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Total Cross Sections for Inelastic Scattering of Charged Particles by Atoms and Molecules. VI. Metastable Helium†

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Sum rules for the asymptotic Born cross sections have been applied to the evaluation of various inelastic-scattering cross sections of metastable He ($2\,^1S$ and $2\,^3S$). The ionization cross sections for the two species are similar in magnitude, and each constitutes only a small part of the total cross section for inelastic scattering. Although the first Born approximation is inappropriate for the scattering of slow charged particles, the energy dependence exhibited in the recent experiment by Long and Geballe for the ionization of He ($2\,^3S$) by low-energy electrons (≤ 16 eV) is compatible with the high-energy behavior predicted by the theory. The exchange correction evaluated from the Mott formula has been included in the ionization cross section by electron impact. Optical oscillator strengths for the first three transitions to doubly excited states [$2\,^1S \rightarrow (2lnl')^1P$] are also given.

I. INTRODUCTION

Rigorous applications of the Bethe procedure[1-3] to obtain various inelastic-scattering cross sections so far have been restricted to one- and two-electron atoms in the ground state.[4] The theory is not restricted to the ground state, and in this paper we present an example of its application to metastable He in the $2\,^3S$ and $2\,^1S$ states. Moreover, these metastable species have open-shell structure, and serve as a prototype for the application of the theory to complex atoms.

The Bethe procedure in its extended form[4] provides an asymptotic expression for the total cross section for inelastic scattering

$$\sigma_{\text{tot}} = A\,(\ln T)/T + B/T + C/T^2 + \cdots , \qquad (1)$$

where A, B, and C are constants determined solely from the properties of the target atom and T is proportional to the square of the incident particle velocity. The constants A and C are readily calculated from the initial-state wave function of the atom. To determine B, however, the oscillator-strength distribution (OSD) must be known, in addition to the initial-state wave function.[1,3] When the cross section is given in the form of Eq. (1) with only two constants A and B, we shall refer to it as the Bethe cross section.

For metastable He, various wave functions and expectation values derived from them are available in the literature.[5] We have used the correlated wave functions determined by Weiss.[6] As was shown earlier,[7] the Weiss wave functions are in many ways as reliable as the Pekeris wave functions.

The OSD of metastable He, however, has many uncertainties. Theoretical or experimental data on the OSD of higher continua such as ($\mathrm{He}^* \rightarrow \mathrm{He}^{++} + 2e$) are not available. The data for the autoionizing states are very scarce.[8] On the other hand, there are many qualitative aspects which are shared by the $2\,^3S$ and $2\,^1S$ states of He, particularly in the OSD. These features. including the uncertainties in the OSD's, are expected to be common in complex atoms, and the experience gained in the present investigation should provide a valuable guide for future applications.

Individual cross sections can also be written in the form of Eq. (1) with three constant – we shall call such expressions the Born asymptotes – which are determined from the generalized oscillator strength (GOS).[7,9] By subtracting the sum of the Born asymptotes for the discrete excitations from the total cross section, we get the Born asymptote for ionization. The ionization cross section thus obtained represents a simple sum of cross sections for all events leading to ionization and is known as the counting ionization cross section. The Born asymptotes for ionization have been further improved by adding the correction for electron exchange evaluated from the Mott formula.[4] The ionization cross sections of metastable He based on the first Born approximation have not been reported in the literature.

So far the ionization cross sections for metastable He have been measured with slow electrons only,[10–12] in which case the first Born approximation is not appropriate. Nevertheless, comparison with the theory will provide a consistency check, and our results may eventually be used to normalize experimental cross sections when high-velocity data become available.

II. OPTICAL OSCILLATOR-STRENGTH DISTRIBUTIONS

To evaluate B in Eq. (1), it is necessary to know the value of

$$L(-1)=\sum_n (f_n R/E_n)\ln(E_n/R)\,, \tag{2}$$

where f_n is the optical oscillator strength for the transition to state n, E_n is the corresponding excitation energy, R is the rydberg, and the summation is over all states, both discrete and continuous.[3] The use of differential oscillator strength df/dE is implied in Eq. (2) for the states in the continua. Many aspects of the OSD's for the singlet and triplet excitations are common. Therefore, the discussion below for the singlet excitations is limited to the aspects which are sufficiently different from those in the triplet excitations.

