Total Cross Sections for Inelastic Scattering of Charged Particles by Atoms and Molecules. IV. Positive Lithium Ion*

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The Born cross sections for several important discrete excitations of Li^+ from its ground state have been calculated with correlated wave functions. By extrapolation, cross sections for higher excitations have also been determined. Subtraction of the sum σ_{ex} of these excitation cross sections from the total inelastic-scattering cross section σ_{tot} obtained through a sum rule for the Bethe cross sections yields a reliable "counting" ionization cross section σ_i. The cross sections thus obtained are

$$\sigma_{tot} = (z/\beta)^2(0.536\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 5.216 \pm 0.002) \times 10^{-20}\ \text{cm}^2 \quad ,$$

$$\sigma_{ex} = (z/\beta)^2(0.265\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 2.295 \pm 0.002) \times 10^{-20}\ \text{cm}^2 \quad ,$$

and $$\sigma_i = (z/\beta)^2(0.271\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 2.921 \pm 0.004) \times 10^{-20}\ \text{cm}^2 \quad ,$$

where ze is the charge of the incident particle and β is its velocity divided by that of light. The ionization cross section is in excellent agreement with experimental data in the asymptotic region (incident electron energy $\gtrsim$ 5 keV).

I. INTRODUCTION

The first Born cross sections for the inelastic scattering of fast charged particles can conveniently be expressed in terms of a few parameters, all of which are uniquely determined from the wave functions of the states involved.[1–4] Furthermore, these parameters obey sum rules and lead to the total inelastic-scattering cross section σ_{tot}. The sum rules actually enable one to evaluate σ_{tot} from the knowledge of the ground-state wave function and the optical oscillator-strength distribution.[3]

Very accurate wave functions for the ground state, as well as for some important discrete excited states of Li^+, have been calculated by Weiss[5] and Perkins,[6] and from these wave functions one can evaluate accurate Born cross sections. Cross sections for other discrete excitations can be obtained by extrapolation utilizing their dependence on effective quantum numbers.

With the ground-state wave function by Weiss and the optical oscillator-strength distribution available in the literature,[5, 7–10] one can determine σ_{tot} to high precision. Then, by subtracting the sum σ_{ex} of discrete-excitation cross sections from σ_{tot}, one can obtain a reliable "counting" ionization cross section σ_i, without using any continuum wave function explicitly. This method, which depends on the discrete-state wave functions only, has a definite advantage over a more conventional method of calculating σ_i by direct use of continuum wave functions in that discrete-state wave functions can usually be determined with far better precision than continuum wave functions. Previously, our method has been applied successfully to obtain σ_i of He.[11]

II. DISCRETE-EXCITATION CROSS SECTIONS

The Born cross section for a discrete excitation from the ground state to the state n is given by[4]

$$\sigma_n = \frac{4\pi a_0^2 z^2}{T/R}\left\{M_n^2\left[\ln\left(\frac{\beta^2}{1-\beta^2}\right) - \beta^2\right] + C_n + \frac{\gamma_n}{T/R} + O(E_n^2/T^2)\right\} \qquad (1)$$

when the transition is (optically) allowed, and

$$\sigma_n = \frac{4\pi a_0^2 z^2}{T/R}\left(b_n + \frac{\gamma_n}{T/R} + O(E_n^2/T^2)\right) \qquad (2)$$

when it is forbidden, where: a_0 is the Bohr radius; ze the charge of the incident particle; $T = \frac{1}{2}mv^2$, with m the *electron* mass and v the velocity of the incident particle; R the Rydberg energy; $\beta = v/c$ with c the speed of light, and E_n the excitation energy. The parameters M_n^2, C_n, b_n, and γ_n are characteristic of the transition as described below. In particular, M_n^2 is related to the optical oscillator strength f_n:

$$M_n^2 = f_n R / E_n \quad . \tag{3}$$

For all practical purposes, the terms $O(E_n^2/T^2)$ in Eqs. (1) and (2) can be neglected for the range of v such that the Born approximation is valid.[4] The leading terms in σ_n, up to and including the terms of order $1/T$ in Eqs. (1) and (2), are known as the Bethe cross section.

For the actual evaluation of the parameters M_n^2, C_n, b_n, and γ_n, one needs the generalized oscillator strengths $f_n(K)$ where $K\hbar$ is the momentum transfer.[1,2,4] We have evaluated $f_n(K)$, and thence these parameters for the excitations from the ground state to the 2^1S, 2^1P, 3^1S, 3^1P, and 3^1D states from the correlated wave functions computed by Weiss,[5] and to the 4^1S, 5^1S, 6^1S, and 7^1S states from those computed by Perkins.[6] The Weiss wave functions all contain over 50 terms, and the Perkins wave functions contain 40 terms each. The Weiss wave functions compare very favorably with the more elaborate Pekeris wave functions[7] in terms of total energies and some other expectation values. The total energies and other expectation values are given in Table I.

