relativity than $F_0'(0)$. As can be seen from Eqs. (21) and (24), $S(-1)$ and $F_0'(0)$ are different by the two electron operators $\vec{r}_k\cdot\vec{r}_l$ and it is difficult to explain the behavior of the relativistic and nonrelativistic data in simple terms. Closeness of the relativistic and nonrelativisitic values of $F_0'(0)$ does not imply that the mean values of r^2 for each orbital shows no relativistic effect. On the contrary, the relativistic effect on the mean values of r^2 is such that the contraction of inner orbitals is compensated by the dilation of outer orbitals.

Smaller relativisitc values of $S_{\rm inc}(K)$ at large momentum transfers reflect the fact that the core electrons, which are more likely to be involved in violent collisions, have less probability of interaction than that implied by nonrelativistic calculations because of tighter relativistic binding for them. As expected from the similarity of relativistic and nonrelativistic orbital sizes,[10] we hardly notice relativistic effects in any of the Cs^+ data.

In addition to the relativistic effects, electron correlation affects $S_{\rm inc}(K)$ significantly for large atoms. For instance, $S_{\rm inc}(K)$ for Ar is reduced by 10% or more for $a_0K<5$ by the correlation while $F(K)$ is hardly changed.[11] The values of $S_{\rm inc}(K)$ in Tables I and II and hence the integrals (6) and (7) could be reduced by ~20% by this effect.

IV. CALCULATION OF THE CROSS-SECTION PARAMETERS

With the ion form factors and incoherent scattering functions described in the previous section, we have evaluated the integrals given by Eqs. (5)–(7), (11), and (12) for a variety of atomic and molecular targets. Targets considered include H, H_2, He, C, N, and O, which are characteristic of the residual background gases that may be found in accelerator vacuum systems. For the target form factors and incoherent scattering functions, we have used results available from the literature,[9,12-16] with some minor low- and high-momentum transfer extrapolations which have been described elsewhere.[1]

The results of the numerical integrations are summarized in Table IV. For atomic hydrogen, analytic expressions for $F_0(K)$ and $S_{\rm inc}(K)$ have been used; for H_2 the tables of Liu and Smith[12] have been used which include a room temperature thermal average over vibrational states. The He data are from Kim and Inokuti[9]; we have used their tables for a 20-term Hylleraas wave function. Results for C, N, and O are based on wave functions which include some configuration interaction[13,14,16]; for comparison, values of the integrals for nitrogen are also calculated from the Hartree-Fock wave function.[14,15] Table IV also compares cross-section data obtained from both relativistic and nonrelativistic wave functions for Au^+. The differences between the relativistic and nonrelativistic form factors (Table II) are reflected in the integrals presented in Table IV. For instance, relativistic values of $F(K)$ are slightly larger than the corresponding nonrelativistic values, leading to a better screening of the nucleus [i.e., relativistic $F_0(K)$ is smaller]. Smaller $F_0(K)$ values then produce smaller $I_{\rm el,el}$. The relativistic values of $I_{\rm in,el}$ reflects the relativistic change in $S(-1)$, the leading term for small momentum transfer in $S_{\rm inc}(K)$. [Calculations we have made

TABLE I. Atomic form factors $F(K)$ and incoherent scattering functions $S_{inc}(K)$ for Cs^+. Results for the nonrelativistic Hartree-Fock wave function are given in the columns labeled NR, those for the relativistic Hartree-Fock wave function, in the columns labeled R. Powers of ten are denoted in parentheses following each entry.