A. Triplet Excitations

The quantity $L(-1)$ was calculated from an OSD adopted from data largely available in the literature. The distribution was chosen so as to satisfy the sum rules for the moments

$$S(k)=\sum_n f_n(E_n/R)^k \tag{3}$$

for $k=-2$, -1, 0, and 1. The moment $S(-2)$ is proportional to the polarizability, $S(0)$ is equal to the number of electrons, and the other moments are initial-state properties.[13] The values of these moments are known to high accuracy and are given in Table I (labeled as "Total"). An OSD constructed in this way is designed to provide an accurate value of $L(-1)$, which is strongly influenced by low-lying states. The distribution will not necessarily give a reliable value of other quantities, for example $S(2)$, which are decided largely by the transitions to highly excited states. An adoption of the OSD for metastable He was made by Dalgarno and Kingston in 1958.[14] Our revised version uses more accurate data which have become available since that time and will provide more reliable values for the spectral moments with $k<0$.

Transitions to the low-lying discrete states, in particular to $2\,^3P$, dominate the moments with $k<0$ as may be seen from Table I. This results from a combination of large oscillator strength and low excitation energy. Accurate values of f_n for the first two excitations have been evaluated by Schiff and Pekeris.[15] Fairly reliable values for other discrete excitations are also available.[6,16] An extrapolation formula as a function of the effective quantum number for excitations to $n\geq 5$ states was adopted (Table II), guided by the f_n calculated by Green *et al.*[16] and the quantum-defect method of Bates and Damgaard.[17] The quantum-defect method provides surprisingly accurate f_n even for the $2\,^3P$ and $3\,^3P$ excitations,[17] so that the extrapolation is likely to be equally reliable.

TABLE I. Contributions to $S(k)$ and $L(-1)$.[a]

Final state	$S(-2)$	$S(-1)$	$S(0)$	$S(1)$	$L(-1)$
			Triplet transitions		
$2\,^3P$	76.17	6.408	0.539	0.015	−15.86
$n\geq 3$, $n\,^3P$ (1s np)	1.83	0.477	0.126	0.065	−0.82
1st continuum (1s ϵp)	0.80	0.441	0.314	0.428	−0.22
Doubly excited ($2lnl'$)	0.04	0.126	0.367	1.072	0.14
Remainder[b]	0.06	0.152	0.654	4.241	0.18
Total[b]	78.90	7.604	2.000	5.821	−16.58
			Singlet transitions		
$2\,^1P$	192.10	8.503	0.376	0.017	−26.51
$n\geq 3$, $n\,^1P$ (1s np)	6.43	1.290	0.265	0.056	−2.06
1st continuum (1s ϵp)	1.43	0.631	0.354	0.390	−0.46
Doubly excited ($2lnl'$)	0.05	0.135	0.402	1.199	0.15
Remainder[b]	0.48	0.126	0.603	4.086	0.07
Total[b]	200.49	10.685	2.000	5.748	−28.81

[a] See Eqs. (2) and (3) for definitions.

[b] The contributions from the "remainder" were adjusted so that the accurate values of the "total" $S(k)$ were reproduced. The values of the "total" $S(k)$ were obtained from K. T. Chung and R. P. Hurst, Phys. Rev. 152, 35 (1966) for $k=-2$, and C. L. Pekeris, *ibid.* 126, 1470 (1962); 115, 1216 (1959) for $k=-1$ and 1.

TABLE II. Dipole oscillator strengths for the 1s 2s→ 1s *np* transitions of He.