Furthermore, we find that the values of $f_n(K)$ computed from the length and velocity formulas agree within 1% or better for the values of K for which the magnitudes of $f_n(K)$ are significant. The large volume of the numerical data on $f_n(K)$ of Li^+ prevents us from presenting them here.[12] Qualitatively, the $f_n(K)$ of Li^+ are very similar to those of He. The values of M_n^2, C_n, b_n, and γ_n computed from the Weiss and Perkins wave functions are given in Tables II and III.

The dependence of these parameters for the higher excited states on the effective quantum numbers has been determined by extrapolation from those calculated with the Weiss, Perkins, and hydrogenic ($n = 4$, 5, and 6) wave functions.[12] Actually, we have used the effective quantum number $n^* = n + \delta$, where n is the principal quantum number and δ is deduced from available theoretical and spectroscopic data.[7,13,14] The formulas for the extrapolated values of the parameters are given in Table IV.

From the parameters in Tables II–IV, we get the sum of the Bethe cross sections for the discrete excitations

$$\sigma_{ex} = \frac{4\pi a_0^2 z^2}{T/R}\left\{M_{ex}^2\left[\ln\left(\frac{\beta^2}{1-\beta^2}\right) - \beta^2\right] + C_{ex}\right\} \quad , \tag{4}$$

where $$M_{ex}^2 = \sum_n M_n^2 = 0.1415 \quad , \tag{5}$$

and $$C_{ex} = \sum_n (C_n + b_n) = 1.225 \pm 0.001 \tag{6}$$

TABLE I. Expectation values for some discrete states of Li^+ in a.u.

State	Source	− (Total energy)	r_1	r_{12}	r_1^2	r_{12}^2
1^1S	Weiss[a]	7.279913	0.572774	0.862316	0.446279	0.927065
1^1S	Pekeris[b]	7.2799134	0.572774	0.862315	0.446279	0.927065
2^1S	Weiss	5.040873	1.64415	2.84435	4.69439	9.43577
2^1S	Pekeris	5.0408767	1.64420	2.84445	4.69510	9.43710
2^1P	Weiss	4.993348	1.52190	2.59241	4.04113	8.07321
2^1P	Schiff[c]	4.9933511	1.52193	2.59247	4.04163	8.07421
3^1S	Weiss	4.733732	3.46040	6.44606	23.5741	47.1716
3^1P	Weiss	4.720181	3.40580	6.33457	23.1011	46.2104
3^1D	Weiss	4.722377	2.87243	5.27268	15.8868	31.7985
4^1S	Perkins[d]	4.629778	6.0311	11.576	75.372	150.76
5^1S	Perkins	4.582424	9.3507	18.210	185.71	371.42
6^1S	Perkins	4.556951	13.418	26.341	387.57	775.15
7^1S	Perkins	4.541692	18.258	36.021	723.48	1447.0

[a]Reference 5.
[b]Reference 7.
[c]B. Schiff, H. Lifson, C. L. Pekeris, and P. Rabinowitz, Phys. Rev. 140, A1104 (1965).
[d]Reference 6.

TABLE II. Parameters for the Born cross sections of Li^+ [see Eq. (1) of the text]. Optically allowed excitations.[a]

Excited state	M_n^2	C_n	$\gamma_n^{(e)}$	$\gamma_n^{(\infty)}$	f_n
2^1P	0.0998	0.835	0.0391	0.267	0.4565
3^1P	0.0216	0.182	0.0486	−0.0068	0.1107

[a] For the allowed excitations, the values of γ_n depend on the reduced mass of the incident and target particles; $\gamma_n^{(e)}$ is for the incident electrons, and $\gamma_n^{(\infty)}$ for the case of a reduced mass infinite compared to that of the electron, a good approximation for protons and heavier incident particles.

Note that M_{ex}^2 is determined only by optically allowed transitions, whereas C_{ex} contains contributions from forbidden transitions as well. The uncertainty in Eq. (6) comes mainly from the n^1P excitations with $n \geq 4$.

