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Generalized Oscillator Strengths of the Helium Atom. III. Transitions from the Ground State to the 3^1D and 4^1P States*

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The generalized oscillator strengths of He for the $1^1S \to 3^1D$ and 4^1P transitions have been calculated with correlated wave functions, according to both the length and velocity formulas. The agreement between the two alternative results is within 3% or less for moderate values of the momentum transfer. The resulting Born cross sections for charged-particle impact are also given. Compared with our values, available experimental data on the 3^1D excitation are substantially larger, while for the 4^1P excitation they agree within ± 50%.

1. INTRODUCTION

To test rigorously the validity of the Born approximation, it is essential to minimize those uncertainties in the generalized oscillator strength (GOS) which come from the inaccuracy in the wave functions. We have extended our earlier work[1,2] by calculating with the Weiss correlated wave functions[3] the GOS of He for the $1^1S \to 3^1D$, 4^1P transitions.

The Born excitation cross sections for charged-particle impact are computed and compared with other theoretical and experimental data.

2. DEFINITIONS

The following notation is the same as those used in paper I: $f_n(K)$ is the GOS for the transition from the ground state to the state n; f_n is the optical oscillator strength; $\lim f_n(K) = f_n$, as $K \to 0$; $\vec{K}\hbar$ is the momentum transfer; a_0 is the Bohr radius; E_n/R is the excitation energy for state n in Rydbergs; $T = mv^2/2$, where m is the electron rest mass, and v the incident particle velocity; and finally, ze is the charge of the incident particle. We also take over the following equations.

Formula I (the "length" formula):

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

Formula II (the "velocity" formula):

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

Formula III (the "expansion" formula), for small K only:

$$f_n(K) = \sum_{\lambda=0}^{\infty} (Ka_0)^{2\lambda} f_n^{(\lambda)}/\lambda! \ . \tag{3}$$

The Born cross section, represented by the Bethe procedure:

For an optically allowed transition,

$$\sigma_s = \frac{4\pi a_0^2 z^2}{T/R} \left[\frac{f_s}{E_s/R} \ln\left(\frac{4c_s T}{R}\right) + \frac{\gamma_s}{T/R} + O\left(\frac{E_s^2}{T^2}\right) \right]. \tag{4}$$

For an optically forbidden transition,

$$\sigma_{s'} = \frac{4\pi a_0^2 z^2}{T/R} \left[b_{s'} + \frac{\gamma_{s'}}{T/R} + O\left(\frac{E_s^2}{T^2}\right) \right] . \tag{5}$$

The parameters c_s, $b_{s'}$, γ_s, and $\gamma_{s'}$ are determined from the GOS. [See Eqs. (12), (13), (15), and (16) of paper I.] The parameter γ_s depends on the mass of the incident particle, and we denote by $\gamma_s^{(e)}$ the value for electrons, and by $\gamma_s^{(\infty)}$ that for infinite reduced mass (compared to the electron mass), a very good approximation to protons and other heavy particles.

The Weiss wave functions[3] are of Hylleraas type and contain 53, 52, and 18 terms for the ground, 3^1D and 4^1P states, respectively. The excitation energies and other properties computed from the Weiss wave functions are in very good accord with the best available theoretical and experimental information (Table I). The computational method is essentially the same as that described in Sec. 3 of paper I, except for the fact that the spherical Bessel function $j_3(Kr)$ appears in the "velocity" calculation for $f_{3^1D}(K)$ and that the computation is cumbersome. [See Eqs. (9) and (10), paper I.]

TABLE I. Comparison of properties calculated from the Weiss wave functions and those from other sources in atomic units.

Property	Source	1^1S	3^1D	4^1P
Excitation energy E_n	Experiment[a]		0.848 07	0.872 63
(Total energy for the 1^1S state)	Weiss (Ref. 3)	2.903 724	0.848 11	0.872 77
	Green[b]	2.903 383	0.847 77	0.872 32
	Pekeris[c]	2.903 724		0.872 65
Expectation value of r_1^2	Weiss[d]	1.193 48	63.178	294.86
	Pekeris[c]	1.193 48		304.06
Expectation value of r_{12}^2	Weiss[d]	2.516 43	126.42	589.72
	Pekeris[c]	2.516 44		608.14
Optical oscillator strength, "length"	Weiss[e]			0.030 2
	Green[b]			0.029 6
Optical oscillator strength, "velocity"	Weiss[e]			0.030 3
	Green[b]			0.029 6

[a]W. C. Martin, J. Res. Natl. Bur. Std. (U.S.) 64A, 19 (1960); includes relativistic effects. Other energy values are nonrelativistic.

