Generalized Oscillator Strengths of the Helium Atom. I*

Yong-Ki Kim and Mitio Inokuti
Argonne National Laboratory, Argonne, Illinois
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The generalized oscillator strengths $f_n(K)$ ($\vec{K}\hbar$ = momentum transfer) for the transitions of He from its ground state to excited states $n = 2^1P$, 3^1P, 2^1S, and 3^1S are computed from the Weiss correlated wave functions of over 50 terms each. For $(Ka_0)^2 \lesssim 2$ (a_0 = the Bohr radius), the results by two alternative formulas, corresponding to the "length" and "velocity" formulas in the optical limit, agree with each other within 0.5% for the 2^1P and 2^1S excitations, and within 1.5% for the 3^1P and 3^1S excitations. Our $f_{2^1P}(K)$ is in accord with electron-scattering experiments by Lassettre and his co-workers. For $(Ka_0)^2 \gtrsim 0.2$, our $f_{2^1S}(K)$ departs from experimental data at 500 eV, but its slope at $K = 0$ is consistent with experiment. Our results are very probably accurate within a few percent, and thus should provide a sound basis to test the validity of the (first) Born approximation. The representation of the Born excitation cross section for charged-particle impact is greatly simplified by a generalization of the Bethe procedure; it is shown that a few definite parameters can convey the essential content of the Born approximation. As an illustration, the cross sections for the excitations to the four states in He are evaluated and compared with experiments.

1. INTRODUCTION

The generalized oscillator strength of an atom or molecule is an important property representing the response of the system to sudden transfer of a given momentum to its electrons. In particular, it constitutes the essential part of the differential cross section [Eq. (3)] for inelastic scattering of sufficiently fast charged particles.[1-3] The well-known prescription for its evaluation [Eq. (1)] requires the wave functions for the initial and final states of the system, which are in general known only approximately, often only crudely, except for atomic hydrogen. This deficiency has hampered the application of the Bethe theory to its full extent even to the relatively simple case of the helium atom. For its transitions from the ground state to low-lying excited states, many calculations are found in the literature,[4-14] but the approximate nature of the wave functions used does not always convince one of the reliability of the results,[15] which appear in many cases quite sensitive to the choice of the wave functions.

Current experiments on inelastic scattering of electron beams with high resolution in energy and good collimation are providing data of remarkable quality.[5,6,8,16-20] Indeed, one is frequently impressed with a claim for a precision of a few percent in measured differential cross sections. This circumstance has led us to perform a *definitive* calculation, hopefully within an accuracy of a few percent or better, of the generalized oscillator strengths for some discrete transitions in the helium atom. The primary purpose of the present paper is to report results for the transitions to the 2^1S, 3^1S, 2^1P, and 3^1P states. Our data shoud provide a trustworthy basis to test the validity of the (first) Born approximation; and when applicable, they may be used to normalize experimental data for a particular transition and thereby determine other cross sections on an absolute scale.

The information on the generalized oscillator strength has several different areas of application, such as the Bethe (total) cross section for inelastic scattering of fast charged particles[1,2,21] and atom-atom inelastic-collision cross sections.[22]

The secondary purpose of this paper is to elucidate the nature of the Bethe approximation, which has often been misunderstood, and to demonstrate its application to the four transitions in He.

2. DEFINITIONS

The generalized oscillator strength $f_n(K)$ for the transition of an N-electron atom from its ground state to the nth excited state with momentum transfer $\vec{K}\hbar$ is defined as,[1,2,15]

$$f_n(K) = \frac{E_n/R}{(Ka_0)^2}\left|\sum_{j=1}^{N}\int \psi_n^* e^{i\vec{K}\cdot\vec{r}_j}\psi_0 d\vec{r}_1\cdots d\vec{r}_N\right|^2, \quad (1)$$

where a_0 is the Bohr radius, E_n the excitation energy from the ground state, R the Rydberg energy, $\vec{r}_j$ the position of the jth electron, and ψ_n and ψ_0 the excited-state and the ground-state wave functions, respectively. When the states involved are degenerate, customary average and summation over substates are implied.

In analogy to the "velocity" formula for the optical oscillator strength, an alternative formula for $f_n(K)$ may be used[4,23]:

$$f_n(K) = \frac{R}{E_n}a_0^2\left|\sum_{j=1}^{N}\int e^{iKz_j} \times(\psi_n^*\partial\psi_0/\partial z_j - \psi_0\partial\psi_n^*/\partial z_j) \times d\vec{r}_1\cdots d\vec{r}_N\right|^2, \quad (2)$$

with $z_j = (\vec{K}\cdot\vec{r}_j)/K$. In the limit $K \to 0$, Eq. (1) reduces to the "length" formula, and Eq. (2) to the "velocity" formula for the optical oscillator strength f_n. Although the two formulas give identical results with the exact wave functions, the contributions of various regions of the configuration space are weighted differently by these formulas.[24] Hence, when approximate wave functions are used, comparison of usually different results from the two formulas should provide a *qualitative* measure of accuracy.[25]

The generalized oscillator strength is the essential factor in the differential cross section for inelastic scattering of a charged particle in the Born approximation, i.e.,[1,2,15]

$$d\sigma_n = \frac{4\pi a_0^2 z^2}{T/R}\frac{f_n(K)}{E_n/R}\, d\ln(Ka_0)^2 , \tag{3}$$

where ze is the charge of the incident particle, and $T = mv^2/2$, m being the *electron* mass and v the incident particle velocity.

As can be seen from Eq. (1), $f_n(K)$ is an even function of Ka_0 and therefore it can be expanded in powers of $(Ka_0)^2$ for small Ka_0[3,26]:

$$f_n(K) = \sum_{\lambda=0}^{\infty} (Ka_0)^{2\lambda} f_n^{(\lambda)}/\lambda\,!, \tag{4}$$

where

$$f_n^{(\lambda)}/\lambda\,! = (\lambda\,!)^{-1}[d/d(Ka_0)^2]^{\lambda} f_n(K)\big|_{K=0}$$
$$= \frac{E_n}{R}\sum_{\mu=1}^{2\lambda+1}\frac{(-1)^{\lambda-\mu+1}}{\mu\,!(2\lambda+2-\mu)\,!} \times Z_n^{(\mu)} Z_n^{(2\lambda+2-\mu)*}, \tag{5}$$

with

$$Z_n^{(\mu)} = a_0^{-\mu}\sum_j \int \psi_n^* z_j^{\mu}\psi_0 \, d\vec{r}_1\cdots d\vec{r}_N. \tag{6}$$

In Eq. (5), $Z_n^{(\nu)*}$ denotes the complex conjugate of $Z_n^{(\nu)}$. The first expansion coefficient $f_n^{(0)}$ is the optical oscillator strength f_n. For optically allowed transitions, $Z_n^{(\mu)}$ vanishes for all even μ, and for optically forbidden transitions it vanishes either for all odd or all even μ depending on the parity of the excited state.

3. COMPUTATIONAL METHOD

Many previous investigations of f_n for He[27-32] suggest that it is necessary to use accurate wave functions for both the ground and the excited states to obtain trustworthy values of $f_n(K)$. We chose the Hylleraas wave functions computed by Weiss with 53 terms for the ground state, 54 terms for the excited ^1S states, and 52 terms for the ^1P states.[32] The excitation energies and other properties such as f_n and the expectation values of r^2 computed from the Weiss wave functions indicate that they are sufficiently accurate for our purpose. (See Table I.)

The Weiss wave functions for the singlet states identified by the usual quantum numbers n, l, and m are written as

$$\psi_{nlm} = \sum_{pq\mu} c_{pq\mu,n}\varphi_{pq\mu,lm}, \tag{7}$$

where the $c_{pq\mu,n}$ are variation coefficients, and

$$\varphi_{pq\mu,lm} = 2^{-\frac{1}{2}}\xi^{p+q+\mu+l+3}|\vec{r}_1-\vec{r}_2|^{\mu} \times\{r_1^{p} r_2^{q+l}\exp[-\xi(r_1+\eta r_2)]Y_{00}(1)Y_{lm}(2) + r_1^{q+l} r_2^{p}\exp[-\xi(\eta r_1+r_2)]Y_{lm}(1)Y_{00}(2)\}. \tag{8}$$

In Eqs. (7) and (8), the indices p, q, and μ are nonnegative integers, ξ and η variational exponents, and $Y_{lm}(1)$ and $Y_{lm}(2)$ the spherical harmonics for the angular variables of electrons 1 and 2, respectively.