III. TOTAL INELASTIC-SCATTERING CROSS SECTION

We have shown earlier[3] that the sum σ_{tot} of the Bethe cross sections for all inelastic scattering is given by the same analytical form as Eq. (4) with the parameters M_{ex}^2 and C_{ex} replaced by M_{tot}^2 and C_{tot}, respectively.

The value of M_{tot}^2 is determined from the ground-state wave function alone. To evaluate C_{tot}, however, the value of the sum

$$L(-1) \equiv \sum_n (f_n R/E_n)\ln(E_n/R) . \quad (7)$$

over all discrete and continuum states is needed in addition to the values of integrals I_1 and I_2 in the notations of Ref. 3, both of which can be computed from the ground-state wave function.

TABLE III. Parameters for the Born cross sections of Li^+ [see Eq. (2) of the text]. Optically forbidden excitations.

Excited state	b_n	γ_n
2^1S	0.0224	−0.0447
3^1S	0.0050	−0.0099
3^1D	0.0020	−0.0095
4^1S	0.0019	−0.0037
5^1S	0.00093	−0.0018
6^1S	0.00052	−0.0010
7^1S	0.00032	−0.00063

TABLE IV. Extrapolated cross-section parameters and their sums (see Sec. 2).

For excitations to the n^1P ($n \geq 4$) states

$$f_n = 2.58(n^*)^{-3} + 3.70(n^*)^{-5} + 2.95(n^*)^{-7}$$
$$M_n^2 = 0.465(n^*)^{-3} + 1.00(n^*)^{-5} + 1.25(n^*)^{-7}, \text{ and}$$
$$C_n = 3.97(n^*)^{-3} + 7.75(n^*)^{-5} + 12.5(n^*)^{-7} ,$$

where $n^* = n + 0.0136$.

For excitations to the n^1S ($n \geq 4$) states

$$b_n = 0.104(n^*)^{-3} + 0.173(n^*)^{-5} ,$$

where $n^* = n - 0.074$.

For excitations to the n^1D ($n \geq 4$) states

$$b_n = 0.0760(n^*)^{-3} - 0.148(n^*)^{-5} - 0.375(n^*)^{-7},$$

where $n^* = n - 0.0012$.

Sum of the parameters[a]

	f_n	M_n^2	C_n	$b(n^1S)$	$b(n^1D)$
$\sum_{n=2}^{3}$	0.567	0.1214	1.017	0.0274	0.0020 ($n = 3$)
$\sum_{n=4}^{\infty}$	0.109	0.0201	0.171	0.0046	0.0028
$\sum_{n=2}^{\infty}$	0.676	0.1415	1.188	0.0320	0.0048

[a] The sum of b_n for the n^1F and other excitations is estimated at about 1 % of $\sum b(n^1D)$ and is neglected in evaluating C_{ex}.

For discrete excitations, the values of f_n are given in Tables II and IV. Our discrete oscillator strengths, though independently determined, are very similar to those of Dalgarno and Parkinson.[10] We have adopted the continuum oscillator strengths from those calculated by Stewart and Webb,[8] after adjusting their Hartree-Fock length results to match the discrete f_n at the ionization threshold, and also to be consistent with various sum-rule values of the oscillator strengths (see Tables V and VI). Our adopted continuum oscillator strengths only partially account for double excitations and ionizations through the sum rule, but the resulting error in $L(-1)$ is expected to be insignificant.

From the Weiss wave function for the ground state, we get

$$M_{tot}^2 = 0.2860 , \quad (8)$$

TABLE V. Moments of oscillator strengths of Li^+. $S(\mu) \equiv \sum_n f_n (E_n/R)^\mu$.

μ	Accurate total[a]	Discrete	Present work continuum	Total
2	688.837	15.6	>424.3	>439.9
1	20.1837	3.24	>16.78	>20.02
0	2	0.676	1.324	2.000
−1	0.286017	0.1415	0.1445	0.2860
−2	0.0481	0.0298	0.0183	0.0481

[a]Accurate values of $S(2)$, $S(1)$, and $S(-1)$ can be evaluated from the expectation values in Ref. 7, $S(0)$ from the Thomas-Kuhn-Reiche sum rule, and $S(-2)$ from the dipole polarizability computed by M. N. Grasso, K. T. Chung, and R. P. Hurst, Phys. Rev. 167, 1 (1968).

$$I_1 = 0.6549 \ , \tag{9}$$

and $$I_2 = 0.0269 \ . \tag{10}$$

From Eqs. (8)–(10) and Tables V and VI, we also get [see Eqs. (21) and (23) of Ref. 3]

$$C_{\text{tot}} = -2L(-1) + I_1 - I_2 + M_{\text{tot}}^2 \times 11.2268$$
$$= 2.784 \pm 0.001 \ . \tag{11}$$

The uncertainty in Eq. (11) is mainly due to that in the value of $L(-1)$.