$(a_0K)^2$	$F(K)$		$Z_e S_{inc}(K)$	
	R	NR	R	NR
0.0	5.400(1)	5.400(1)	0.0	0.0
0.01	5.391(1)	5.391(1)	9.360(−2)	9.430(−2)
0.02	5.383(1)	5.383(1)	1.861(−1)	1.875(−1)
0.03	5.375(1)	5.374(1)	2.775(−1)	2.796(−1)
0.04	5.366(1)	5.365(1)	3.678(−1)	3.706(−1)
0.05	5.358(1)	5.357(1)	4.570(−1)	4.605(−1)
0.06	5.350(1)	5.348(1)	5.452(−1)	5.494(−1)
0.07	5.341(1)	5.340(1)	6.324(−1)	6.373(−1)
0.08	5.333(1)	5.331(1)	7.185(−1)	7.242(−1)
0.09	5.325(1)	5.323(1)	8.037(−1)	8.100(−1)
0.10	5.317(1)	5.315(1)	8.879(−1)	8.950(−1)
0.20	5.238(1)	5.234(1)	1.680(0)	1.694(0)
0.30	5.163(1)	5.158(1)	2.393(0)	2.414(0)
0.40	5.092(1)	5.085(1)	3.038(0)	3.066(0)
0.50	5.025(1)	5.016(1)	3.626(0)	3.662(0)
0.60	4.961(1)	4.951(1)	4.167(0)	4.209(0)
0.70	4.899(1)	4.889(1)	4.667(0)	4.716(0)
0.80	4.841(1)	4.829(1)	5.132(0)	5.187(0)
0.90	4.785(1)	4.773(1)	5.567(0)	5.628(0)
1.00	4.732(1)	4.719(1)	5.976(0)	6.042(0)
2.00	4.305(1)	4.289(1)	9.161(0)	9.257(0)
3.00	4.008(1)	3.991(1)	1.143(1)	1.152(1)
4.00	3.785(1)	3.769(1)	1.317(1)	1.325(1)
5.00	3.608(1)	3.593(1)	1.454(1)	1.462(1)
6.00	3.460(1)	3.445(1)	1.567(1)	1.574(1)
7.00	3.333(1)	3.318(1)	1.662(1)	1.669(1)
8.00	3.220(1)	3.205(1)	1.744(1)	1.752(1)
9.00	3.119(1)	3.104(1)	1.818(1)	1.826(1)
10.00	3.027(1)	3.011(1)	1.886(1)	1.895(1)
20.00	2.401(1)	2.376(1)	2.387(1)	2.403(1)
30.00	2.062(1)	2.035(1)	2.729(1)	2.750(1)
40.00	1.855(1)	1.830(1)	2.983(1)	3.004(1)
50.00	1.713(1)	1.689(1)	3.175(1)	3.196(1)
60.00	1.603(1)	1.579(1)	3.324(1)	3.346(1)
70.00	1.510(1)	1.486(1)	3.444(1)	3.467(1)
80.00	1.427(1)	1.403(1)	3.543(1)	3.567(1)
90.00	1.351(1)	1.326(1)	3.628(1)	3.652(1)
100.00	1.281(1)	1.254(1)	3.702(1)	3.727(1)
200.00	8.123(0)	7.838(0)	4.166(1)	4.192(1)
300.00	6.184(0)	5.942(0)	4.417(1)	4.439(1)
400.00	5.319(0)	5.099(0)	4.580(1)	4.601(1)
500.00	4.818(0)	4.597(0)	4.698(1)	4.718(1)
600.00	4.440(0)	4.209(0)	4.787(1)	4.807(1)
700.00	4.110(0)	3.869(0)	4.857(1)	4.878(1)
800.00	3.810(0)	3.561(0)	4.914(1)	4.935(1)
900.00	3.533(0)	3.281(0)	4.961(1)	4.981(1)
1000.00	3.281(0)	3.029(0)	5.000(1)	5.019(1)
2000.00	1.840(0)	1.664(0)	5.186(1)	5.199(1)
3000.00	1.375(0)	1.256(0)	5.251(1)	5.261(1)
4000.00	1.179(0)	1.083(0)	5.287(1)	5.297(1)
5000.00	1.062(0)	9.732(−1)	5.311(1)	5.321(1)
6000.00	9.731(−1)	8.862(−1)	5.329(1)	5.338(1)
7000.00	8.979(−1)	8.109(−1)	5.342(1)	5.351(1)
8000.00	8.313(−1)	7.438(−1)	5.352(1)	5.360(1)
9000.00	7.714(−1)	6.837(−1)	5.360(1)	5.368(1)

TABLE I. *(Continued)*

$(a_0K)^2$	$F(K)$		$Z_e S_{inc}(K)$	
	R	NR	R	NR
10 000.00	7.173(−1)	6.297(−1)	5.366(1)	5.373(1)
20 000.00	3.845(−1)	3.111(−1)	5.392(1)	5.394(1)
30 000.00	2.397(−1)	1.825(−1)	5.397(1)	5.398(1)
40 000.00	1.648(−1)	1.195(−1)	5.399(1)	5.399(1)
50 000.00	1.211(−1)	8.423(−2)	5.399(1)	5.400(1)
60 000.00	9.313(−2)	6.252(−2)	5.400(1)	5.400(1)
70 000.00	7.417(−2)	4.824(−2)	5.400(1)	5.400(1)
80 000.00	6.066(−2)	3.834(−2)	5.400(1)	5.400(1)
90 000.00	5.067(−2)	3.120(−2)	5.400(1)	5.400(1)
100 000.00	4.306(−2)	2.588(−2)	5.400(1)	5.400(1)

using the Cs^+ relativistic wave function results for $F(K)$ and $S_{inc}(K)$ from Table I show very little difference (~2% or less) from the cross-section parameters given in Table IV for the nonrelativistic case.]