Initial state	$2\,^3S$	$2\,^1S$
Final state		
$n=2$[a]	0.5391	0.3764
3[a]	0.0645	0.1514
4	0.0259[b]	0.0508[c]
≥ 5[d]	$1.338\,(n^*)^{-3}$	$2.271\,(n^*)^{-3}$
	$+3.80\,(n^*)^{-5}$	$+12.1\,(n^*)^{-5}$
		$+43.8\,(n^*)^{-7}$
Sum	0.6654	0.6415

[a] Reference 15.

[b] Reference 16.

[c] Reference 6.

[d] n^* (triplet) $= n - 0.068$, n^* (singlet) $= n + 0.0121$.

The extrapolated quantum-defect method of Burgess and Seaton,[18] combined with recent spectroscopic data,[19] was used to compute df/dE from threshold to $E_n/R \sim 2$ for the $(1s\epsilon p)\,^3P$ continuum, beyond which the df/dE of Huang[20] was used. Huang used a six-term Hylleraas wave function for the bound state and hydrogenic wave functions for the free states. The df/dE of the quantum-defect method and that of Huang are in closest agreement (~ 3%) around $E_n/R = 2$.

The positions of the lowest members of the autoionizing series of doubly excited states converging on the $\mathrm{He}^+(n=2)$ threshold have been well established.[21–23] The detailed shape of the continuum OSD in this energy region for the metastable species has not been calculated, nor has the photoabsorption or electron-impact spectrum been observed. However, the widths of these levels are small[21] and it is not expected that the coupling to the background $(1s\epsilon p)$ continuum will affect significantly their contribution to $L(-1)$. Consequently, the oscillator strength of these autoionizing states has been estimated by treating them as stationary states.

Knox and Rudge[8] have calculated the positions and oscillator strengths of the doubly excited triplet states using wave functions represented by a superposition of Sturmian functions. We have also evaluated the f_n in both length and velocity form using the $2\,^3S$ wave function by Weiss[6] and the wave functions of Lipsky and Russek[23] for the doubly excited states. For the first few states the results agree with those of Knox and Rudge. However, for higher transitions our results do not agree as well. We have used the f_n by Knox and Rudge for the doubly excited triplet states. We note from these results that the first autoionizing state $(2s2p)$ has an unusually large fraction (14%) of the total oscillator strength and should show up as a prominent peak in the photoabsorption spectrum. As may be seen from the data of Ref. 8, the members of the "−" series have larger f_n than those of the "+" series, unlike the situation in the absorption from the ground state. Although the sum of f_n for the autoionizing levels amounts to almost 20% of the total (Table I), their contribution to $L(-1)$ represents only ~ 1% of the total because of the large energy denominators involved.

From Table I, we see that the sum of f_n for discrete states $(1snp)$ and the first continuum $(1s\epsilon p)$ is almost unity. The autoionizing states below the $\mathrm{He}^+(n=2)$ threshold contribute about 0.37 so that to satisfy the Thomas-Reiche-Kuhn sum rule[13] we must assign about 0.65 (out of 2) to all other excitations. There are no data for these higher excitations. However, their contribution represents less than 0.1% of $S(-2)$ and only 2% of $S(-1)$. We expect the relative importance of the contribution of the higher excitations to $L(-1)$ and to $S(-1)$ to be similar. Therefore, we have adopted two artificial discrete states, whose f_n and E_n have been chosen so as to satisfy the accurately known values of $S(k)$ for $k = 1$, 0, -1, and -2, when combined with the known f_n and E_n. With this model, the higher excitations contribute only about 1% of $L(-1)$.

As shown in Table I, $L(-1)$ depends heavily upon the discrete excitations, particularly the first one $(2\,^3P)$. This relative importance of the discrete excitations in the evaluation of $L(-1)$ is also expected to hold in other atoms with low-lying states such as the alkali atoms. Finally, from Table I, we conclude that $L(-1) = 16.58 \pm 0.18$ for the $2\,^3S$ state.