With the substitution of Eqs. (7) and (8) into (1) and (2), $f_n(K)$ can be expressed in terms of integrals

$$\mathcal{J} \equiv \int_0^{\infty} dr_1 r_1^{\kappa} e^{-ar_1} j_{\lambda}(Kr_1)\int_0^{\infty} dr_2 r_2^{\nu} e^{-br_2}, \tag{9}$$

and

$$\mathcal{K} \equiv \int_0^{\infty} dr_1 r_1^{\kappa} e^{-ar_1} j_{\lambda}(Kr_1) \times \int_{r_1}^{\infty} dr_2 r_2^{\nu} e^{-br_2}, \tag{10}$$

where $j_{\lambda}(Kr_1)$ is the spherical Bessel function of the first kind, and λ, κ, and ν are integers covering the ranges $0 \le \lambda \le 2$, $-1 \le \kappa$, and $0 \le \nu$ for the states of interest. When $\kappa > \lambda$, the integration for

TABLE I. Comparison of properties of He calculated from the Weiss wave functions with those from other sources (atomic units).

Properties	State = n: 1^1S	2^1S	3^1S	2^1P	3^1P
Excitation energy E_n:					
Weiss[a]		0.757 75	0.842 47	0.779 88	0.848 59
Experiment[b]		0.757 72	0.842 42	0.779 86	0.848 55
$\langle n\|r_1^2\|n\rangle$: Weiss	1.193 48	16.084	85.770	15.755	91.966
Pekeris[35]	1.193 48	16.089		15.766	91.873
f_n by "length" formula:					
Weiss[32]				0.2759	0.0734
Schiff and Pekeris[30]				0.2762	0.0736
f_n by "velocity" formula:					
Weiss[32]				0.2761	0.0730
Schiff and Pekeris[30]				0.2762	0.0734
Overlap integral with 1^1S		-7.00×10^{-5}	9.20×10^{-5}	0.0	0.0

[a]Reference 32, nonrelativistic.

[b]Reference 34, includes relativistic effects.

TABLE II. The generalized oscillator strengths for the 2^1P and 3^1P excitations of He.

	2^1P		3^1P	
$(Ka_0)^2$	Formula I[a]	Formula II	Formula I	Formula II
0.05	2.5440×10^{-1}	2.5453×10^{-1}	6.8954×10^{-2}	6.8589×10^{-2}
0.10	2.3486×10^{-1}	2.3492×10^{-1}	6.4743×10^{-2}	6.4407×10^{-2}
0.15	2.1705×10^{-1}	2.1706×10^{-1}	6.0793×10^{-2}	6.0480×10^{-2}
0.20	2.0080×10^{-1}	2.0078×10^{-1}	5.7088×10^{-2}	5.6794×10^{-2}
0.25	1.8596×10^{-1}	1.8591×10^{-1}	5.3618×10^{-2}	5.3339×10^{-2}
0.30	1.7239×10^{-1}	1.7232×10^{-1}	5.0367×10^{-2}	5.0100×10^{-2}
0.35	1.5996×10^{-1}	1.5988×10^{-1}	4.7323×10^{-2}	4.7068×10^{-2}
0.40	1.4857×10^{-1}	1.4849×10^{-1}	4.4475×10^{-2}	4.4228×10^{-2}
0.45	1.3812×10^{-1}	1.3804×10^{-1}	4.1809×10^{-2}	4.1570×10^{-2}
0.50	1.2852×10^{-1}	1.2844×10^{-1}	3.9315×10^{-2}	3.9083×10^{-2}
0.55	1.1969×10^{-1}	1.1961×10^{-1}	3.6981×10^{-2}	3.6755×10^{-2}
0.60	1.1156×10^{-1}	1.1149×10^{-1}	3.4797×10^{-2}	3.4577×10^{-2}
0.65	1.0408×10^{-1}	1.0401×10^{-1}	3.2754×10^{-2}	3.2540×10^{-2}
0.70	9.7177×10^{-2}	9.7108×10^{-2}	3.0841×10^{-2}	3.0632×10^{-2}
0.75	9.0804×10^{-2}	9.0740×10^{-2}	2.9051×10^{-2}	2.8848×10^{-2}
0.80	8.4916×10^{-2}	8.4856×10^{-2}	2.7376×10^{-2}	2.7177×10^{-2}
0.85	7.9471×10^{-2}	7.9415×10^{-2}	2.5807×10^{-2}	2.5613×10^{-2}
0.90	7.4430×10^{-2}	7.4379×10^{-2}	2.4337×10^{-2}	2.4148×10^{-2}
0.95	6.9761×10^{-2}	6.9713×10^{-2}	2.2961×10^{-2}	2.2775×10^{-2}
1.00	6.5431×10^{-2}	6.5387×10^{-2}	2.1671×10^{-2}	2.1490×10^{-2}
1.2	5.0986×10^{-2}	5.0953×10^{-2}	1.7267×10^{-2}	1.7101×10^{-2}
1.4	4.0141×10^{-2}	4.0114×10^{-2}	1.3848×10^{-2}	1.3697×10^{-2}
1.6	3.1903×10^{-2}	3.1879×10^{-2}	1.1179×10^{-2}	1.1041×10^{-2}
1.8	2.5577×10^{-2}	2.5555×10^{-2}	9.0816×10^{-3}	8.9548×10^{-3}
2.0	2.0672×10^{-2}	2.0649×10^{-2}	7.4232×10^{-3}	7.3063×10^{-3}
2.2	1.6832×10^{-2}	1.6810×10^{-2}	6.1034×10^{-3}	5.9955×10^{-3}
2.4	1.3801×10^{-2}	1.3779×10^{-2}	5.0466×10^{-3}	4.9467×10^{-3}
2.6	1.1389×10^{-2}	1.1367×10^{-2}	4.1953×10^{-3}	4.1025×10^{-3}
2.8	9.4555×10^{-3}	9.4338×10^{-3}	3.5055×10^{-3}	3.4193×10^{-3}
3.0	7.8948×10^{-3}	7.8736×10^{-3}	2.9435×10^{-3}	2.8631×10^{-3}
3.2	6.6267×10^{-3}	6.6061×10^{-3}	2.4831×10^{-3}	2.4081×10^{-3}
3.4	5.5902×10^{-3}	5.5702×10^{-3}	2.1040×10^{-3}	2.0340×10^{-3}
3.6	4.7381×10^{-3}	4.7187×10^{-3}	1.7902×10^{-3}	1.7248×10^{-3}
3.8	4.0337×10^{-3}	4.0150×10^{-3}	1.5294×10^{-3}	1.4682×10^{-3}
4.0	3.4485×10^{-3}	3.4305×10^{-3}	1.3116×10^{-3}	1.2542×10^{-3}
4.2	2.9599×10^{-3}	2.9426×10^{-3}	1.1289×10^{-3}	1.0751×10^{-3}
4.4	2.5502×10^{-3}	2.5336×10^{-3}	9.7509×10^{-4}	9.2461×10^{-4}
4.6	2.2052×10^{-3}	2.1891×10^{-3}	8.4502×10^{-4}	7.9760×10^{-4}
4.8	1.9133×10^{-3}	1.8979×10^{-3}	7.3464×10^{-4}	6.9006×10^{-4}
5.0	1.6655×10^{-3}	1.6506×10^{-3}	6.4062×10^{-4}	5.9868×10^{-4}
5.5	1.1932×10^{-3}	1.1796×10^{-3}	4.6064×10^{-4}	4.2448×10^{-4}
6.0	8.6991×10^{-4}	8.5734×10^{-4}	3.3673×10^{-4}	3.0541×10^{-4}
6.5	6.4421×10^{-4}	6.3260×10^{-4}	2.4985×10^{-4}	2.2260×10^{-4}
7.0	4.8389×10^{-4}	4.7314×10^{-4}	1.8792×10^{-4}	1.6411×10^{-4}
7.5	3.6819×10^{-4}	3.5823×10^{-4}	1.4310×10^{-4}	1.2223×10^{-4}
8.0	2.8348×10^{-4}	2.7426×10^{-4}	1.1022×10^{-4}	9.1859×10^{-5}
8.5	2.2064×10^{-4}	2.1211×10^{-4}	8.5793×10^{-5}	6.9590×10^{-5}
9.0	1.7346×10^{-4}	1.6557×10^{-4}	6.7427×10^{-5}	5.3093×10^{-5}
9.5	1.3763×10^{-4}	1.3034×10^{-4}	5.3470×10^{-5}	4.0761×10^{-5}
10.0	1.1015×10^{-4}	1.0342×10^{-4}	4.2757×10^{-5}	3.1465×10^{-5}
20	4.2007×10^{-6}		1.5615×10^{-6}	
30	5.4225×10^{-7}		1.9010×10^{-7}	
40	1.2431×10^{-7}		4.1316×10^{-8}	
50	3.9441×10^{-8}		1.2545×10^{-9}	
60	1.5373×10^{-8}		4.7197×10^{-9}	
70	6.9002×10^{-9}		2.0591×10^{-9}	
80	3.4324×10^{-9}		1.0009×10^{-9}	
90	1.8464×10^{-9}		5.2837×10^{-10}	
100	1.0565×10^{-9}		2.9762×10^{-10}	