The parameter $\ln c_{el,in}$ defined by Eq. (10), which is analogous to the Bethe-theory parameter $\ln c_{tot}$ for a structureless projectile[5] and appears in the leading order for the cross section $\sigma_{el,in}$ of Eq. (4), has been calculated for each of the collision partners considered in this work. In addition to the integral $\mathcal{G}_1 - \mathcal{G}_2$, given in Table IV, $\ln c_{el,in}$ requires values of $S(-1)$ and $L(-1)$ for the targets, as well as the net charge $[F_0(0)]$ of the incident ion. [For all the ions considered here, $F_0(0)$ is simply one.] Values of these constants, as well as $S(1)$ and $S'(1)$, for the various target particles are given in Table V. The values for $S(-1)$, $S(1)$, and $L(-1)$ have been extracted from previous work.[5,12,17,18] The methods used to evaluate these energy moments of the dipole oscillator strengths vary considerably. The values for $S(-1)$ and $S(1)$ given in Table V should be reliable. The values of $L(-1)$ (except for H and He) may be less accurate than indicated.[18] However, this uncertainty has little impact on the cross sections reported here. The values for $S'(1)$ have been calculated simply from the approximate expression (25) with the exceptions of H [for which Eq. (25) is exact] and He, for which more accurate values are available.[5]

The results for $\ln c_{el,in}$ are given in Table VI. For comparison, values from both the Hartree-Fock and a configuration interaction wave function for the nitrogen-target atom are given. For the Hartree-Fock case [indicated by N(HF)], a value of $S(-1)$ of 2.9 has been used in calculating $\ln c_{el,in}$ from Eq. (10). This value is common to the Hartree-Fock calculation via the sum rule (21), rather than the value of 2.6 given in Table V, which is obtained from the configuration interaction wave function. Also given in Table VI are results for the next-order cross-section parameters $\gamma_{el,in}$, $\gamma_{in,el}$, and $\gamma_{in,in}$ as calculated from Eqs. (16)–(18). Besides the nuclear and electronic charges of the incident ion and target, all of the required atomic properties for these contributions to the cross sections have been given in Tables III and V. [The only other parameter, $\gamma_{el,el}$, required for the first two orders to the cross sections examined, may be readily calculated from Eq. (15). However, it is significantly less than one for all the cases considered in this work. Consequently, it is most likely negligible, always of order $(m_e/M)^2$, compared to other nonleading order contributions such as those which would arise from higher Born amplitudes.]

Cross sections for a molecular target may be calculated with reasonable accuracy by simply summing the cross sections for the atomic constituents of the molecule. In the case of an H_2 target this procedure gives results which are no more than about 15% above the cross sections calculated directly with the H_2 molecular wave functions. For molecules consisting of heavier atoms, such as N_2, O_2, CO, etc., the error using this approximation should be less.

V. DISCUSSION

The parameters tabulated in Tables IV–VI may be used to calculate the various cross sections according to Eqs. (1)–(4). Certain of the inelastic cross sections can be combined to determine total excitation plus ionization cross sections. These in turn provide upper bounds on the collisional electron-loss cross sections, which are of interest in establising vacuum requirements for accelerators or storage rings using partially stripped heavy ions. As an example, by combining Eqs. (2) and (3) and utilizing the parameter values calculated in Sec. IV, we obtain for the total cross

TABLE II. Atomic form factors $F(K)$ and incoherent scattering functions $S_{inc}(K)$ for Au^+. Results for the nonrelativistic Hartree-Fock wave function are given in the columns labeled NR, those for the relativistic Hartree-Fock wave function, in the columns labeled R. Powers of ten are denoted in parentheses following each entry.