B. Singlet Excitations

Principal results for the OSD are given in Table I. The singlet f_n were adopted from the same source as the corresponding triplet f_n, except in the case of the doubly excited states. For these states the f_n were calculated from the $2\,^1S$ wave function of Weiss and the excited-state wave functions of both Refs. 22 and 23. The two sets of results agree to within 1% for the low-lying states. The length and velocity f_n are in closer agreement than in the triplet case. The value of $L(-1)$ is unaffected by the use of either the length or velocity f_n. We used the velocity results calculated from

TABLE III. Oscillator strengths for the $2\,^1S \rightarrow (2lnl')\,^1P$ transitions of He.[a]

Final state	E_n/R	f_n
$2s2p$	2.920	0.268
(23) −	3.100	0.116
(24) −	3.200	0.018

[a] Based on the velocity results evaluated from the $2\,^1S$ wave function by Weiss (Ref. 6) and the doubly excited state wave functions by Altick and Moore (Ref. 22).

the excited-state wave functions of Ref. 22. In Table III, we present those f_n which are larger than 0.01. For the singlet excitation, we have $L(-1) = -28.81 \pm 0.15$.

III. CROSS SECTIONS FOR INELASTIC SCATTERING

A. Total Cross Section

In the notation used previously,[3,4] the total cross section for inelastic scattering [Eq. (1)] is given by

$$\sigma_{\text{tot}} = 4\pi a_0^2 z^2 (R/T)\left[M_{\text{tot}}^2 \ln(4c_{\text{tot}}\, T/R) + \gamma_{\text{tot}}(R/T)\right] , \tag{4}$$

where a_0 is the Bohr radius, ze is the charge of the incident particle, and $T = \frac{1}{2}mv^2$ with m the electron mass and v the velocity of the incident particle.

The first constant M_{tot}^2 in Eq. (4) is an initial-state expectation value defined as[3]

$$M_{\text{tot}}^2 = \langle (\textstyle\sum_j \vec{r}_j)^2 \rangle , \tag{5}$$

where the summation is over all atomic electrons and $\vec{r}_j$ is the position vector of the jth electron.

The second constant $\ln c_{\text{tot}}$ is defined as[3]

$$M_{\text{tot}}^2 \ln c_{\text{tot}} = -2L(-1) + I_1 - I_2 , \tag{6}$$

where $L(-1)$ is given by Eq. (2), and I_1 and I_2 are integrals which are evaluated from the initial-state wave function (see Ref. 3 for definitions). The integrands for I_1 and I_2 contain the incoherent-scattering function, which is sensitive to electron correlation.

The third constant γ_{tot} has different values depending on the type of incident particle[4]:

$$\gamma_{\text{tot}} = \begin{cases} -N[\frac{3}{2} + S'(1)/4N] & \text{for positrons} \qquad (7\text{a}) \\ -N[\frac{5}{2} + S'(1)/4N] & \text{for electrons} \qquad (7\text{b}) \\ -N[\frac{1}{4} + S'(1)/4N] & \text{for heavy particles,} \quad (7\text{c}) \end{cases}$$

where N is the total number of electrons in the atom. In Eqs. (7), $S'(1)$ is another initial-state expectation value defined as[4]

$$S'(1) = N^2 + 2\sum_j \sum_{k \neq j} \left\langle (z_j - z_k)^2 \frac{\partial^2}{\partial z_j \partial z_k} \right\rangle , \tag{8}$$

where z is a Cartesian component of $\vec{r}$ and the summations are over all electrons of the atom. As is shown in Ref. 4,

$$S'(1) = N + \text{small correction terms} , \tag{9}$$

where the correction terms depend on the electron correlation.

The values of the atomic constants in Eqs. (4)–(8) are given in Table IV. The uncertainties in the values of $M_{\text{tot}}^2 \ln 4c_{\text{tot}}$ arise entirely from those in the values of $L(-1)$.

