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Electron-impact ionization cross sections and bound-free generalized oscillator strengths for atomic systems

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Within the Born approximation, a general formulation is given for differential cross sections corresponding to electron-impact ionization of an arbitrary L-S–coupled atomic system. Expressions for the generalized oscillator strength and total cross section are also given. Correlation effects are explicitly included in the formulation through the use of a configuration-interaction wave function to describe the initial bound target state, and a close-coupling wave function to describe the final free target state. Two independent computer codes have been constructed which allow these functions to be of arbitrary complexity for any atom. The codes use recently developed, but different, techniques for solving the close-coupling equations. Test results are obtained for the helium atom, and they agree well with previous correlated calculations.

I. INTRODUCTION

Many calculations of electron-impact ionization cross sections for atomic systems have been performed using the Born approximation and its variants. A more sophisticated theoretical treatment of the problem would be desirable. However, the practical difficulties of dealing with the double-continuum wave function make this goal seem somewhat far off. One aspect of Born calculations which has not yet been investigated in depth is the effect of using well-correlated wave functions for the initial bound and final free states of the target system. It is the purpose of this paper to present a general evaluation of Born ionization amplitudes for any atomic system in which arbitrarily complex L-S–coupled configuration-interaction (CI) wave functions are used. We use an orthonormal basis of radial functions throughout, and always ensure that the initial- and final-state target functions are orthogonal. There is no restriction that the initial target state be a ground state or even the lowest state of a particular symmetry, and ionization is not confined to outer-shell electrons.

We take for our representation of the bound state CI wave functions as described by Hibbert,[1] and for the free or continuum state we solve appropriate close-coupling equations. In practice the close-coupling functions are obtained from computer codes which use either (a) the noniterative-integral-equation method (NIEM) of Smith and Henry,[2] or (b) the R-matrix method of Burke *et al.*[3]

In Sec. II we present the general formulation of the problem, for an arbitrarily complex neutral atom, assuming that L-S coupling is valid throughout. Section II contains explicit formulas for differential and total cross sections as well as generalized oscillator strengths. In Sec. III we present results for ionization of helium which were used to test the computer codes. Excellent numerical agreement is obtained between identical calculations which use the NIEM and R-matrix continuum wave functions. The present results show very clearly the effects of increasing the amount of correlation included in the wave functions, and thus they help tie together many of the previous calculations.

In future papers we shall perform calculations for more complex systems. Calculations of Born ionization cross sections for other systems of astrophysical interest are compiled in the review article of Bely and Van Regemorter.[4]

II. THEORY

The triple differential cross section for electron-impact ionization of an atom A in the Born approximation is given by

$$d\sigma = \frac{4k_f}{K^4 k_0} k^2 |\epsilon_{0\vec{k}}(\vec{K})|^2 \, d\omega \, d\omega_k \, dk, \tag{1}$$

where $d\omega$ is an element of solid angle about the direction of the scattered electron, $\vec{k}$ is the wave vector for the ejected electron, $\vec{k}_0$ and $\vec{k}_f$ are the initial and final wave vectors, respectively, of the incident electron, and

$$\vec{K} = \vec{k}_0 - \vec{k}_f \tag{2}$$

is the momentum transfer. The cross section σ is in units of a_0^2, and $\vec{k}_f^2$, $\vec{k}_0^2$, and $\vec{k}^2$ are in Rydbergs. The form factor is expressed by

$$\epsilon_{0\vec{k}}(\vec{K}) = \int \Psi_f^{(-)}(\vec{k}) \left(\sum_{q=1}^{N+1} e^{i\vec{K}\cdot\vec{r}_q} \right) \Phi_0 \, dV, \tag{3}$$

where Φ_0 is the initial bound state of the atom and $\Psi_f^{(-)}(\vec{k})$ is the continuum final state of $(e^-_{\text{ejected}} + A^+)$ with boundary conditions corresponding to an outgoing wave in channel f plus ingoing spherical waves in all open channels. $N+1$ is the number of electrons in the atom. The continuum function is normalized to a δ function in $\vec{k}$ space, i.e.,

$$\int \Psi_f^{*(-)}(\vec{k}) \Psi_{f'}^{(-)}(\vec{k}') \, dV = \delta(\vec{k} - \vec{k}')\delta_{ff'}. \tag{4}$$

If the continuum functions are normalized to a δ function in E space, then

$$d\sigma = \frac{4k_f}{K^4 k_0} |\epsilon_{0E}(\vec{K})|^2 \, d\omega \, d\omega_E \, dE, \tag{5}$$

where $E = \vec{k}^2$ is the energy of the ejected electron, and the normalization becomes

$$\int \Psi_f^{*(-)}(E, \hat{k}) \Psi_{f'}^{(-)}(E', \hat{k}') \, dV = \delta(E - E')\delta(\hat{k}, \hat{k}')\delta_{ff'}. \tag{6}$$

$\hat{k}$ is the unit vector in the direction of $\vec{k}$ and

$$\epsilon_{0E}(\vec{K}) = \int \Psi_f^{*(-)}(E, \hat{k}) \left(\sum_{q=1}^{N+1} e^{i\vec{K}\cdot\vec{r}_q} \right) \Phi_0 \, dV. \tag{7}$$

We will work with the E-space-normalized continuum functions.