[c]C. L. Pekeris, Phys. Rev. 115, 1216 (1959); B. Schiff, H. Lifson, C. L. Pekeris, and P. Rabinowitz, *ibid.* 140, A1104 (1965).

[b]L. C. Green, E. K. Kolchin, and N. C. Johnson, Phys. Rev. 139, A373 (1965); Astrophys. J. 144, 369 (1966).

[d]Computed from the Weiss wave functions by the present authors.

[e]Reference 3.

3. GENERALIZED OSCILLATOR STRENGTHS

The GOS's are tabulated in Table II, and the expansion coefficients for Formula III [Eq. (3)] are given in Table III. The agreement between the length and velocity results is within 3% for $(Ka_0)^2 \lesssim 5$ and within 1% for more significant region $(Ka_0)^2 \lesssim 1$.

Although the 4^1P wave function is not as elaborate as the other Weiss wave functions, it yields a reliable $f_{4^1P}(K)$ judged from the close agreement of the length and velocity results. Because of close

TABLE II. The generalized oscillator strengths for the 3^1D and 4^1P excitations of He.

	3^1D		4^1P	
$(Ka_0)^2$	Formula I	Formula II	Formula I	Formula II
0.05	4.2206×10^{-4}	4.2652×10^{-4}	2.848×10^{-2}	2.860×10^{-2}
0.10	7.4421×10^{-4}	7.5052×10^{-4}	2.688×10^{-2}	2.701×10^{-2}
0.15	9.8603×10^{-4}	9.9255×10^{-4}	2.536×10^{-2}	2.550×10^{-2}
0.20	1.1634×10^{-3}	1.1691×10^{-3}	2.393×10^{-2}	2.408×10^{-2}
0.25	1.2892×10^{-3}	1.2936×10^{-3}	2.258×10^{-2}	2.273×10^{-2}
0.30	1.3739×10^{-3}	1.3768×10^{-3}	2.130×10^{-2}	2.145×10^{-2}
0.35	1.4260×10^{-3}	1.4273×10^{-3}	2.010×10^{-2}	2.025×10^{-2}
0.40	1.4522×10^{-3}	1.4520×10^{-3}	1.896×10^{-2}	1.911×10^{-2}
0.45	1.4582×10^{-3}	1.4567×10^{-3}	1.789×10^{-2}	1.804×10^{-2}
0.50	1.4486×10^{-3}	1.4458×10^{-3}	1.689×10^{-2}	1.704×10^{-2}
0.55	1.4268×10^{-3}	1.4231×10^{-3}	1.594×10^{-2}	1.609×10^{-2}
0.60	1.3959×10^{-3}	1.3914×10^{-3}	1.505×10^{-2}	1.520×10^{-2}
0.65	1.3582×10^{-3}	1.3532×10^{-3}	1.421×10^{-2}	1.436×10^{-2}
0.70	1.3157×10^{-3}	1.3102×10^{-3}	1.342×10^{-2}	1.356×10^{-2}
0.75	1.2698×10^{-3}	1.2640×10^{-3}	1.268×10^{-2}	1.282×10^{-2}
0.80	1.2218×10^{-3}	1.2158×10^{-3}	1.199×10^{-2}	1.212×10^{-2}
0.85	1.1726×10^{-3}	1.1665×10^{-3}	1.133×10^{-2}	1.146×10^{-2}
0.90	1.1230×10^{-3}	1.1169×10^{-3}	1.071×10^{-2}	1.084×10^{-2}
0.95	1.0736×10^{-3}	1.0676×10^{-3}	1.013×10^{-2}	1.026×10^{-2}
1.00	1.0248×10^{-3}	1.0189×10^{-3}	9.590×10^{-3}	9.714×10^{-3}

TABLE II. (*Cont.*)