$(a_0K)^2$	$F(K)$		$Z_e S_{inc}(K)$	
	R	NR	R	NR
0.0	7.800(1)	7.800(1)	0.0	0.0
0.01	7.792(1)	7.792(1)	9.123(−2)	8.477(−2)
0.02	7.784(1)	7.784(1)	1.816(−1)	1.688(−1)
0.03	7.776(1)	7.776(1)	2.711(−1)	2.521(−1)
0.04	7.769(1)	7.769(1)	3.598(−1)	3.347(−1)
0.05	7.761(1)	7.761(1)	4.477(−1)	4.166(−1)
0.06	7.753(1)	7.753(1)	5.348(−1)	4.977(−1)
0.07	7.745(1)	7.745(1)	6.210(−1)	5.782(−1)
0.08	7.738(1)	7.737(1)	7.065(−1)	6.580(−1)
0.09	7.730(1)	7.730(1)	7.912(−1)	7.371(−1)
0.10	7.722(1)	7.722(1)	8.751(−1)	8.156(−1)
0.20	7.647(1)	7.647(1)	1.674(0)	1.565(0)
0.30	7.575(1)	7.574(1)	2.406(0)	2.256(0)
0.40	7.505(1)	7.504(1)	3.079(0)	2.896(0)
0.50	7.438(1)	7.436(1)	3.700(0)	3.489(0)
0.60	7.373(1)	7.370(1)	4.275(0)	4.042(0)
0.70	7.309(1)	7.306(1)	4.809(0)	4.558(0)
0.80	7.248(1)	7.244(1)	5.306(0)	5.042(0)
0.90	7.189(1)	7.184(1)	5.772(0)	5.497(0)
1.00	7.131(1)	7.125(1)	6.209(0)	5.926(0)
2.00	6.637(1)	6.621(1)	9.525(0)	9.246(0)
3.00	6.253(1)	6.227(1)	1.184(1)	1.162(1)
4.00	5.942(1)	5.908(1)	1.372(1)	1.356(1)
5.00	5.683(1)	5.644(1)	1.535(1)	1.527(1)
6.00	5.462(1)	5.420(1)	1.683(1)	1.680(1)
7.00	5.271(1)	5.227(1)	1.817(1)	1.819(1)
8.00	5.103(1)	5.058(1)	1.941(1)	1.948(1)
9.00	4.953(1)	4.908(1)	2.055(1)	2.066(1)
10.00	4.819(1)	4.773(1)	2.161(1)	2.175(1)
20.00	3.920(1)	3.883(1)	2.908(1)	2.932(1)
30.00	3.380(1)	3.341(1)	3.345(1)	3.369(1)
40.00	2.989(1)	2.942(1)	3.652(1)	3.679(1)
50.00	2.689(1)	2.633(1)	3.894(1)	3.926(1)
60.00	2.453(1)	2.390(1)	4.098(1)	4.135(1)
70.00	2.265(1)	2.197(1)	4.275(1)	4.317(1)
80.00	2.113(1)	2.043(1)	4.431(1)	4.477(1)
90.00	1.990(1)	1.919(1)	4.572(1)	4.621(1)
100.00	1.889(1)	1.818(1)	4.699(1)	4.752(1)
200.00	1.406(1)	1.341(1)	5.553(1)	5.607(1)
300.00	1.166(1)	1.094(1)	5.994(1)	6.049(1)
400.00	9.792(0)	9.040(0)	6.260(1)	6.319(1)
500.00	8.358(0)	7.626(0)	6.445(1)	6.506(1)
600.00	7.301(0)	6.617(0)	6.585(1)	6.644(1)
700.00	6.535(0)	5.906(0)	6.697(1)	6.754(1)
800.00	5.981(0)	5.398(0)	6.789(1)	6.843(1)
900.00	5.573(0)	5.024(0)	6.866(1)	6.919(1)
1000.00	5.264(0)	4.738(0)	6.933(1)	6.984(1)
2000.00	3.768(0)	3.206(0)	7.301(1)	7.351(1)
3000.00	2.852(0)	2.304(0)	7.457(1)	7.499(1)
4000.00	2.249(0)	1.779(0)	7.539(1)	7.573(1)
5000.00	1.871(0)	1.479(0)	7.589(1)	7.617(1)
6000.00	1.630(0)	1.300(0)	7.621(1)	7.647(1)
7000.00	1.471(0)	1.184(0)	7.645(1)	7.669(1)
8000.00	1.359(0)	1.103(0)	7.663(1)	7.687(1)
9000.00	1.277(0)	1.040(0)	7.678(1)	7.701(1)

TABLE II. (*Continued*)