[a]Formula I: Evaluated from Eq. (1) of the text. Formula II: Evaluated from Eq. (2) of the text.

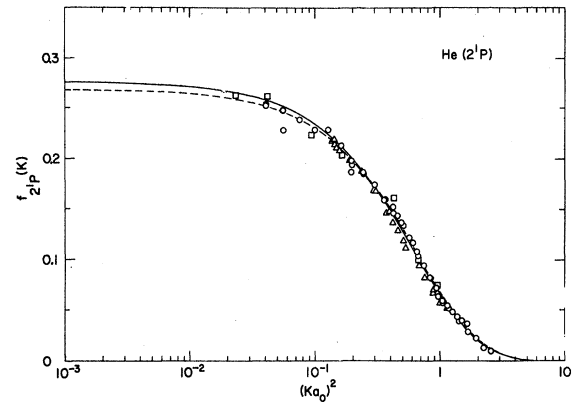

FIG. 1. The generalized oscillator strength for the 2^1P excitation of He. The experimental data are those of Geiger (□) (Ref. 6), of Lassettre *et al.* (○) [Refs. 8, 16, and J. Chem. Phys. 45, 3214 (1966)], and of Vriens *et al.* (△) (Ref. 20). The broken line represents theoretical values calculated by Lassettre *et al.* (Refs. 7 and 8), and the solid line the present work. Differences between "Formula I" and "Formula II" results (see Tables II and III) are indiscernible in Figs. 1 and 2. As is pointed out by Miller and Platzman (Ref. 15), the area under the curve in $f_n(K)$ versus $\ln(Ka_0)^2$ plot, taken between appropriate limits of Ka_0, determines the excitation cross section σ_n. [See Eqs. (3), (11), and (14).]

$\mathcal{J}$ is elementary. For $\kappa \leq \lambda$, however, $\mathcal{J}$ is expressed in terms of a hypergeometric function with the aid of Eq. (3), p. 385 of Ref. 33. The integral $\mathcal{K}$ is computed in a similar way after an elementary integration over r_2. The integrals encountered in the evaluation of $Z_n(\mu)$ [see Eq. (6)] are similar to but simpler than $\mathcal{J}$ and $\mathcal{K}$, namely, without $j_\lambda(Kr_1)$.

The evaluation of $f_n(K)$ by Eq. (2) for large K poses an additional difficulty on the numerical accuracy owing to the near cancellation of the two terms in Eq. (2). Most of our computation was carried out on an IBM 360 Model 75 computer in double-precision arithmetic to prevent the accumulation of round-off errors.

For the excitation energies E_n which appear both in Eqs. (1) and (2), we have used the values computed from the Weiss wave functions (Table I). The computed energies are so close to the spectroscopic data[34] as well as to those computed by Pekeris *et al.*[35] that the use of these alternative values would have slightly affected the fourth significant figure of our $f_n(K)$.[24]

4. RESULT AND DISCUSSION

A. Excitations to the 2^1P and 3^1P States

The results for the allowed transitions are presented in Table II. (See also Figs. 1 and 2.) The values in the columns labeled as "Formula I" were computed from Eq. (1), and those labeled as "Formula II" from Eq. (2). The "Formula II" results for $(Ka_0)^2 \gtrsim 10$ have been judged unreliable because of heavy cancellation of integrals (see Sec. 3) and are not presented in Table II. The agreement for the 2^1P excitation between the results from the two formulas is excellent for $(Ka_0)^2 \lesssim 3$. In view also of the fact that the optical oscillator strengths computed from the Weiss wave functions[32] agree to three significant figures with those computed by Schiff and Pekeris[30] (see Table I) we believe our $f_{2^1P}(K)$ to be accurate to 1% for $(Ka_0)^2 \lesssim 2$. The $f_{2^1P}(K)$ computed by Eq. (2) is probably the better for small K because its optical limit agrees better with f_{2^1P} calculated from the Pekeris wave functions.

Our result for the 3^1P excitation is less conclusive than that for the 2^1P excitation, because of the lower accuracy of the 3^1P wave function. For the physically interesting region $(Ka_0)^2 \lesssim 2$, we believe our $f_{3^1P}(K)$ to be accurate to 3%. For comparison with experimental data for the 3^1P excitation, we recommend the $f_{3^1P}(K)$ computed from Eq. (1) because its optical limit agrees better with the result of Schiff and Pekeris.[30]

B. Excitations to the 2^1S and 3^1S States

Our results for the forbidden transitions are given in Table III, arranged in a manner similar to that in Table II. (See also Fig. 3.) Although the orthogonality of the Weiss wave functions (which were computed without constraints of orthogonality to the ground state) is excellent (see Table I), the small nonvanishing overlap integral causes some uncertainty in the values of $f_n(K)$ computed from Eq. (1). To reduce this type of uncertainty we have used the expansion formula [Eq. (4) whose derivation assumes the orthogonality]; the results thereby obtained (from 10-term expansions) are also given in Table III under "Formula III." It is evident from Table III that either the "Formula II" or "Formula III" result may be used for small K. At present, it is difficult to judge which of them is better.

We believe our results for the 2^1S excitation to be accurate probably to 1%, and for the 3^1S excitation to 3% in the region $(Ka_0)^2 \lesssim 5$. For large K, again the "Formula II" results suffer from near cancellation, and the "Formula I" results are recommended.

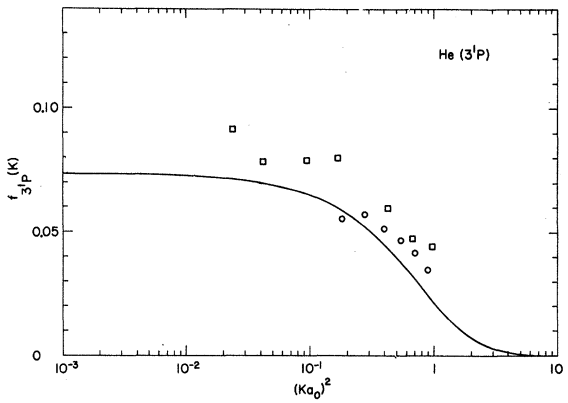

FIG. 2. The generalized oscillator strength for the 3^1P excitation of He. The experimental data are those of Geiger (□) (Ref. 6), and of Lassettre *et al.* (○) (Ref. 16). The solid line represents the present calculation.

TABLE III. The generalized oscillator strengths for the 2^1S and 3^1S excitations of He.