TABLE IV. Constants for the total cross section.[a,b]

	$2\,^3S$	$2\,^1S$
M_{tot}^2	7.604	10.685
$L(-1)$	-16.58 ± 0.18	-28.81 ± 0.15
I_1	1.444	1.463
I_2	11.262	18.387
$S'(1)$	1.912	2.113
$M_{\text{tot}}^2 \ln 4c_{\text{tot}}$	33.88 ± 0.36	55.51 ± 0.30
$\gamma_{\text{tot}}{}^{(a)}$	-3.48	-3.53
$\gamma_{\text{tot}}{}^{(b)}$	-5.48	-5.53
$\gamma_{\text{tot}}{}^{(\infty)}$	-0.978	-1.03

[a] See Eqs. (7a)–(7c) for the definitions of $\gamma^{(a)}$, $\gamma^{(b)}$, and $\gamma^{(\infty)}$, respectively.

[b] The values of I_1, I_2, and $S'(1)$ were calculated from the Weiss wave functions (Ref. 6).

B. Discrete Excitations

The Born asymptote for a discrete excitation to the state n is written as

$$\sigma_n = 4\pi a_0^2 z^2 (R/T)\left[M_n^2 \ln(4c_n T/R) + \gamma_n(R/T)\right] \tag{10a}$$

for a dipole-allowed transition, and

$$\sigma_n = 4\pi a_0^2 z^2 (R/T)\left[b_n + \gamma_n(R/T)\right] \tag{10b}$$

for a forbidden transition, where the constants M_n^2, $\ln c_n$, b_n, and γ_n are determined from the GOS for the excitation.[1-3,9] In particular, $M_n^2 \equiv f_n R/E_n$ and, by definition, $S(-1)$ is related to M_{tot}^2 [see Eq. (3)]:

$$S(-1) = \textstyle\sum_n M_n^2 = M_{\text{tot}}^2 .$$

Therefore, the data in the "$S(-1)$" column in Table I represent the sums of M_n^2 over different types of transitions.

The constants for several excitations to the low-lying states have been reported earlier.[7] For higher-P excitations, the quantum-defect method[17] has been used to extrapolate the values of M_n^2, and $\ln c_n$ has been assumed independent of n for $n \geq 4$. This near constancy of $\ln c_n$ is observed in the excitations of He and Li$^+$ from the ground state.[24] The constants for higher-D excitations have been extrapolated as functions of the effective quantum numbers, based on the values obtained from the Weiss wave functions for the metastable states and the hydrogenic wave functions for the excited states. For the excitations to S states, correlated wave functions by Perkins[25] have been used. The results are given in Tables V and VI.

As can be seen from the values of $M_n^2 \ln c_n$ and b_n in Tables V and VI, and also from the values of GOS in Ref. 7, the cross sections for the $3D$ excitations are larger than those for the $3S$ excitations (at all T) and for the $3P$ excitations (for $T/R \lesssim 100$), contrary to the situation in the excitations from the ground state of He.[9] This abnormality is

TABLE V. Constants for the triplet excitation cross sections.

Allowed transitions[a]

Final state ($n\,^3P$)	M_n^2	$M_n^2 \ln c_n$	$\gamma_n^{(e)}$	$\gamma_n^{(\infty)}$
$n=2$	6.408	16.228	−0.195	0.075
3	0.275	−0.242	0.100	0.132
4	0.091	−0.082	0.024	0.036
$\sum (n \geq 5)$	0.111	−0.100	0.014	0.032
Sum	6.885	15.804	−0.057	0.275

Forbidden transitions

Final state ($n\,^3S$)	b_n	γ_n	Final state ($n\,^3D$)	b_n	γ_n
$n=3$	0.705	−0.088	3	1.419	−0.213
4	0.141	−0.018	4	0.343	−0.041
$\sum (n \geq 5)$	0.132	−0.016	$\sum (n \geq 5)$	0.389	−0.036
Sum	0.978	−0.122		2.151	−0.290

Sum of discrete excitations[a,b]

M_{ex}^2	$M_{ex}^2 \ln 4c_{ex}$	$\gamma_{ex}^{(e)}$	$\gamma_{ex}^{(\infty)}$
6.885 ± 0.014	28.58 ± 0.10	−0.47 ± 0.02	−0.14 ± 0.02

[a] For electrons and positrons, use $\gamma^{(e)}$, and for heavy particles $\gamma^{(\infty)}$.