IV. IONIZATION CROSS SECTION

We can now obtain the parameters [to be used with Eq. (4)] for the ionization cross section σ_i by subtracting σ_{ex} from σ_{tot},

$$M_i^2 = M_{\text{tot}}^2 - M_{\text{ex}}^2 = 0.1445 \ , \tag{12}$$

and from Eqs. (6) and (11),

$$C_i = C_{\text{tot}} - C_{\text{ex}} = 1.559 \pm 0.002 \, . \tag{13}$$

With these values of the parameters, we get from Eqs. (4)–(6), (8), and (11)–(13)

$$\sigma_{\text{tot}} = (z^2/\beta^2)(0.536\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 5.216 \pm 0.002) \times 10^{-20}\ \text{cm}^2 \ , \tag{14}$$

$$\sigma_{\text{ex}} = (z^2/\beta^2)(0.265\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 2.295 \pm 0.002) \times 10^{-20}\ \text{cm}^2 \ , \tag{15}$$

and

$$\sigma_i = (z^2/\beta^2)(0.271\{\ln[\beta^2/(1-\beta^2)] - \beta^2\} + 2.921 \pm 0.004) \times 1^{-20}\ \text{cm}^2 \ . \tag{16}$$

Since σ_{tot} includes double ionization, σ_i given by Eq. (16) is the "counting" ionization cross section, a simple sum over all ionization events.

There seem to be no experimental data either for discrete excitations or for the total inelastic scattering by Li^+. There are, however, some experimental data on the single- as well as double-ionization cross sections of Li^+ by electron impact measured by the crossed-beam method.[15–18]

It is appropriate to compare our σ_i with the sum of the experimental cross sections for the single and double ionization. The data of Peart, Martin, and Dolder,[18] however, show that the cross section for the double ionization is about 2 orders of magnitude smaller than that for the single ionization, and it is not essential to include the experimental data on the double ionization. In Fig. 1, we compare σ_i with the single-ionization data only. In consequence, our σ_i becomes an upper limit to the cross section for the single ionization.

In Fig. 1, we plot various cross sections multiplied by β^2/z^2 as a function of $\ln[\beta^2/(1-\beta^2)] - \beta^2$. As can be seen from Eqs. (14)–(16), the Bethe cross sections are represented by straight lines in such a plot. It is clear from the figure that the experimental data[18] are in excellent agreement with theory for the incident electron energies $\gtrsim 5$ keV. The experimental data below 3-keV incident energy[15–18] also show a nearly "straight-line" behavior but with a steeper slope, a phenomenon which could lead to misinterpretation when high-energy data were not available. It is interesting to note that the asymptotic behavior of the ionization cross section is achieved when the incident energy is ~60 times the threshold energy. A similar situation was also observed for the ionization

TABLE VI. The values of $L(\mu) \equiv \sum_n f_n (E_n/R)^\mu \ln(E_n/R)$ of Li^+.

μ	Discrete	Continuum	Total
1	5.09	>47.19	>52.28
0	1.058	3.090	4.148
−1	0.2209	0.3068	0.5277