	2^1S			3^1S		
$(Ka_0)^2$	Formula I[a]	Formula II	Formula III	Formula I	Formula II	Formula III
0.05	3.9807×10^{-3}	3.9006×10^{-3}	3.8840×10^{-3}	8.6951×10^{-4}	8.0251×10^{-4}	8.0768×10^{-4}
0.10	7.3163×10^{-3}	7.2510×10^{-3}	7.2234×10^{-3}	1.5915×10^{-3}	1.5231×10^{-3}	1.5319×10^{-3}
0.15	1.0174×10^{-2}	1.0119×10^{-2}	1.0085×10^{-2}	2.2364×10^{-3}	2.1673×10^{-3}	2.1785×10^{-3}
0.20	1.2613×10^{-2}	1.2565×10^{-2}	1.2526×10^{-2}	2.8097×10^{-3}	2.7405×10^{-3}	2.7534×10^{-3}
0.25	1.4683×10^{-2}	1.4639×10^{-2}	1.4599×10^{-2}	3.3168×10^{-3}	3.2481×10^{-3}	3.2620×10^{-3}
0.30	1.6430×10^{-2}	1.6389×10^{-2}	1.6349×10^{-2}	3.7631×10^{-3}	3.6952×10^{-3}	3.7098×10^{-3}
0.35	1.7893×10^{-2}	1.7854×10^{-2}	1.7815×10^{-2}	4.1536×10^{-3}	4.0867×10^{-3}	4.1018×10^{-3}
0.40	1.9107×10^{-2}	1.9069×10^{-2}	1.9032×10^{-2}	4.4931×10^{-3}	4.4272×10^{-3}	4.4426×10^{-3}
0.45	2.0103×10^{-2}	2.0066×10^{-2}	2.0030×10^{-2}	4.7860×10^{-3}	4.7213×10^{-3}	4.7369×10^{-3}
0.50	2.0907×10^{-2}	2.0870×10^{-2}	2.0837×10^{-2}	5.0365×10^{-3}	4.9730×10^{-3}	4.9887×10^{-3}
0.55	2.1544×10^{-2}	2.1507×10^{-2}		5.2486×10^{-3}	5.1862×10^{-3}	
0.60	2.2034×10^{-2}	2.1997×10^{-2}		5.4257×10^{-3}	5.3645×10^{-3}	
0.65	2.2396×10^{-2}	2.2359×10^{-2}		5.5713×10^{-3}	5.5111×10^{-3}	
0.70	2.2646×10^{-2}	2.2609×10^{-2}		5.6884×10^{-3}	5.6292×10^{-3}	
0.75	2.2799×10^{-2}	2.2762×10^{-2}		5.7798×10^{-3}	5.7216×10^{-3}	
0.80	2.2866×10^{-2}	2.2830×10^{-2}		5.8481×10^{-3}	5.7908×10^{-3}	
0.85	2.2860×10^{-2}	2.2825×10^{-2}		5.8957×10^{-3}	5.8394×10^{-3}	
0.90	2.2790×10^{-2}	2.2755×10^{-2}		5.9248×10^{-3}	5.8693×10^{-3}	
0.95	2.2665×10^{-2}	2.2631×10^{-2}		5.9374×10^{-3}	5.8828×10^{-3}	
1.00	2.2493×10^{-2}	2.2460×10^{-2}		5.9352×10^{-3}	5.8814×10^{-3}	
1.2	2.1456×10^{-2}	2.1427×10^{-2}		5.8102×10^{-3}	5.7595×10^{-3}	
1.4	2.0083×10^{-2}	2.0058×10^{-2}		5.5576×10^{-3}	5.5099×10^{-3}	
1.6	1.8572×10^{-2}	1.8551×10^{-2}		5.2343×10^{-3}	5.1895×10^{-3}	
1.8	1.7040×10^{-2}	1.7023×10^{-2}		4.8778×10^{-3}	4.8358×10^{-3}	
2.0	1.5555×10^{-2}	1.5541×10^{-2}		4.5123×10^{-3}	4.4732×10^{-3}	
2.2	1.4153×10^{-2}	1.4141×10^{-2}		4.1532×10^{-3}	4.1168×10^{-3}	
2.4	1.2853×10^{-2}	1.2843×10^{-2}		3.8094×10^{-3}	3.7756×10^{-3}	
2.6	1.1660×10^{-2}	1.1651×10^{-2}		3.4861×10^{-3}	3.4549×10^{-3}	
2.8	1.0575×10^{-2}	1.0566×10^{-2}		3.1857×10^{-3}	3.1569×10^{-3}	
3.0	9.5909×10^{-3}	9.5831×10^{-3}		2.9090×10^{-3}	2.8824×10^{-3}	
3.2	8.7028×10^{-3}	8.6954×10^{-3}		2.6555×10^{-3}	2.6311×10^{-3}	
3.4	7.9027×10^{-3}	7.8956×10^{-3}		2.4244×10^{-3}	2.4019×10^{-3}	
3.6	7.1827×10^{-3}	7.1758×10^{-3}		2.2141×10^{-3}	2.1935×10^{-3}	
3.8	6.5352×10^{-3}	6.5285×10^{-3}		2.0232×10^{-3}	2.0044×10^{-3}	
4.0	5.9528×10^{-3}	5.9465×10^{-3}		1.8502×10^{-3}	1.8330×10^{-3}	
4.2	5.4290×10^{-3}	5.4229×10^{-3}		1.6934×10^{-3}	1.6778×10^{-3}	
4.4	4.9576×10^{-3}	4.9517×10^{-3}		1.5514×10^{-3}	1.5372×10^{-3}	
4.6	4.5330×10^{-3}	4.5274×10^{-3}		1.4228×10^{-3}	1.4098×10^{-3}	
4.8	4.1502×10^{-3}	4.1449×10^{-3}		1.3062×10^{-3}	1.2944×10^{-3}	
5.0	3.8048×10^{-3}	3.7997×10^{-3}		1.2005×10^{-3}	1.1898×10^{-3}	
5.5	3.0795×10^{-3}	3.0751×10^{-3}		9.7699×10^{-4}	9.6874×10^{-4}	
6.0	2.5127×10^{-3}	2.5090×10^{-3}		8.0081×10^{-4}	7.9445×10^{-4}	
6.5	2.0661×10^{-3}	2.0631×10^{-3}		6.6104×10^{-4}	6.5617×10^{-4}	
7.0	1.7116×10^{-3}	1.7091×10^{-3}		5.4942×10^{-4}	5.4570×10^{-4}	
7.5	1.4279×10^{-3}	1.4259×10^{-3}		4.5965×10^{-4}	4.5682×10^{-4}	
8.0	1.1992×10^{-3}	1.1975×10^{-3}		3.8697×10^{-4}	3.8480×10^{-4}	
8.5	1.0134×10^{-3}	1.0121×10^{-3}		3.2772×10^{-4}	3.2604×10^{-4}	
9.0	8.6148×10^{-4}	8.6041×10^{-4}		2.7911×10^{-4}	2.7780×10^{-4}	
9.5	7.3640×10^{-4}	7.3555×10^{-4}		2.3897×10^{-4}	2.3793×10^{-4}	
10.0	6.3279×10^{-4}	6.3211×10^{-4}		2.0564×10^{-4}	2.0478×10^{-4}	
20	6.4906×10^{-5}			2.1274×10^{-5}		
30	1.4706×10^{-5}			4.8037×10^{-6}		
40	4.8620×10^{-6}			1.5813×10^{-6}		
50	2.0020×10^{-6}			6.4882×10^{-7}		
60	9.5185×10^{-7}			3.0765×10^{-7}		
70	5.0112×10^{-7}			1.6165×10^{-7}		
80	2.8475×10^{-7}			9.1722×10^{-8}		
90	1.7173×10^{-7}			5.5257×10^{-8}		
100	1.0864×10^{-7}			3.4929×10^{-8}		

TABLE III. (*continued*)

	2^1S			3^1S		
$(Ka_0)^2$	Formula I[a]	Formula II	Formula III	Formula I	Formula II	Formula III
200	4.7591×10^{-9}			1.5265×10^{-9}		
300	7.0851×10^{-10}			2.2729×10^{-10}		
400	1.7908×10^{-10}			5.7465×10^{-11}		
500	6.0972×10^{-11}			1.9572×10^{-11}		

[a]Formula I: Evaluated from Eq. (1) of the text. Formula II: Evaluated from Eq. (2) of the text. Formula III: Evaluated from Eq. (4) of the text.

The expansion coefficients $f_n^{(\lambda)}/\lambda!$ [see Eq. (4)] are tabulated in Table IV, and the matrix elements $Z_n^{(\mu)}$ [see Eq. (6)] in Table V.

C. Comparison with Experiment

The use of experimental $d\sigma_n$ (usually for fast electrons) in the left-hand side of Eq. (3) allows one to define operationally an "apparent" generalized oscillator strength.[36] A necessary (though not sufficient) condition for the validity of the Born approximation is that the experimental $d\sigma_n$ at different T produce the same "apparent" $f_n(K)$.