[b] $\sum_{L=3}^{\infty} b(^3L)$ is estimated to be ~ 0.10. $\sum_{L=3}^{\infty} \gamma(^3L) \equiv 0$ (see Ref. 4).

a direct consequence of the minima in the GOS of the $3P$ excitations, which is normally expected to have the largest cross section. We can interpret it as the Bethe sum rule[1] [$\sum_n f_n(K) = N$ for any K] operating locally; the missing part near the minimum of a GOS is taken up by the GOS of energetically nearby states. A similar situation also exists in the transitions between the excited states of H.[26]

TABLE VI. Constants for the singlet excitation cross sections.

Allowed transitions[a]

Final state ($n\,^1P$)	M_n^2	$M_n^2 \ln c_n$	$\gamma_n^{(e)}$	$\gamma_n^{(\infty)}$
$n=2$	8.503	30.188	−0.153	0.035
3	0.833	−0.552	0.159	0.232
4	0.221	−0.156	0.035	0.061
$\sum (n \geq 5)$	0.236	−0.160	0.021	0.054
Sum	9.793	29.320	−0.062	0.382

Forbidden transitions

Final state ($n\,^1S$)	b_n	γ_n	Final state ($n\,^1D$)	b_n	γ_n
$n=1$	0.045	−0.032			
3	0.974	−0.101	3	2.630	−0.267
4	0.202	−0.023	4	0.446	−0.033
$\sum (n \geq 5)$	0.194	−0.021	$\sum (n \geq 5)$	0.487	−0.018
Sum	1.415	−0.177		3.563	−0.318

Sum of discrete excitations[a,b]

M_{ex}^2	$M_{ex}^2 \ln 4c_{ex}$	$\gamma_{ex}^{(e)}$	$\gamma_{ex}^{(\infty)}$
9.793 ± 0.014	48.02 ± 0.15	−0.43 ± 0.02	−0.11 ± 0.02

[a] See Table V, footnote a.

[b] $\sum_{L=3}^{\infty} b(^1L)$ is estimated to be ~ 0.15. $\sum_{L=3}^{\infty} \gamma(^1L) \equiv 0$ (see Ref. 4.

TABLE VII. Constants for the ionization cross section.[a]

	M_i^2	$M_i^2 \ln 4c_i$	$\gamma_i^{(a)}$	$\gamma_i^{(b)}$	$\gamma_i^{(\infty)}$
Triplet	0.719 ± 0.014	5.30 ± 0.45	−3.01	−5.01	−0.84
Singlet	0.892 ± 0.014	7.49 ± 0.45	−3.10	−5.10	−0.92

[a] For positrons use $\gamma^{(a)}$, for electrons $\gamma^{(b)}$, and for heavy particles $\gamma^{(\infty)}$. The uncertainty in the values of γ is estimated to be ± 0.02.

By summing the constants in Eqs. (10) for all (singly excited) discrete states, we can express the cross section for the discrete excitations in the same form as Eq. (4):

$$\sigma_{ex} = 4\pi a_0^2 z^2 (R/T)\left[M_{ex}^2 \ln(4c_{ex}T/R) + \gamma_{ex}(R/T)\right] , \tag{11a}$$

where

$$M_{ex}^2 = \textstyle\sum_{\text{discrete}} M_n^2 , \tag{11b}$$

$$M_{ex}^2 \ln c_{ex} = \textstyle\sum_{\text{discrete}} (M_n^2 \ln c_n + b_n) , \tag{11c}$$

$$\gamma_{ex} = \textstyle\sum_{\text{discrete}} \gamma_n . \tag{11d}$$

The values of M_{ex}^2, $M_{ex}^2 \ln 4c_{ex}$, and γ_{ex} are also listed in Tables V and VI.

Note that the contribution from the superelastic transition ($2\,^1S \rightarrow 1\,^1S$) must be added to other cross sections to obtain σ_{ex}, unlike the situation in the stopping power where its contribution must be subtracted.