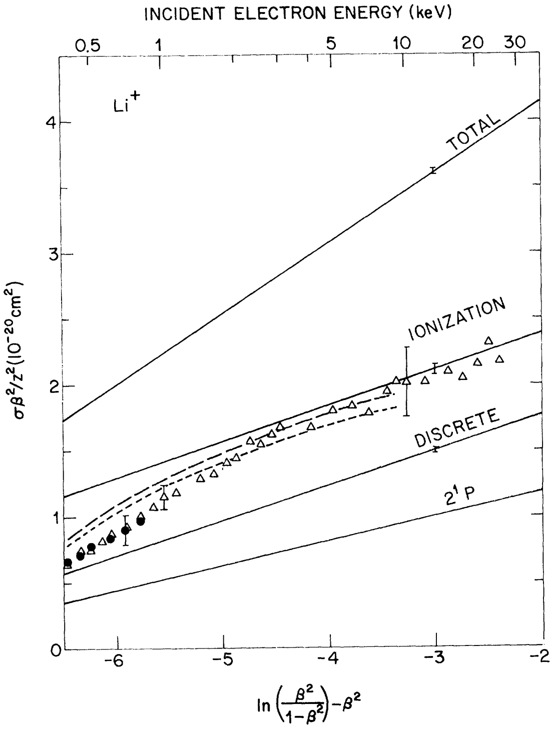

FIG. 1. Cross sections for the excitation of $Li^+(1^1S)$ by incident particles of charge ze and velocity βc. Note that the ordinate is the cross section multiplied by $(\beta/z)^2$. The straight lines represent the Bethe (asymptotic) cross sections for total inelastic scattering (TOTAL), for ionization (IONIZATION), for the sum of discrete excitations (DISCRETE), and for the excitation to the 2^1P state of Li^+ (2^1P). The long broken line curve and dashed line curve represent the ionization cross sections calculated by Economides and McDowell (Ref. 20) using the length and velocity forms, respectively. The closed circles (●) are the ionization cross section by electron impact measured by Lineberger, Hooper and McDaniel (Ref. 15), and the open triangles (Δ) are those by Peart, Martin, and Dolder (Ref. 18). Typical error limits are given for the experimental data. The error limits for the theoretical cross sections in this plot are independent of incident energy.

cross sections[11, 19] of He and H^-.

Also we have shown in Fig. 1 the single-ionization cross sections calculated by Economides and McDowell.[20] From a two-parameter ground state and the Hartree-Fock continuum wave functions, they computed the cross section both in the length and velocity formulas. Their length result is in good agreement with our σ_i in the asymptotic region.

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Coulomb T Matrix and Electron Capture by Protons Passing through Hydrogen †

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Using Nutt's expression for the two-particle off-shell Coulomb T matrix, and neglecting multiple-scattering terms in Faddeev's expansion for the transition matrix, an expression for the charge-exchange amplitude in proton-hydrogen scattering is derived. The results of numerical calculations are compared with the corresponding results of Brinkman and Kramers, of Jackson and Schiff, and of Drisko. An analytical expression for the total cross section at high energies is obtained from our formalism. In the high-energy limit, our results approach the Brinkman-Kramers formula.

I. INTRODUCTION

The problem of three particles interacting with each other through the Coulomb potential has fundamental importance in atomic scattering, and a very considerable amount of work has been done in this connection. There are two principal difficulties: First, the mathematical complexity present in solving the three-particle Schrödinger equation; second, special problems arise from the long-range nature of the Coulomb potential and require the scattering amplitude to be defined with respect to the Coulomb-distorted asymptotic states rather than plane-wave states. However, the work of Faddeev[1] on the expansion of three-body T matrix in terms of two-body T matrices has revived hopes of obtaining reasonable approximations to the three-body problem. For example, if we have the expression for the two-body off-shell Coulomb T matrix, Faddeev's procedure enables us, in principle, to obtain the corresponding three-body Coulomb T matrix. Schwinger[2] obtained a set of integral representations for the two-particle Coulomb Green's function and subsequently, Nutt[3] derived expression for the Coulomb T matrix and investigated its analytic structure. In addition, Nutt's work indicates how the problem of describing the scattering of a particle from a bound system of two particles may be treated using the Coulomb T matrix in Faddeev's expansion. Most of the difficulties associated with the Coulomb-distorted asymptotic states appear to be resolved in the formulations of Schwinger and Nutt. These results encourage us to reinvestigate the old problem of proton-hydrogen (p-H) charge exchange at high energies within the framework of Faddeev's theory.

In order to appreciate the present approach, a brief summary of the status of the p-H charge-exchange problem is desirable. Our discussion is restricted to the high-energy limit. Extensive reviews have been given by Bransden.[4,5] The problem can be stated: Does the first Born approximation describe the process correctly in the high-energy limit, and if so, what is the correct potential to use in the Born formula? Brinkman and Kramers[6] (BK) first evaluated the Born amplitude for charge exchange neglecting the internuclear potential V_{12}. It was argued that at high energies the internucleon potential should not affect the charge-exchange cross section. Later, Jackson and Schiff[7] (JS) evaluated the Born approximation including V_{12}, and found that the cross section was reduced by a factor of 0.66 at high energies in comparison with that of BK. This result presents a serious problem. Subsequently, Drisko[8] evaluated the cross section in the high-energy limit, taking into account the first three terms of the Born series, and found the cross section to be given by

$$\sigma_B{}^{(3)} = \sigma_{BK}(0.319 + 5\pi v/2^{12}) , \qquad (1.1)$$

where σ_{BK} is the BK cross section, and v is the velocity of incident proton in a.u. in the laboratory system. The result appears to indicate that, no matter how high the energy is, the Born series does not converge to its first term.

It is not known whether the Born series for the transition amplitude for rearrangement collisions