$(a_0K)^2$	$F(K)$		$Z_eS_{inc}(K)$	
	R	NR	R	NR
10 000.00	1.212(0)	9.877(−1)	7.690(1)	7.713(1)
20 000.00	8.543(−1)	6.495(−1)	7.752(1)	7.770(1)
30 000.00	6.461(−1)	4.502(−1)	7.775(1)	7.787(1)
40 000.00	5.062(−1)	3.271(−1)	7.786(1)	7.794(1)
50 000.00	4.087(−1)	2.474(−1)	7.791(1)	7.797(1)
60 000.00	3.382(−1)	1.934(−1)	7.794(1)	7.798(1)
70 000.00	2.856(−1)	1.552(−1)	7.796(1)	7.799(1)
80 000.00	2.451(−1)	1.272(−1)	7.797(1)	7.799(1)
90 000.00	2.133(−1)	1.061(−1)	7.798(1)	7.799(1)
100 000.00	1.878(−1)	8.984(−2)	7.798(1)	7.800(1)

section for collisions leading to the excitation or ionization of a high-velocity Li^+ ion incident on a hydrogen molecule

$$\sigma(Li^+)_{ex+ion} = 8\pi a_0^2[1.07(\alpha^2/\beta^2) - 5.78(\alpha^4/\beta^4)]. \quad (27)$$

This two-term cross section, as well as the leading term only, are shown in Fig. 1. Also shown is the Padé approximant cross section[19] (solid curve) constructed from Eq. (27). For comparison the corresponding Li^+ cross sections for atomic H targets are also shown. Data indicated in the figure are for the single-electron-loss cross section $\sigma_{1,2}$ of Li^+ colliding with H_2 targets as measured by Allison *et al.*[20] and Pivovar *et al.*[21] Figure 2 gives similar results for Li^+ incident on He and N_2 gases, with additional data from Dmitriev and co-workers.[22]

The total excitation and ionization cross sections calculated in this work should provide upper limits to the single-electron-loss (ionization) cross sections, $\sigma_{1,2}$ of Li^+. Other processes which contribute to this total are multiple-electron-loss cross sections, ($\sigma_{1,3}$, etc.) and collisional excitation of the Li^+ ion to a discrete bound state. For Li^+, $\sigma_{1,3}$ is generally an order-of-magnitude smaller than $\sigma_{1,2}$,[20-22] consequently the data shown in Figs. 1 and 2 are essentially the total Li^+-ionization cross sections.

There are a number of points which are apparent upon examining the figures, but which also should be emphasized. It is clear that considerable discrepancies exist in the various experimental data for the Li^+-ionization cross sections.[23] In addition most of the available data are in too low a velocity region to apply the Born approximation, with the possible exception of the data by Dmitriev *et al.*[22] for He targets near 750 keV/nucleon. Consequently any conclusions which are drawn from a comparison between theory and experiment must be prefaced with some caution. With this caveat in mind, however, some further analysis is enlightening. The theoretical asymptotic (leading term only) and Padé cross sections are above the ionization cross sections $\sigma_{1,2}$ as expected. In contrast, the two-term expansion fails to preserve the upper-bound character of these cross sections, eventually dropping below the data at a sufficiently low energy. This is in accord with the experience in other ion-atom calculations[1,19] and with similar Bethe cross sections for the ionization of light atoms by electron impact.[5] For electron impact collisions, the Bethe cross sections equivalent

TABLE III. Atomic properties $F_0'(0)$, $S(-1)$, and $S(1)$ for Li^+, Cs^+, and Au^+. The values for Cs^+ and Au^+ are based on the Hartree-Fock wave functions. Those for Li^+ are from a correlated wave function by Pekeris (Ref. 17).

Ion	$F_0'(0)$		$S(-1)$		$S(1)$
	Relativistic	Nonrelativistic	Relativistic[a]	Nonrelativistic	Nonrelativistic
Li^+		0.148 760		0.286 017	20.1837
Cs^+	8.537	8.757	9.417	9.486	1.37×10^4
Au^+	7.914	7.923	9.166	8.514	3.01×10^4

[a] Calculated from Eq. (21) simply by replacing the charge distribution by a relativistic one.

TABLE IV. Values of the integrals $I_{el,el}$, $I_{in,el}$, $I_{in,in}$, and $\mathcal{I}_1 - \mathcal{I}_2$ as defined by Eqs. (5)–(7) and (9)–(10) for the ions Li^+, Cs^+, and Au^+ on various target gases. Models for the target atoms and H_2 molecules are described in the references indicated; all the atomic models include some configuration interaction in the wave function except for N(14,15) which is Hartree-Fock only. The columns marked NR show data based on nonrelativistic wave functions for the ions, and those marked R show data based on relativistic wave functions. Numerical integration errors are typically less than one unit in the last significant figure.