C. Ionization Cross Section

By subtracting Eq. (11a) from (4), we obtain the counting ionization cross section

$$\sigma_i = 4\pi a_0^2 z^2 (R/T)\left[M_i^2 \ln(4c_i T/R) + \gamma_i (R/T)\right] , \tag{12a}$$

where

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

$$M_i^2 \ln 4c_i = M_{\text{tot}}^2 \ln 4c_{\text{tot}} - M_{ex}^2 \ln 4c_{ex} , \tag{12c}$$

$$\gamma_i = \gamma_{\text{tot}} - \gamma_{ex} . \tag{12d}$$

The values of M_i^2, $M_i^2 \ln 4c_i$, and γ_i are given in Table VII. It is clear from the values of the constants for the total and discrete-excitation cross sections that a major part of σ_{tot} comes from σ_{ex}. It is important, therefore, to determine σ_{tot} and σ_{ex} accurately to obtain reliable σ_i by our method in this case.

A few points should be noted here about the ionization cross section: (a) The magnitude of σ_i for the triplet excitation is about $\frac{1}{3}$ larger than that for the singlet excitation for $T/R \lesssim 100$. (b) The correction to the Bethe cross section represented by γ_i is almost entirely from $\gamma_{\rm tot}$. This is also true for the ionization of He and Li$^+$ in the ground state.[4] (c) The first autoionizing state $(2s2p)$ has an unusually large cross section because its M_n^2(equal to $f_n R/E_n$) is more than 10% of M_i^2 (Table III). For the excitation from the ground state,[22] the $(2s2p)$ state accounts for only 0.2% of the corresponding M_i^2.

For incident electrons, a further correction for electron exchange must be included, for the exchange effect contributes to the order $(\ln T)/T^2$ and $1/T^2$ in σ_i. The exchange correction based on the Mott formula is given by[4]

$$\sigma_{\rm exch} = 4\pi a_0^2 N(R/T)^2 [1+\ln(I/T)]\ , \tag{13}$$

where I is the ionization potential (IP) of the atom.

Each orbital in metastable He contributes almost equally to the sum of the optical oscillator strengths [see $S(0)$ in Table III] as if the atomic electrons were independent of each other. Hence, tentatively we evaluated $\sigma_{\rm exch}$ by summing the contributions from each orbital with appropriate orbital energy and electron occupation number. The cross sections for the ionization of He$(2\,^3S)$ by electron impact, with and without the exchange correction, are plotted in Fig. 1, along with the Bethe cross section. In Fig. 1, σ_i times T is plotted as a function of $\ln T$, whereby the Bethe cross section is represented by a straight line, and the γ_i term is shown as the departure from the straight line.

D. Comparison with Other Data

Recently, Long and Geballe[12] measured the cross section for the ionization of He$(2\,^3S)$ by electron impact for $T \leq 16$ eV. The measurement was relative and was indirectly normalized at $T = 12$ eV through a theoretical cross section for the ionization of He in the ground state. Their results are included in Fig. 1. Although the incident energy used in the experiment is too low to permit a direct comparison with the Born cross section, the experimental data are certainly compatible with the high-T behavior of σ_i given by Eq. (12a) combined with the exchange correction (13).

Earlier, Fite and Brackmann[10] and Vriens[11] measured cross sections for the ionization of a mixture of the triplet and singlet metastable He of unknown composition. The uncertainty in the concentration of the two metastable species, however, is largely offset by the similar magnitudes of σ_i for the two species as mentioned in Sec. III C. Again, these experiments were done at low T and a comparison with the Born cross section is not appropriate. The cross sections measured by Fite and Brackmann[10] are almost a factor of 2 smaller than those by Long and Geballe,[12] whereas those by Vriens[11] lie in between these two experiments.