For the 2^1P excitation, published experimental data have so far been relative,[37] and have been normalized to some theoretical data.[6,16-18,20] A better comparison, therefore, would be possible after experimental data are renormalized against our results. The shape of the "apparent" $f_n(K)$, however, should be free of uncertainties due to the normalization. For a tentative comparison, we quote in Fig. 1 some published experimental data without renormalization. The experimental data of Lassettre *et al.*[8,16,18] at $T\cong 400$–500 eV agree with our calculated $f_{2^1P}(K)$ very well. Average deviation of their data from our $f_{2^1P}(K)$ is about 2.5% except for the large-angle data for which the cross sections become extremely difficult to measure.[38] Their data are normalized to $f_{2^1P}(K)$ calculated by Lassettre and Jones[7] (see further discussion in Sec. 4D) in the neighborhood of $(Ka_0)^2\sim 0.3$ to 0.4, where their calculated values happen to agree very well with ours. (See Fig. 1.) Therefore, renormalization against our result will not change to any appreciable extent Lassettre's "apparent" $f_n(K)$ not only of He, but also of all other atoms and molecules, which are normalized against $f_{2^1P}(K)$ of He.

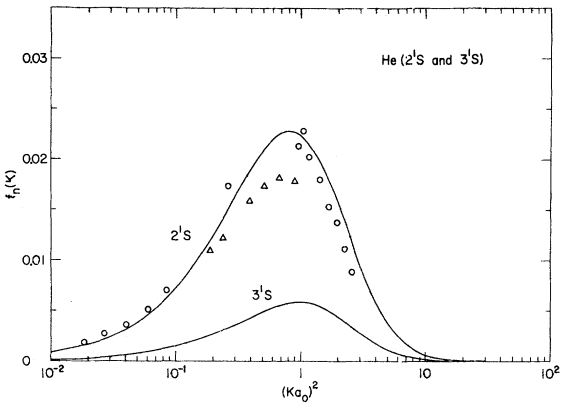

FIG. 3. The generalized oscillator strengths for the 2^1S and 3^1S excitations of He. The experimental data for the 2^1S excitation are those of Lassettre *et al.* (○) (Refs. 8 and 17, $T=500$ eV), and of Vriens *et al.* (△) (Ref. 20, $T=300$ and 400 eV). The solid curves represent the present calculation. There are no experimental data available for the 3^1S excitation. Differences between "Formula II" and "Formula III" results are indiscernible in this figure.

The experimental data of Vriens, Simpson, and Mielczarek[20] for $T\leq 400$ eV are normalized against an anlaytic formula for $f_{2^1P}(K)$ (Sec. 4D) whose optical limit is chosen to be the value by Schiff and Pekeris.[30] These data are consistently smaller than our result except for the small angle (5°) data. The deviation from our $f_{2^1P}(K)$ is about 5%, somewhat greater than the claimed experimental uncertainty of 2%. The small difference may have come from uncertainty in the normalization procedure, or may represent a departure from the Born approximation. The latter possibility, however, seems to be in disagreement with implications of extensive experimental data of Lassettre and coworkers.

Although the normalization of Geiger's data[6] by use of a calculated elastic-scattering cross section

TABLE IV. Power-series expansion coefficients for the generalized oscillator strengths of He for small momentum transfers. [See Eq. (4) of the text.]

	$f_n^{(\lambda)}/\lambda!$			
λ	2^1S	3^1S	2^1P	3^1P
0	0.0	0.0	0.275 87	0.073 438
1	0.083 616	0.017 028	−0.450 15	−0.092 490
2	−0.123 938	−0.017 897	0.429 45	0.057 131
3	0.107 984	0.008 014	−0.311 55	−0.016 248
4	−0.071 770	0.000 193 5	0.189 54	−0.006 065
5	0.040 092	−0.003 192		

TABLE V. Matrix elements $Z_n^{(\mu)}$ [see Eq. (6) of the text] between the ground and excited states of He.

μ \ n	2^1S	3^1S	2^1P	3^1P
1			0.420 556	0.208 015
2	0.469 780	−0.201 060		
3			2.058 69	0.785 943
4	4.177 95	−1.267 86		
5			22.4849	4.760 31
6	62.7593	−7.038 98		
7			426.415	−9.924 23
8	1459.87	230.165		
9			12 230.7	−4039.80
10	48 284.2	25 035.7		

may be subject to reconsideration,[39] his large-angle data($\gtrsim 2\times10^{-2}$ rad) for the 2^1P excitation agree reasonably well with our result. Relativistic kinematics has been used to redetermine the "apparent" $f_n(K)$ from his experimental $d\sigma_n$. (Figure 1.) We omitted from Figs. 1 and 2 some small-angle data ($\lesssim 10^{-2}$ rad) which show a larger scatter presumably due to the difficulty in photographic detection and in the geometry.

The close agreement of our $f_{2^1P}(K)$ and available experimental data, particularly those of Lassettre *et al.*, seems to support the general belief[40] that the 2^1P differential cross section is well represented by the Born approximation to rather low-incident energies (~200 eV).

The experimental data for the 3^1P excitation are less reliable than those for the 2^1P excitation because of the difficulty in separating the contributions from the 3^1S and 3^1D excitations. The experimental data of Lassettre *et al.*[16] and of Geiger[6] are presented in Fig. 2. It is clear from Fig. 2 that the shape of the former agrees in general with theory, though not as precisely as for the 2^1P excitation.

The magnitudes of Geiger's data for the 3^1P excitation are substantially larger than our result, possibly because of insufficient energy resolution, but the shape is in somewhat better agreement with theory than the data of Lassettre *et al.*[16] A renormalization, however, would seriously affect his 2^1P data that were simultaneously measured.

As for the 2^1S excitations,[8,16,17,20] all experimental data for $(Ka_0)^2 \gtrsim 0.2$ depart in various ways from our calculation. (See Fig. 3.) We can detect in Fig. 3 a tendency for the shape of the "apparent" $f_{2^1S}(K)$ to become closer to that of our result as the incident electron energy is increased. The Born approximation is probably valid only at much higher incident electron energy ($\gtrsim 800$ eV) for this excitation. Note also that the slope of the $f_{2^1S}(K)$ vs. $(Ka_0)^2$ plot as $K \to 0$ measured by Skerbele and Lassettre[17] with 500-eV incident energy is 0.099, slightly larger than our $f_{2^1S}^{(1)} = 0.0836$. (See Tables IV and VI.)

No experimental $d\sigma_n$ for the 3^1S excitation ap-

TABLE VI. Values of $f_n^{(1)}$ for the 2^1S and 3^1S excitations of He.

2^1S	$f_{2^1S}^{(1)}$	Comments
Experiment		
Lassettre *et al.*[a]	0.089	$T=500$ eV, $(Ka_0)^2 \geq 0.177$.
	0.092	
Skerbele and Lassettre[17]	0.099	$T=500$ eV, $0.09 > (Ka_0)^2 > 0.02$.
Boersch, Geiger, and Schröder[19]	0.116	$T=25$ keV, $(Ka_0)^2 \geq 3.3\times10^{-4}$.
Vriens, Simpson, and Mielczarek[20]	0.0773	$T=400$ eV, $(Ka_0)^2 \geq 0.235$.
Theory		
Altshuler[4]	0.0366	Method I, hydrogenic wave functions
	0.0557	Method II, hydrogenic wave functions
Fox[9]	0.072	Hartree ground-state wave function
	0.11	Eckart ground-state wave function
Garstang[45]	0.13	Hartree-Fock wave functions
van den Bos[11]	0.0611	BJ-BE combination of Ref. 11.
Present work	0.0836	Weiss wave functions
3^1S	$f_{3^1S}^{(1)}$	
Theory		
Garstang[45]	0.021	Hartree-Fock wave functions
van den Bos[11]	0.0266	BJ-BE combination of Ref. 11
Present work	0.0170	Weiss wave functions

[a]Obtained by Lassettre (Ref. 17) from experimental data quoted in Ref. 67.

pears to be available, except for some relative measurements of the zero-angle electron-scattering cross sections $d\sigma_n(0)$.[41] The ratios $R_P = d\sigma_{3^1P}(0)/d\sigma_{2^1P}(0)$ and $R_S = d\sigma_{3^1S}(0)/d\sigma_{2^1S}(0)$ have been measured by Lassettre *et al.*[42] at 202 eV ($R_P = 0.22$, $R_S = 0.22$), and by Chamberlain *et al.*[43] at 81 eV and below ($R_P = 0.20$, $R_S = 0.25$ at 81 eV). The experimental ratios compare very favorably with our calculated ratios ($R_P = 0.206$, $R_S = 0.183$ at $T = 202$ eV, and $R_P = 0.203$, $R_S = 0.189$ at $T = 81$ eV), though the Born approximation is expected to be valid only for the R_P measurement of Lassettre *et al.*[42]

D. Comparison with Other Theoretical Results

As discussed in A of this section, the optical oscillator strengths of Schiff and Pekeris[30] and of Weiss[32] provide an indispensable guide in judging the accuracy of our result.