$(Ka_0)^2$	3^1D Formula I	3^1D Formula II	4^1P Formula I	4^1P Formula II
1.2	8.4200×10^{-4}	8.3679×10^{-4}	7.712×10^{-3}	7.825×10^{-3}
1.4	6.8499×10^{-4}	6.8059×10^{-4}	6.237×10^{-3}	6.338×10^{-3}
1.6	5.5510×10^{-4}	5.5139×10^{-4}	5.072×10^{-3}	5.163×10^{-3}
1.8	4.4964×10^{-4}	4.4647×10^{-4}	4.148×10^{-3}	4.229×10^{-3}
2.0	3.6480×10^{-4}	3.6203×10^{-4}	3.412×10^{-3}	3.484×10^{-3}
2.2	2.9682×10^{-4}	2.9434×10^{-4}	2.821×10^{-3}	2.884×10^{-3}
2.4	2.4236×10^{-4}	2.4012×10^{-4}	2.345×10^{-3}	2.401×10^{-3}
2.6	1.9869×10^{-4}	1.9664×10^{-4}	1.958×10^{-3}	2.008×10^{-3}
2.8	1.6358×10^{-4}	1.6169×10^{-4}	1.644×10^{-3}	1.687×10^{-3}
3.0	1.3525×10^{-4}	1.3351×10^{-4}	1.386×10^{-3}	1.424×10^{-3}
3.2	1.1231×10^{-4}	1.1071×10^{-4}	1.174×10^{-3}	1.207×10^{-3}
3.4	9.3660×10^{-5}	9.2194×10^{-5}	9.985×10^{-4}	1.027×10^{-3}
3.6	7.8435×10^{-5}	7.7096×10^{-5}	8.527×10^{-4}	8.776×10^{-4}
3.8	6.5954×10^{-5}	6.4735×10^{-5}	7.309×10^{-4}	7.524×10^{-4}
4.0	5.5679×10^{-5}	5.4574×10^{-5}	6.289×10^{-4}	6.474×10^{-4}
4.2	4.7186×10^{-5}	4.6187×10^{-5}	5.430×10^{-4}	5.589×10^{-4}
4.4	4.0137×10^{-5}	3.9238×10^{-5}	4.704×10^{-4}	4.840×10^{-4}
4.6	3.4264×10^{-5}	3.3456×10^{-5}	4.088×10^{-4}	4.203×10^{-4}
4.8	2.9352×10^{-5}	2.8627×10^{-5}	3.564×10^{-4}	3.661×10^{-4}
5.0	2.5228×10^{-5}	2.4579×10^{-5}	3.116×10^{-4}	3.197×10^{-4}
5.5	1.7519×10^{-5}	1.7028×10^{-5}	2.254×10^{-4}	2.304×10^{-4}
6.0	1.2391×10^{-5}	1.2022×10^{-5}	1.657×10^{-4}	1.683×10^{-4}
6.5	8.9127×10^{-6}	8.6337×10^{-6}	1.236×10^{-4}	1.245×10^{-4}
7.0	6.5097×10^{-6}	6.2982×10^{-6}	9.340×10^{-5}	9.316×10^{-5}
7.5	4.8219×10^{-6}	4.6605×10^{-6}	7.144×10^{-5}	7.037×10^{-5}
8.0	3.6181×10^{-6}	3.4939×10^{-6}	5.525×10^{-5}	5.360×10^{-5}
8.5	2.7473×10^{-6}	2.6507×10^{-6}	4.316×10^{-5}	4.114×10^{-5}
9.0	2.1091×10^{-6}	2.0333×10^{-6}	3.404×10^{-5}	3.178×10^{-5}
9.5	1.6356×10^{-6}	1.5755×10^{-6}	2.708×10^{-5}	2.470×10^{-5}
10.0	1.2804×10^{-6}	1.2323×10^{-6}	2.172×10^{-5}	1.929×10^{-5}
20.0	3.4514×10^{-8}		8.101×10^{-7}	
30.0	3.3703×10^{-9}		9.678×10^{-8}	
40.0	6.0339×10^{-10}		2.035×10^{-8}	
50.0	1.5379×10^{-10}		5.961×10^{-9}	
60.0	4.9386×10^{-11}		2.169×10^{-9}	
70.0	1.8668×10^{-11}		9.182×10^{-10}	
80.0	7.9670×10^{-12}		4.348×10^{-10}	
90.0	3.7348×10^{-12}		2.244×10^{-10}	
100.0	1.8870×10^{-12}		1.239×10^{-10}	

TABLE III. Power-series expansion coefficients $f_n^{(\lambda)}/\lambda!$ [see Eq. (3)] for the generalized oscillator strengths of He.