Incident ion	Target (references)	$I_{el,el}$ NR	$I_{el,el}$ R	$I_{in,el}$ NR	$I_{in,el}$ R	$I_{in,in}$ NR	$I_{in,in}$ R	$\mathcal{I}_1 - \mathcal{I}_2$ NR	$\mathcal{I}_1 - \mathcal{I}_2$ R
Li^+	H	0.689		0.198		0.394		1.59	
	H_2(12)	1.24		0.348		0.720		3.23	
	He(9)	1.48		0.447		0.534		2.83	
	C(13,14)	1.55×10^1		4.45		1.51		7.12	
	N(14,15)	1.87×10^1		5.54		1.68		8.38	
	N(16)	1.85×10^1		5.56		1.57		7.75	
	O(16)	2.17×10^1		6.54		1.64		8.76	
Cs^+	H	9.47×10^1		3.33		7.86		2.84×10^2	
	H_2(12)	1.71×10^2		5.94		1.40×10^1		5.40×10^2	
	He(9)	2.51×10^2		7.25		9.88		4.44×10^2	
	C(13,14)	2.24×10^3		7.59×10^1		2.90×10^1		1.21×10^3	
	N(14,15)	2.90×10^3		9.29×10^1		3.18×10^1		1.37×10^3	
	N(16)	2.88×10^3		9.20×10^1		2.94×10^1		1.31×10^3	
	O(16)	3.56×10^3		1.08×10^2		3.04×10^1		1.42×10^3	
Au^+	H	1.51×10^2	1.47×10^2	3.67	3.71	8.08	8.32	4.10×10^2	4.01×10^2
	H_2(12)	2.75×10^2	2.69×10^2	6.58	6.64	1.45×10^1	1.49×10^1	7.92×10^2	7.73×10^2
	He(9)	4.27×10^2	4.17×10^2	8.40	8.40	1.05×10^1	1.07×10^1	6.78×10^2	6.62×10^2
	C(13,14)	3.63×10^3	3.55×10^3	8.46×10^1	8.52×10^1	3.04×10^1	3.11×10^1	1.84×10^3	1.79×10^3
	N(14,15)	4.77×10^3	4.66×10^3	1.05×10^2	1.05×10^2	3.36×10^1	3.43×10^1	2.09×10^3	2.04×10^3
	N(16)	4.75×10^3	4.64×10^3	1.04×10^2	1.04×10^2	3.12×10^1	3.18×10^1	2.02×10^3	1.98×10^3
	O(16)	5.94×10^3	5.80×10^3	1.24×10^2	1.24×10^2	3.24×10^1	3.31×10^1	2.21×10^3	2.16×10^3

to Eq. (4) agree well with experiments only in the high-energy range beyond the main peak of the cross section. For incident energies near the peak and below, higher-order terms in the Born cross sections omitted from Eqs. (1)–(4) as well as contributions from non-Born terms (distortions of the target and projectile wave functions, electron exchange, etc.) are important.

TABLE V. Atomic and molecular properties $S(-1)$, $S(1)$, $L(-1)$, and $S'(1)$ for the targets H, H_2, He, C, N, and O. The values given have been extracted from, or estimated from, data appearing in the references indicated in parentheses. For $S'(1)$ Eq. (25) has been used for all targets except H and He.

Target (references)	$S(-1)$	$S(1)$	$L(-1)$	$S'(1)$
H(5)	1	$\frac{4}{3}$	−0.073 25	1
H_2(12)	1.55	3.34	0.278	2.0
He(5,17)	0.7525	8.167	0.638	2.047
C(1,18)	2.9	1.0×10^2	−0.141	6.0
N(1,18)	2.6	1.5×10^2	1.05	7.0
O(1,18)	2.3	2.0×10^2	1.73	8.0

Another cross section of interest in certain applications is that for ionization of the target atom or molecule. Again an upper bound to this type of cross section may be calculated from the results of this work by combining Eqs. (3) and (4). For the example of Li^+ impact on an H_2 molecular target, we obtain, for the total cross section for excitation and ionization of the H_2 molecule,

$$\sigma(H_2)_{ex+ion} = 4\pi a_0^2\{(\alpha^2/\beta^2)[1.55\ln(4\beta^2/\alpha^2) + 4.12] - 16.3(\alpha^4/\beta^4)\}. \quad (28)$$

This cross section is of the same form as the Bethe-Born asymptotic cross section for inelastic scattering of structureless ions by atoms or molecules. Pivovar *et al.*[21] have determined for several gases the ratio of the cross section for ionization by Li^+ to that due to proton impact at the same projectile velocity. Their data does not take into account excitation processes to bound states, but some similarities in the cross-section ratios might still be expected. In the energy range from $\frac{1}{7}$ to $\frac{2}{7}$ MeV per nucleon ($\beta \simeq 0.017$ to 0.025) they obtained ratios of 1.6, 2.0, and 1.8, respec-