Altshuler[4] computed $f_n(K)$ for the 2^1S, 2^1P, and 3^1P excitations from hydrogenic wave functions using the two alternative formulas [Eqs. (1) and (2)]. Considering the crudeness of the wave functions, it is remarkable that his $f_n(K)$ for the ^1P excitations computed from Eq. (2) are close to ours in shape and magnitude within $\lesssim 5\%$ for $(Ka_0)^2 \lesssim 1$. For $(Ka_0)^2 \gtrsim 1$, his results from Eq. (1) are in better agreement with ours, though they are poor for small K. His $f_{2^1S}(K)$ computed from Eq. (2) agrees with ours in shape, but is smaller in magnitude by 20 to 30%.

Lassettre and Jones[7] calculated $f_{2^1P}(K)$ from Eq. (1) using a six-term Hylleraas ground-state wave function and a variational 2^1P wave function (similar to a screened hydrogenic function in accuracy). Their calculation was later extended to cover a wider range of K by Silverman and Lassettre.[8] This $f_{2^1P}(K)$ is in very good agreement with ours in the region $0.3 \leq (Ka_0)^2 \leq 1.0$. (See Fig. 1.)

A similar calculation, by use of Eqs. (1) and (2), was reported by Kennedy and Kingston,[12] presumably with an improved ground-state wave function. We find, however, that the result in Ref. 12 is larger than our result by a few percent, contrary to their claimed accuracy of 1%.[25]

Van den Bos[11] calculated $f_n(K)$ for many excited states of He using Eq. (1) with various combinations of ground and excited-state wave functions comparable to the Hartree-Fock wave functions or somewhat inferior. Of the many combinations, the $f_n(K)$ for the ^1P excitations computed with a two-term Hartree-Fock-Roothaan ground-state wave function and Eckart ^1P wave functions agree within 5% with our result for $(Ka_0)^2 \lesssim 2$.

Bell, Kennedy, and Kingston[13] calculated $f_{3^1P}(K)$ using a six-term Hylleraas ground-state wave function and a hydrogenic excited-state wave function. Their $f_{3^1P}(K)$ is larger than ours by several percent, indicating the importance of accurate wave functions not only for the ground but also for the excited states.

As mentioned earlier, the nonvanishing overlap integrals between the ground and excited ^1S state wave functions lead to less accurate $f_n(K)$ for small K when Eq. (1) is used.[44] Fox[9] studied the dependence of $f_n(K)$ on the choice of ground-state wave functions when the orthogonality constraint was enforced. His result for the 2^1S excitation with the Hartree ground-state wave function agrees reasonably with our result. The results of Fox[9] and of Altshuler[4] clearly indicate, however, that an accurate evaluation of $f_n(K)$ for the ^1S excitation requires much more sophisticated wave functions than for the ^1P excitation.

Another quantity of interest for the ^1S excitation is $f_n^{(1)}$, the first nonvanishing coefficient of the expansion Eq. (4).[3,45] (See Table IV, and comment on the experimental data of Skerbele and Lassettre[17] in Sec. 4C.) This coefficient may be used as a measure of the reliability of $f_n(K)$ for small K. For the 2^1S and 3^1S excitations, values of $f_n^{(1)}$ from various sources are tabulated in Table VI. Clearly no combination of Hartree-Fock or inferior wave functions produces a reliable value of $f_n^{(1)}$ because its essential factor $Z_n^{(2)}$ emphasizes the contribution from large r.

In view of the remarkable success of Altshuler for the ^1P excitations by use of Eq. (2), as a prelude to the calculation of $f_n(K)$ for large atoms or molecules, it would be interesting to calculate $f_n(K)$ for the allowed transitions using *bona-fide* Hartree-Fock wave functions both for the ground and excited states of He.

Rau and Fano[46] have shown that the leading term of $f_n(K)$ as $K \to \infty$ is proportional to $(Ka_0)^{-2(l+5)}$, where l is the azimuthal quantum number of the excited state. We found that this asymptotic behavior could be described by the leading term alone for $(Ka_0)^2 > 900$.

The generalized oscillator strengths for other transitions from the ground as well as metastable states will be reported in a later publication.

5. The Bethe Total Cross Sections for Excitation

The (total) cross section σ_n for excitation to a particular state n is simply an integral of $d\sigma_n$ [Eq. (3)], the upper and lower limits being determined by kinematics. In the region of validity of the Born approximation, where $T = mv^2/2$ is sufficiently larger than the binding energies of atomic electrons, σ_n can conveniently be treated in terms of an expansion in inverse powers of T. The leading term is known as the Bethe *asymptotic* cross section.[1,2,15,21] Thus, the excitation cross section σ_S for an optically allowed transition to the state s is

$$\sigma_S = \frac{4\pi a_0^2 z^2}{T/R}\left[\frac{f_S}{E_S/R}\ln(4c_S T/R) + \frac{\gamma_S}{T/R} + O\left(\frac{E_S^2}{T^2}\right)\right], \tag{11}$$

where the constants c_S and γ_S are defined by

$$\ln[c_S(E_S/R)^2] = \int_0^\infty [f_S(K)/f_S]\,d\ln(Ka_0)^2 - \int_{-\infty}^0 \{1-[f_S(K)/f_S]\}\,d\ln(Ka_0)^2, \tag{12}$$

and

$$\gamma_S = -(m/2M)f_S - (E_S/4R)f_S^{(1)}, \tag{13}$$

$f_S^{(1)}$ being defined by Eq. (5) and M denoting the reduced mass of the incident particle and the atom.

TABLE VII. Parameters for the excitation cross sections of He.

Optically allowed transitions

Excited state s	Rf_s/E_s	$\ln c_s$	$Rf_s/E_s \ln(4c_s)$	$\gamma_s^{(e)}$ [a]	$\gamma_s^{(\infty)}$ [a]
2^1P	0.177	−1.868	−0.0852	0.0376	0.175
3^1P	0.0433	−1.833	−0.0193	0.00252	0.0392

Optically forbidden transitions

Excited state s'	$b_{s'}$	γ_s
2^1S	0.0455	−0.0317
3^1S	0.0103	−0.00717

[a]Because γ_s for allowed transitions depend on M, we give values for an electron $\gamma_s^{(e)}$ and for a charged particle with $M\to\infty$ $\gamma_s^{(\infty)}$. The latter hardly differs from the value for a proton.

The excitation cross section $\sigma_{s'}$ for an optically forbidden transition to the state s' is

$$\sigma_{s'}=\frac{4\pi a_0^2 z^2}{T/R}\left[b_{s'}+\frac{\gamma_{s'}}{T/R}+O\left(\frac{E_{s'}^2}{T^2}\right)\right], \tag{14}$$

where $b_{s'}$ and $\gamma_{s'}$ are defined by

$$b_{s'}=\int_{-\infty}^{\infty}\frac{f_{s'}(K)}{E_{s'}/R}d\ln(Ka_0)^2, \tag{15}$$

and $$\gamma_{s'}=-(E_{s'}/4R)f_{s'}^{(1)}. \tag{16}$$

The derivation of Eqs. (11) through (16) is given in the Appendix. Equations (13) and (16) represent a generalization of a similar treatment by Vriens,[47] who utilizes a presumed analytic form for $f_n(K)$.