λ	Final state 3^1D	Final state 4^1P
0		0.030 1676
1	0.009 5930	−0.034 6558
2	−0.024 7254	0.017 8689
3	0.035 6259	−0.001 8249
4	−0.037 5938	−0.005 0664
5	0.032 2414	

spacing of levels it is very difficult at present to resolve electron-impact differential cross sections for the 3^1D and 4^1P excitations, and we are unaware of experimental data on these individual excitations to be compared with our result.

The GOS's calculated in the length formula by van den Bos[4] with a two-term Hartree-Fock-Roothaan wave function for the ground-state and Eckart wave functions for the excited states are in good agreement [lower by ~6% than our result for 3^1D at $(Ka_0)^2 = 0.5$ and higher by ~ 6% for 4^1P at $(Ka_0)^2 = 0.1$] with ours.

Bell, Kennedy, and Kingston[5] calculated the

GOS's from a six-term Hylleraas ground-state wave function and modified hydrogenic excited-state wave functions in both the length and velocity formulas. For the 3^1D excitation, their velocity result is almost the same as ours [smaller by ~1% at $(Ka_0)^2 = 0.5$] and the length result is lower [by 6% at $(Ka_0)^2 = 0.5$] than our result. Recently, Bell, Kennedy, and Kingston[6] have essentially duplicated our work in the length formula only, using Weiss wave functions; they concluded that their "accurate" GOS for the 3^1D excitation should be accurate to 0.1% and lie about halfway between the length and velocity results of Ref. 5. The values of $f_{3^1D}(K)$ in Table II, however, are a few to several percent larger than those in Ref. 6, particularly for small momentum transfer, and do not support their conclusion at all.[7] As for the 4^1P excitation, the GOS in Ref. 5 is somewhat larger than ours [by ~8% for the velocity result, and by ~5% for the length result at $(Ka_0)^2 = 0.1$], and that in Ref. 6 is essentially identical to our length result as it should be.

In Sec. 4C of paper I, we implied that the "apparent" $f_{3^1P}(K)$ deduced from experiment by Lassettre, Krasnow, and Silverman[8] as well as by Geiger[9] is actually the sum of the GOS's for the 3^1S, 3^1P, and 3^1D excitations, because neither experiment had enough energy resolution to separate the three states. In Fig. 1, we have plotted $f_{3^1P}(K)$ (from paper I), the sum of the three excitations, and the experimental data. Now the agreement between theory and experiment, particularly that of Ref. 8, is improved.

The differential Born cross sections for the 3^1D excitation in the textbook by Mott and Massey[10] (Table VI, p. 481) are almost by a factor of 2 too large, whereas the 4^1P cross sections there are in good agreement with our result.

As is the case for the 2^1S and 3^1S excitations

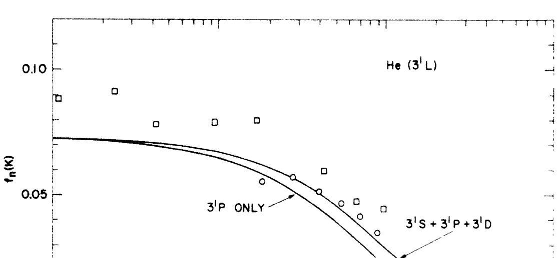

FIG. 1. The generalized oscillator strengths of He for the $1^1S \rightarrow 3^1L$ transitions. The circles (○) are experimental data by Lassettre *et al.* (Ref. 8), and squares (□) those by Geiger (Ref. 9). Neither experiment had sufficient energy resolution to separate the 3^1S, 3^1P, and 3^1D transitions, and their "3^1P" data actually include all three transitions.

TABLE IV. Parameters for the excitation cross sections of He. [See Eqs. (4) and (5).]