TABLE VI. Values of the cross section parameters $\ln c_{el,in}$, $\gamma_{el,in}$, $\gamma_{in,el}$, and $\gamma_{in,in}$ as defined by Eqs. (8) and (16)–(18), for the ions Li^+, Cs^+, and Au^+ incident on various target gases. The values of $\ln c_{el,in}$ use the integrals $\mathcal{I}_1 - \mathcal{I}_2$ given in Table IV; the other properties required are from Tables III and V. N(HF) is based on the Hartree-Fock results for $\mathcal{I}_1 - \mathcal{I}_2$, N on the configuration interaction results for $\mathcal{I}_1 - \mathcal{I}_2$.

Ion	Target	$\ln c_{el,in}$	$\gamma_{el,in}$	$\gamma_{in,el}$	$\gamma_{in,in}$
Li^+	H	1.74	−2.60	$-\frac{1}{4}$	−3.32
	H_2	1.73	−5.25	$-\frac{1}{2}$	−5.53
	He	2.07	−5.62	−1	−3.69
	C	2.55	-2.2×10^1	−9	−16
	N(HF)	2.17	—	—	—
	N	2.17	-2.9×10^1	$-12\frac{1}{4}$	−15
	O	2.30	-3.5×10^1	−16	−19
Cs^+	H	2.84×10^2	-7.62×10^2	$-6\frac{3}{4}$	-1.73×10^3
	H_2	3.48×10^2	-1.53×10^3	$-13\frac{1}{2}$	-2.69×10^3
	He	5.88×10^2	-1.55×10^3	−27	-1.34×10^3
	C	4.17×10^2	-5.0×10^3	−243	-5.2×10^3
	N(HF)	4.72×10^2	—	—	—
	N	5.03×10^2	-6.0×10^3	$-330\frac{3}{4}$	-4.8×10^3
	O	6.16×10^2	-6.9×10^3	−432	-4.3×10^3
Au^+	H	4.10×10^2	-1.57×10^3	$-9\frac{3}{4}$	-3.79×10^3
	H_2	5.11×10^2	-3.13×10^3	$-19\frac{1}{4}$	-5.89×10^3
	He	8.99×10^2	-3.15×10^3	−39	-2.90×10^3
	C	6.35×10^2	-9.8×10^3	−351	-1.1×10^4
	N(HF)	7.20×10^2	—	—	—
	N	7.76×10^2	-1.2×10^4	$-477\frac{3}{4}$	-1.0×10^4
	O	9.59×10^2	-1.3×10^4	−624	-9.1×10^3

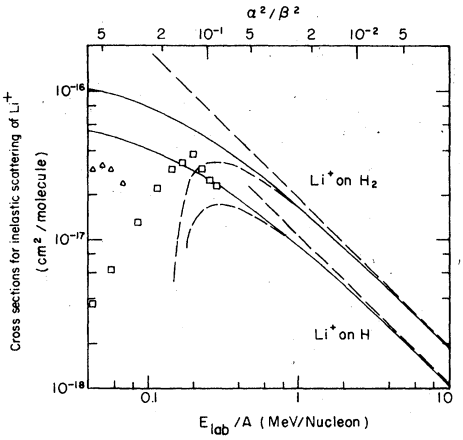

FIG. 1. Excitation and ionization cross sections for Li^+ ions incident on atomic H and molecular H_2. Broken lines are the theoretical results of this work for the Born one-term (upper curves) and two-term (lower curves) expansions in β^{-2}. Solid curves are the Padé approximant cross sections constructed from the two-term expansions. The experimental data for the Li^+ single electron-loss cross section $\sigma_{1,2}$ on H_2 targets are taken from Allison *et al.* (△, Ref. 20) and Pivovar *et al.* (□, Ref. 21). The upper scale gives the expansion parameter α^2/β^2.