Some remarks may be made on the above formulas. Firstly, *a few well-defined parameters f_s/E_s, c_s, and λs (or $b_{s'}$ and $\lambda s'$) determine the essentially meaningful content of the Born approximation*, thus obviating repeated integrations of $d\sigma_n$ at different T. Of these parameters, f_s/E_s, c_s, and $b_{s'}$ are the most important.[21] They also determine the cross section at relativistic velocities ($v=\beta c$, $T\gtrsim 10^4$ eV)[2,48,49]:

$$\sigma_s=\frac{8\pi a_0^2 z^2}{mv^2/R}\left\{\frac{f_s}{E_s/R}\left[\ln\left(\frac{\beta^2}{1-\beta^2}\right)-\beta^2\right]+C_s\right\} \tag{17}$$

for an allowed excitation, C_s being related to c_s by

$$C_s=(Rf_s/E_s)[\ln c_s+\ln(2mc^2/R)],$$

$$\ln(2mc^2/R)=11.2268, \tag{18}$$

and

$$\sigma_{s'}=\frac{8\pi a_0^2 z^2}{mv^2/R}b_{s'} \tag{19}$$

for a forbidden excitation. Secondly, the term with γ_s or $\gamma_{s'}$ represents the most significant part of the difference between the Born cross section and the Bethe asymptotic cross section and thus serves as a measure of the applicability of the Bethe procedure. This term, however, should by no means be confused with the difference between the *true* cross section and the Bethe cross section, because those effects which are neglected in the Born approximation contribute to the cross section within the same order of magnitude as the γ_s or $\gamma_{s'}$ term.[47] Thirdly, γ_s for an allowed transition depends on M and may have either sign while $\gamma_{s'}$ for a forbidden transition is invariably nonpositive.[47] Finally, γ_s and $\gamma_{s'}$, likewise c_s and $b_{s'}$,[21] obey certain sum rules.

We have evaluated c_s and γ_s for excitations to the 2^1P and 3^1P states, and $b_{s'}$ and $\gamma_{s'}$ for the 2^1S and 3^1S states from our $f_n(K)$. The results are presented in Table VII. The total cross sections thereby derived are shown in Figs. 4-7, where the ordinate represents $(T/R)\sigma_n/(4\pi a_0^2 z^2)$ and the abscissa $\ln(T/R)$. Notice that the Bethe asymptotic term, given by the straight lines there, dominates over the correction term with γ_n. Further the remainder $O(E_n^2/T^2)$ is insignificant in the region of interest. Indeed, integration of $d\sigma_n$ between exact kinematical limits shows that the remainder $O(E_n^2/T^2)$, even at $T=100$ eV, is less than 1% for the 2^1S and 3^1S excitations, and even smaller for the 2^1P and 3^1P excitations.

It is worth noting that the important parameters c_s and $b_{s'}$ are often inadequately treated in the literature. An example is the discussions on pp. 496-498 of Ref. 10. The often quoted formulas, Eqs. (117a) and (117b) of Ref. 10, imply in our notation

$$c_s=R/E_s, \tag{20}$$

and

$$b_{s'}=|Z_{s'}^{(2)}|^2|W_0|/(4R), \tag{21}$$

respectively, where W_0 is the total energy of the ground state. These relations neither have a

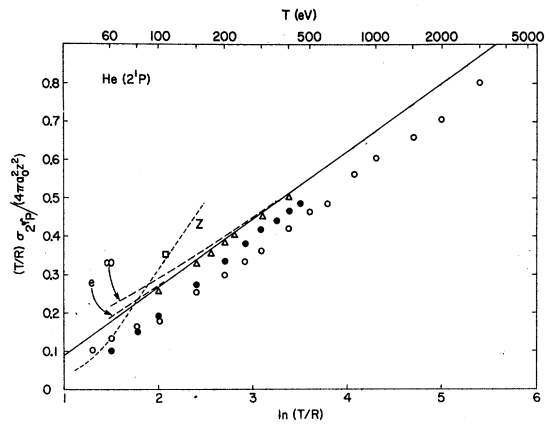

FIG. 4. Cross section for the 2^1P excitation of He. The solid straight line represents the Bethe asymptotic cross section for any charged particle, and the broken curves (---) represent the same with the kinematical correction [Eq. (11)] for an electron (labeled "e") and for charged particles with $M \to \infty$ (labeled "∞"). The dots (●) show the electron-collision data of Jobe and St. John (Ref. 60), the circles (○) those of Moustafa Moussa *et al.* (Ref. 61), and the triangles (△) those of Vriens *et al.* (Ref. 20). The square (□) shows the measurement of Gabriel and Heddle (Ref. 58), and the dashed curve (---, labeled "Z") Zapesochnyi's data (Ref. 62).

sound basis nor can serve as a practical guide. Indeed, for the transitions in He, Eq. (20) gives $\ln c_{2^1P} = -0.445$ and $\ln c_{3^1P} = -0.529$, leading to the cross sections too large by some 40% at $T = 500$ eV. Further, Eq. (21) gives $b_{2^1S} = 0.320$ and $b_{3^1S} = 0.0587$, leading to the asymptotic cross sections several times too large. (See Table VII.)

A. Excitation to the 2^1P and 3^1P States

Earlier theoretical and experimental studies have been extensively reviewed by Moiseiwitsch and Smith,[50] and by Green *et al.*[51]

Among published calculations[4,10-14,51-55], the results within the Born approximation of Altshuler[4] (from his "Method II"), of Bell[53] (for proton and alpha particles), of Mott and Massey (Ref. 10, p. 498), and of Kennedy and Kingston[12] (for 2^1P) are the closest to our result, differing only by a few percent in the region $T \gtrsim 400$ eV. Earlier determination[12-14,47] of the parameters f_S/E_S, $\ln c_S$, and γ_S is, in general, in reasonable agreement with our result in Table VII, except for the γ_{3^1P} values. A study of Rothenstein[56] indicates that the second Born approximation reduces the electron-impact cross section for the 2^1P excitation by about 6% at $T = 200$ eV. However, the use of simple hydrogenic wave functions, which give an erroneous f_{2^1P},[15] prevents one from attaching quantitative significance to this result. Allowance for the electron exchange also seems to reduce the first Born cross section by a few to several percent for $T \lesssim 400$ eV.[47,54,57]

Figures 4 and 5 compare our results with selected experimental data. The cross sections given in Refs. 58–62 were derived from intensities of optical emissions excited by electron impact. For the 2^1P excitation, the data of Jobe and St. John[60] are closer to our result than those of Moustafa Moussa *et al.*[61] (Notice also that the latter measurements were originally relative and were normalized in such a way as to exhibit the correct asymptotic slope.) In contrast, the 3^1P data of Moustafa Moussa *et al.*[61] (in this case measured absolutely) are compatible with our asymptotic cross section but those of St. John *et al.*[59] are not. The data of Zapesochnyi[62] for the 2^1P and the 3^1P excitations are in disagreement with our result.

The 2^1P excitation cross sections in Ref. 20 are semiempirical in origin. The determination of the cross sections is based on the Born approximation [Eq. (3)] and utilizes an analytic form for the "apparent" $f_{2^1P}(K)$ fitted to measured differential cross sections. The resulting cross sections agree well with our theory. (See Fig. 4.) The 3^1P excitation cross sections derived in a similar manner by Silverman and Lassettre[63] are also in good accord with our result.

The measurements for the 3^1P excitation by protons and deuterons[64-66] are in fair agreement with our result.

The cross sections adopted by Miller[27] in 1956 after critical analyses of experimental and theoretical information available at that time are slightly higher than our results for $T \gtrsim 200$ eV.

B. Excitations to the 2^1S and 3^1S States

Again, theoretical and experimental data are summarized in Refs. 50 and 51.