Parameter	Final state 3^1D	Final state 4^1P
Rf_s/E_s		0.0173
$\ln c_s$		−1.816
$Rf_sE_s^{-1}\ln(4c_s)$		−0.00743
b_s'	0.00251	
$\gamma_n^{(e)}$	−0.00407	0.000040
$\gamma_n^{(\infty)}$		0.0151

discussed in paper I, the first nonvanishing coefficient $f_n^{(1)}$ for the 3^1D excitation [see Eq. (3)] is sensitive to the choice of wave functions used. The values of $f_{3^1D}^{(1)}$ in the literature[4,5,10–13]

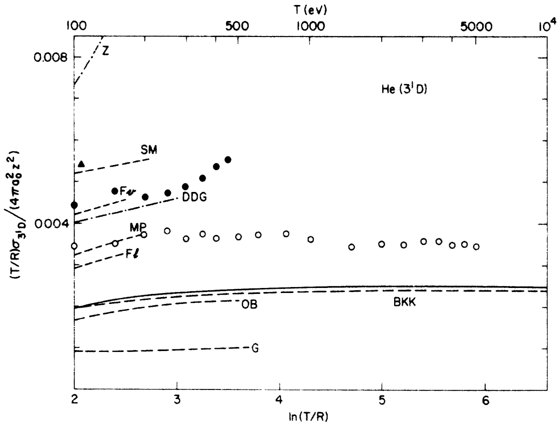

FIG. 2. Excitation cross sections for the $1^1S \rightarrow 3^1D$ excitation of He. Note that the ordinate is the excitation cross section times $T = mv^2/2$. For electrons T as given on the top scale is the incident energy. The open circles (○) are electron-impact experimental data by Moustafa Moussa *et al.* (Ref. 23); the closed circles (●) those by St. John *et al.* (Ref. 20); the closed triangle (▲) by Gabriel and Heddle (Ref. 19); and the chained curve (-·-·-·) on top left corner marked "Z" by Zapesochnyi (Ref. 21). The other chained curve marked "DDG" represents the proton-impact experimental data by Denis *et al.* (Ref. 22). Other theoretical cross sections are represented by broken curves (----); "SM" and "MP" denote the results of impact-parameter approximations by Stauffer and McDowell (Ref. 15) and McDowell and Pluta (Ref. 18), respectively; "Fl" and "Fv" the length and velocity Born calculations, respectively, by Fox (Ref. 12); "BKK" represents the "accurate" Born cross section by Bell *et al.* (Refs. 6 and 14. See comments on the accuracy of their results in Sec. 3, 4 and Footnote 7); "OB" the Born-Ochkur approximation result by Ochkur and Brattsev (Ref. 16); and "G" the Born cross section by Gaillard (Refs. 17 and 22). The solid line gives the present result (the same for both electrons and other heavy charged particles).

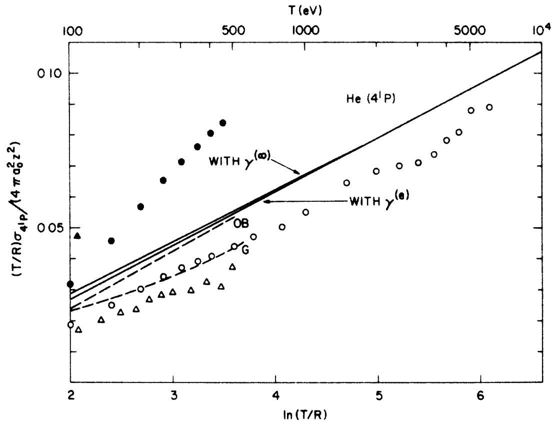

FIG. 3. Excitation cross sections for the $1^1S \rightarrow 4^1P$ excitation of He. The open triangles (△) represent proton-impact experimental data of Thomas and Bent (Ref. 24). Other notations are the same as those in Fig. 2. The solid curves are the present results: The lower one is for incident electrons, and the upper one may be used for incident protons and other heavy particles. See the paragraph below Eq. (5) of the text.

range anywhere from 0.0031 to 0.0195, compared to the accurate value of 0.009593 (Table III).