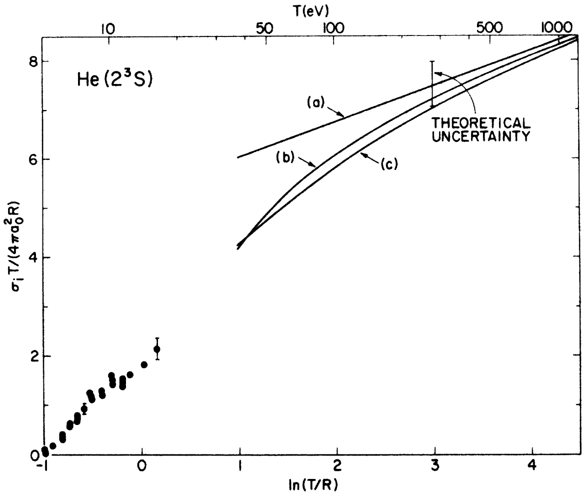

FIG. 1. Cross sections for the ionization of He $(2\,^3S)$ by electron impact. Theoretical cross sections are (a) the Bethe cross section, (b) the Born asymptote for electrons (known as the "Born b" or "modified Born" in the literature), and (c) the Born asymptote with the Mott exchange correction. Uncertainty in the theoretical cross section is common to (a)–(c), and is almost independent of the incident energy T in this plot (σT vs $\ln T$). Dots represent the experiment by Long and Geballe (Ref. 12) and the error limits indicate statistical error only. Normalization of the experimental cross section is subject to an error of ±30%.

Vriens[27] also calculated the ionization cross sections for metastable He by using a "classical" theory. Despite the inconsistencies in the classical theory[28] as used by Vriens, his cross sections are in reasonable agreement with our result (for electrons) for T up to a few keV.

IV. CONCLUDING REMARKS

Using the sum rules for the Born asymptotes, we have determined various cross sections for the inelastic scattering of charged particles by metastable He. For the ionization of ground-state He, the Born asymptote agrees very well with experiment for $T \gtrsim 20I$ ($I = 24.6$ eV).[4] For metastable He, however, the Born asymptote is not expected to be as good because the excitation of the $1s$ core electron shares a substantial part of M_i^2 [see Table I, $S(-1)$ column]. We estimate that our σ_i will be reliable for $T \gtrsim 100I$ ($I \sim 4$ eV). When the inner-shell excitations contribute substantially to $S(-1)$, the first ionization potential alone is not an appropriate parameter to estimate the region of applicability of the Born asymptote.

A. Oscillator-Strength Distribution

The uncertainty in the f_n for the singly excited discrete states $(2s \rightarrow np)$ is amplified in the evaluation of $L(-1)$ because of their small E_n [see Eq. (2)]. Moreover, the excitation (including ionization) of the inner-shell (1s) electron contributes almost one-half of the sum of f_n but very little is known about its OSD. Similar problems are expected to occur, for instance, in alkali atoms. The uncertainty in $L(-1)$ is carried over to the total cross section, and, for the atoms whose σ_{ex} is very large compared to σ_i, the uncertainty becomes large in σ_i though it may be only a small fraction of σ_{tot}. Our method ($\sigma_i = \sigma_{tot} - \sigma_{ex}$) in such cases will be ineffective unless σ_{tot} and σ_{ex} are determined very accurately.

B. Discrete-Excitation Cross Sections

For metastable He, we used excellent wave functions for the first few discrete states,[7] and consequently obtained very reliable σ_{ex}. For more complex atoms, we may not be as fortunate. On the other hand, we find that $\ln c_n$ for high n can be considered constant without introducing large errors. Combined with the M_n^2 values from optical data and the fact that γ_{ex} tends to be rather small, it should be possible to estimate the cross sections for optically allowed discrete transitions within reasonable accuracy, even when reliable wave functions are not available. The occurrence of unusually small cross sections for optically allowed transitions due to minima in the GOS is accompanied by correspondingly large cross sections for the forbidden transitions. The same phenomenon is expected to be common in complex atoms.

To alleviate some of the difficulties mentioned in Secs. IV A and IV B we may partly use experimental cross sections on photoabsorption and differential (angular) inelastic scattering by fast electrons as well as spectroscopic data through the quantum-defect method. A careful application of the sum-rule method will still provide for a reliable test of the compatibility of various inelastic-scattering cross sections.

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