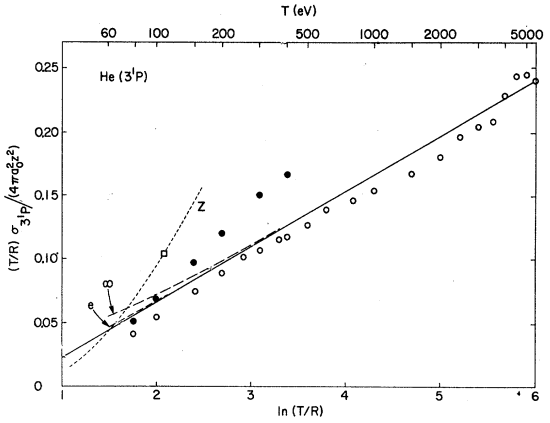

FIG. 5. Cross section for the 3^1P excitation of He. The solid straight line represents the Bethe asymptotic cross section for any charged particle, and the broken curves (---) represent the same with the kinematical corrections [Eq. (11)] for an electron (labeled "e") and for a charged particle with $M \to \infty$ (labeled "∞"). The dots (●) show the electron-collision data of St. John *et al.* (Ref. 59), and the circles (○) those of Moustafa Moussa *et al.* (Ref. 61). The square (□) shows the measurement of Gabriel and Heddle (Ref. 58), and the dashed curve (---, labeled "Z") that of Zapesochnyi (Ref. 62). The data of Silverman and Lassettre (Ref. 63), not shown here, are indistinguishable from the solid line for $T \geq 100$ eV.

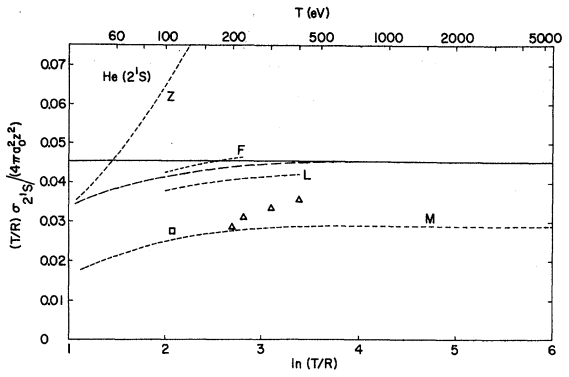

FIG. 6. Cross section for the 2^1S excitation of He. The solid straight line represents the Bethe asymptotic cross section and the broken curve (– – –) the same with the kinematical correction [Eq. (14)] both for any charged particle. The triangles (△) show the electron-collision data of Vriens *et al.* (Ref. 20). The square (□) shows the determination by Gabriel and Heddle (Ref. 58). The dashed curves labeled as *M*, *L*, *F*, and *Z* refer to the adoption of Miller (Ref. 27), the data of Lassettre (Ref. 67), the calculation of Fox (Ref. 9), and of Zapensochnyi (Ref. 62), respectively. The calculation of Altshuler (Ref. 4), which is not shown here, is very close to the adoption of Miller.

The Born cross sections evaluated by Fox[9] are close to ours (Figs. 6 and 7) while those of Altshuler[4] and of van den Bos[11] are very different from ours although all the calculations use wave functions of similar quality. This situation illustrates the need of accurate wave functions for a reliable result in these forbidden transitions, particularly when the states involved belong to the same symmetry so that the orthogonality between them is nontrivial. (See Sec. 4B.)

For the 2^1S excitation by electrons, only a few fragmentary data are available from direct measurements.[27,50] Lassettre,[67] and later Vriens *et al.*[20] evaluated the excitation cross section from "apparent" $f_{2^1S}(K)$ fitted to the measured differential cross sections. Comparison of these cross sections especially those from Ref. 20 with our result on Fig. 6 appears to indicate that the Bethe asymptotic limit is not quite attained at $T = 400$ eV. (See Sec. 4C.)

Among optically measured cross sections for the 3^1S excitation by electrons, the data of Moustafa Moussa *et al.*[61] are compatible with our result and exhibit a gradual attainment of the asymptotic behavior around $T = 10^3$ eV, while the data of St. John *et al.*[59] are incompatible with our result. The data of Zapesochnyi[62] disagree strongly with our asymptote.

The 3^1S excitation cross sections for impact of protons with incident energies around 100 keV[64,66] appear to be in rough agreement with our result, although the Born approximation is not likely to be valid at these low velocities.

The cross sections adopted by Miller[27] for both the 2^1S and 3^1S excitations, in contrast to those for the 2^1P and 3^1P excitations, turn out to be much too low compared to our results. A revised adoption of He cross sections in view of the present work and other recent information[21] is being planned.

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APPENDIX. DERIVATION OF EQS. (11)–(16)

The essential factor in σ_n is the integral[15]

$$A_n = \int_{Q_1}^{Q_2} f_n(K) Q^{-1} dQ,$$

where $Q = (Ka_0)^2$, and the limits Q_1 and Q_2 in nonrelativistic kinematics are

$$Q_1 = [E_n^2/(4RT)][1 + (m/2M)E_n/T + O(E_n^2/T^2)], \quad \text{(A1)}$$

$$Q_2 = [4(M/m)^2 T/R][1 - (m/2M)E_n/T + O(E_n^2/T^2)]. \quad \text{(A2)}$$

Because $f_n(K)$ is known to fall off as a high power of $1/Q$ as $Q \to \infty$,[46] it follows from Eq. (A2) that replacement of Q_2 by infinity introduces an error in A_n only of $o(E_n^2/T^2)$. Thus, after rearranging the interval of integration, we write

$$A_n = \int_1^\infty f_n(K) Q^{-1} dQ + \int_0^1 [f_n(K) - f_n] Q^{-1} dQ - f_n \ln Q_1 - \int_0^{Q_1} [f_n(K) - f_n] Q^{-1} dQ + o(E_n^2/T^2). \quad \text{(A3)}$$

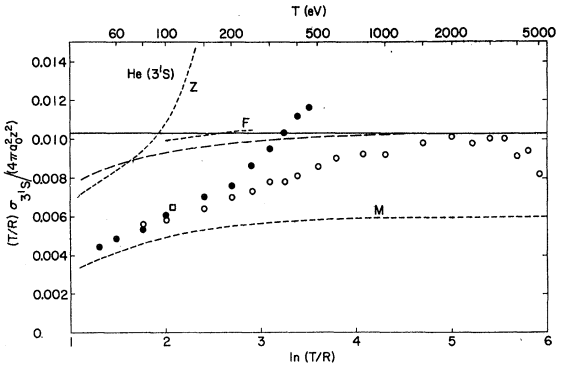

FIG. 7. Cross section for the 3^1S excitation of He. The solid straight line represents the Bethe asymptotic cross section and the broken curve (– – –) the same with the kinematical correction [Eq. (14)], both for any charged particle. The dots (●) show the electron-collision data of St. John *et al.* (Ref. 59), and the circles (○) those of Moustafa Moussa *et al.* (Ref. 61). The square (□) shows the measurement of Gabriel and Heddle (Ref. 58). The dashed curves labeled as *M*, *F*, and *Z* refer to the adoption of Miller (Ref. 27), the calculation of Fox (Ref. 9) and the experimental data of Zapesochnyi (Ref. 62), respectively.

The first two terms on the right-hand side of Eq. (A3) together give either $f_S \ln[c_S(E_S/R)^2]$ for an allowed transition ($n=s$), or $(E_{S'}/R)b_{S'}$ for a forbidden transition ($n=s'$). [See Eqs. (12) and (15).] The third term, present only for an allowed transition, is written, by use of Eq. (A1), as

$$f_S \ln Q_1 = f_S \ln\left(\frac{E_S^2}{4RT}\right) + \left(\frac{m}{2M}\right)\frac{f_S E_S}{T} + O\left(\frac{E_S^2}{T^2}\right). \quad \text{(A4)}$$

The fourth term is expressed, by use of Eq. (4), in the form

$$\int_0^{Q_1}[f_n(K) - f_n^{\cdot}]Q^{-1}dQ$$

$$= f_n^{(1)} E_n^2/(4RT) + O(E_n^2/T^2). \quad \text{(A5)}$$

Combining Eqs. (A3), (A4), and (A5), we obtain

$$A_S = f_S \ln(4c_S T/R) - (m/2M) f_S E_S/T - f_S^{(1)} E_S^2/(4RT) + O(E_S^2/T^2), \quad \text{(A6)}$$

for an allowed transition, and

$$A_{S'} = \left(\frac{E_{S'}}{R}\right) b_{S'} - f_{S'}^{(1)} \frac{E_{S'}^2}{(4RT)} + O\left(\frac{E_{S'}^2}{T^2}\right), \quad \text{(A7)}$$

for a forbidden transition. Equations (A6) and (A7), respectively, lead to Eqs. (11) and (14).

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