tively, for H_2, He, and N_2 target gases and observed only a modest energy dependence. For comparison, the results of this work for the total cross section for excitation and ionization of these target gases due to Li^+ impact have been divided by the corresponding cross section due to proton impact, as evaluated in the traditional Bethe-theory approach.[5,12,18] We obtain for these ratios 1.8, 2.5, and 2.0, respectively, for H_2, He, and atomic N targets at an incident velocity of $\beta = 0.017$, when only the leading terms to the cross sections are used. While this ratio based on the leading terms is only weakly dependent on energy (via the $\ln\beta^2$ terms), it is altered significantly in this velocity region if the next order corrections are included (i.e., terms of order α^4/β^4). For example when these contributions for Li^+ and H^+ impact on He targets are included, the ratio is reduced to 1.5 at $\beta = 0.017$ and to 1.8 at $\beta = 0.025$. At these velocities, the Born approximation is probably no longer useful in predicting the absolute cross sections, but their ratios are still close to what one might expect based on the data of Pivovar *et al.*[21] Also we note that when the projectile velocity approaches that of light, it is necessary to modify the logarithmic term in Eq. (4) as is done in the case of bare ions[24]:

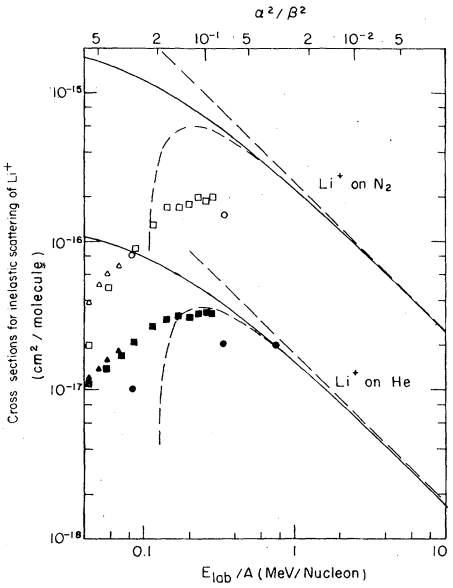

FIG. 2. Excitation and ionization cross sections for Li^+ ions incident on atomic He and molecular N_2. Broken lines are the theoretical results of this work for the Born one-term (upper curves) and two-term (lower curves) expansions in β^{-2}. Solid curves are the Padé approximant cross sections constructed from the two-term expansions. The N_2 theoretical cross sections are taken to be twice the atomic N cross sections calculated in this work. The experimental data for the Li^+ single-electron-loss cross section $\sigma_{1,2}$ on He (solid symbols) and N_2 (open symbols) are taken from Allison *et al.* (▲,△, Ref. 20); Pivovar *et al.* (■,□, Ref. 21) and Dmitriev *et al.* (●,○, Ref. 22). The upper scale gives the expansion parameter α^2/β^2.

$$\sigma_{el,in} = 4\pi a_0^2(\alpha^2/\beta^2)(S^{(2)}(-1)\,|F_0^{(1)}(0)|^2 \times\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + C_{el,in}), \tag{29}$$

with

$$C_{el,in} = S^{(2)}(-1)\,|F_0^{(1)}(0)|^2 \ln(4c_{el,in}/\alpha^2). \tag{30}$$

Unfortunately, existing experimental data are all on light ions and molecules, and provide no clue to the range of validity of the present method on heavy particles. Collisions involving heavy particles with tightly bound electrons are expected to reach the asymptotic Born behavior at higher relative velocities than those for light atoms. We believe, however, the asymptotic cross sections for heavy ions presented in this work would certainly provide better than order-of-magnitude upper limits to the cross sections for ionization of the projectile or the target when the relative velocity is a sizable fraction of the speed of light.

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[7]Derivations of the nonrelativistic expressions for $S^{(j)}(\mu)$ in terms of the ground-state wave function [Eqs. (21) and (22)] depend explicitly on the form of the nonrelativisitc Hamiltonian. Only $S^{(j)}(-1)$ can be adapted to use the nonrelativistic formula with a relativistic charge distribution. Other moments require new definitions if a relativistic formulation is desired owing to the difference in the Hamiltonian and to contributions from negative energy states. In the present work, we do not discuss the relativistic f-sum rules and their related quantities. Only the $S^{(j)}(-1)$ have been calculated for Cs^+ and Au^+ from the relativistic charge distributions using the nonrelativistic formula, Eq. (21).

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[23]Some of the discrepancies in the experimental data may be due to the presence of Li^+ metastable states in the beams used for the cross-section measurements. Dmitriev *et al.* (Ref. 22) have examined this point and determined corrections for the metastable component of their earlier measurements (I. S. Dmitriev, V. S. Nikolaev, L. N. Fateeva, and Ya. A. Teplova, Zh. Eksp. Teor. Fiz. 42, 16 (1962) [Sov. Phys.-JETP 15, 11 (1962)]). Their data given in Fig. 2 includes this correction. However, Pivovar, *et al.* (Ref. 21) have examined this point as well, and apparently not all of the discrepancies can be attributed to a metastable component.
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