4. BORN EXCITATION CROSS SECTIONS

The parameters for the Born excitation cross sections [Eqs. (4) and (5)] are listed in Table IV. There is a variety of experimental and theoretical information on the 3^1D excitation cross section.[4–6,10,12–23] All of the experimental data[19–23] are obtained through optical methods and they may be subject to errors inherent in such a method. All experimental 3^1D cross sections are substantially larger than the Born result, as shown in Fig. 2. Although the electron-impact cross section for the 3^1D excitation measured by Moustafa Moussa, de Heer, and Schutten[23] apparently attains an asymptotic behavior for $T \gtrsim 1000$ eV (Fig. 2), its magnitude is about 40% larger than that predicted by theory. Other experiments seem even less compatible with theory. Among the many theoretical cross sections, that by Bell *et al.*[5,6,13,14] and by van den Bos[4] come close to our result. The 3^1D excitation cross sections in Refs. 6 and 14 are ~4% lower than ours in the asymptotic region (Fig. 2).[7]

The experimental data on the 4^1P excitation cross section[19–24] agree with our result (Fig. 3) within ± 50%. Again, the data of Moustafa Moussa *et al.*[23] exhibit the energy dependence predicted by the Bethe theory, but not the magnitude. The 4^1P excitation cross section calculated by van den Bos[4] is very close to ours, and those by Bell *et al.*[5] are somewhat larger.

Bell, Kennedy, and Kingston[5,6,14] also present their cross sections in the form of Eqs. (4) and (5) (including terms of higher negative powers of T), but they seem to have determined the parameters c_S, b_S', γ_S, and γ_S' by numerically fitting to the Born cross sections evaluated at various incident energies. With the Bethe procedure described in the Appendix of paper I, these parameters are uniquely determined from the GOS itself. The parameters for the 4^1P excitation given by Bell *et al.*[6,14] are in good agreement with those in Table IV, but those for the 3^1D excitation are different from ours.[7] The contributions from the remainder $O(E_n^2/T^2)$ in Eqs. (4) and (5), which represents the difference between the Born cross section and its representation by the Bethe procedure, become significant only at rather low incident velocities where the validity of the Born approximation itself becomes doubtful.

Printing errors in paper I. In Table II, the exponent of $f_{3^1P}(K)$ at $(Ka_0)^2 = 50$ should read "10^{-8}." Seven lines below Eq. (16), "λ_S" and "λ_S'" should read "γ_S" and "γ_S'," respectively.

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[7]The discrepancy between our $f_{3^1D}(K)$ and that in Ref. 6, which should be identical to our length result, is not understood. The fact that the 3^1D length results in Table II for small K can be reproduced precisely by the expansion formula [the coefficients in Table III were calculated by a computer program independent of that

for $f_{3^1D}(K)$] provides a valuable consistency check on our computational method.

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Electron Loss in Heavy-Body Collisions*

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A simple theory based on a free scattering model and the Born approximation is used to describe the loss of electrons from an atomic system during high-energy impact with another atomic system. Calculations for electron loss by atomic hydrogen incident on helium, atomic nitrogen, and argon agree well with the Born approximation and the high-energy experimental data. At high energies the cross sections decrease as aE^{-1}, where E is the laboratory system energy, and for atomic hydrogen projectiles, a has the values 1.6×10^{-11} cm^2 eV, 1.3×10^{-10} cm^2 eV, and 4.7×10^{-10} cm^2 eV for targets of helium, atomic nitrogen, and argon, respectively.

INTRODUCTION

Born approximation calculations[1–3] for the electron-loss cross sections in high-energy collisions involving the few-electron systems of hydrogen and helium show good agreement with experimental data.[4–6] For target and projectile systems with more electrons, the Born approximation calculations become much more difficult. Dmitriev and Nikolaev[7] have done calculations for the few-electron systems using a simpler theory, which gives results identical to the Born approximation at very high energies. The free scattering theory of Dmitriev and Nikolaev[7] assumes that an electron, moving with the same velocity as the projectile nucleus, is removed if, in elastic and inelastic collisions with the target atom, it receives enough momentum transfer to increase its energy above the ionization potential of the projectile system. The Born approximation is used to treat the free electron-target atom scattering, with the use of the closure approximation for the inelastic processes. In view of the simplicity of such a theory, calculations based on it have been performed for heavier target systems. At high energies the agreement between experiment data,[4–6] and calculations for atomic hydrogen incident on helium, atomic nitrogen, and argon is good. The theory should also provide reliable estimates at very high energies for heavier projectile systems, for which no experimental data appear to be available.

THEORY

Let k_0 be the magnitude of the initial momentum vector $\vec{k}_0$ of the incident electron, where it is assumed that the velocity of the incident electron is identical with the relative velocity of the heavy bodies. Let $\vec{k}_f$ be the momentum of the scattered