The partial wave expansion of the final state is

$$\Psi_j^{(-)}(E, \hat{k}) = \sum_{LS\pi} \sum_{l_j m(l_j)} i^{l_j} \mathcal{Y}_{l_j}^{*m(l_j)}(\hat{k}) C(L_j l_j L; M_{L_j} m_{l_j} M_L) \, C(S_j \tfrac{1}{2} S; M_{S_j} m_{1/2} M_S)$$
$$\times \Psi^{(-)}(\alpha_j L_j S_j k_j l_j LS\pi; M_{L_j} M_{S_j} m_{l_j} M_L M_S : \vec{X}), \tag{8}$$

where $\vec{X} = \vec{X}_1, \ldots, \vec{X}_{N+1}$ with $\vec{X}_i$ denoting the space and spin coordinates of the ith electron; $\alpha_j L_j S_j$ specify the final state of the residual ion; $k_j l_j$ are the quantum numbers of the ejected electron; $m(l_j) \equiv m_{l_j}$ for typographical convenience; and we define

$$\mathcal{Y}_l^{m_l}(\hat{k}) = i^l Y_l^{m_l}(\hat{k}), \tag{9}$$

where $Y_l^{m_l}(\hat{k})$ is the spherical harmonic defined by $Y_l^{*m_l}(\hat{k}) = (-1)^m Y_l^{-m_l}(\hat{k})$. The orbital angular momentum of the final state of the residual ion, L_j, is coupled with the angular momentum of the ejected electron, l_j, to give the total angular momentum L. Similarly, the spin angular momentum S_j is coupled with the spin of the ejected electron to give the total spin S. The magnetic projections of L and S are M_L and M_S, respectively. The $N+1$ electron wave function defined by Eq. (8) is a totally antisymmetric eigenstate of L^2, S^2, M_L, M_S, and parity π. For notational convenience, we define

$$\Psi_j^{(-)}(\vec{X}) = \Psi(\alpha_j L_j S_j k_j l_j LS\pi; M_{L_j} M_{S_j} m_{l_j} M_L M_S : \vec{X}). \tag{10}$$

Asymptotically, $\Psi_j^{(-)}$ is defined by

$$\Psi_j^{(-)}(\vec{X}) \underset{r_{N+1}\to\infty}{\sim} \frac{1}{2} \sum_i \Phi_i (\delta_{ij} e^{i\theta_i} - e^{-i\theta_i} S_{ij}^\dagger) \frac{1}{r_{N+1}(\pi k_i)^{1/2}}, \tag{11}$$

where

$$\Phi_i = \sum_{M(L_i) m(l_i) M(S_i) m_{1/2}} \Phi(\vec{X}_1 \cdots \vec{X}_N; L_i S_i M_{L_i} M_{S_i}) \mathcal{Y}_{l_i}^{m(l_i)}(\hat{r}_{N+1}) \, \sigma^{m_{1/2}}(N+1) C(L_i l_i L; M_{L_i} m_{l_i} M_L)$$
$$\times C(S_i \tfrac{1}{2} S; M_{S_i} m_{1/2} M_S). \tag{12}$$

Here $\Phi(\vec{X}_1 \cdots \vec{X}_N; L_i S_i M_{L_i} M_{S_i})$ is the wave function of the final state of the residual ion A^+ and $S_{ij}^\dagger$ is the adjoint of the scattering matrix. The quantity θ_i is defined by

$$\theta_i = k_i r - \tfrac{1}{2} l_i \pi - [(Z - N)/k_i] \ln(2k_i r)$$
$$+ \arg\{\Gamma[l_i + 1 - i(Z - N)/k_i]\}, \tag{13}$$

where Z is the nuclear charge of A. The asymptotic form of $\Psi_j^{(-)}(\vec{X})$ in Eq. (11) is consistent with the normalization specified by Eq. (6).

Now, let us define a function $\Psi_j(\vec{X})$ which satisfies standing-wave boundary conditions, i.e.,

$$\Psi_j(\vec{X}) \underset{r_{N+1}\to\infty}{\sim} \sum_i \Phi_i (\sin\theta_i \delta_{ij} + \cos\theta_i K_{ij}) \frac{1}{r_{N+1}(k_i)^{1/2}}, \tag{14}$$

where $\underline{K}$ is the reactance matrix and

$$\underline{K} = i(\underline{I} - \underline{S})(\underline{I} + \underline{S})^{-1}. \tag{15}$$

The transformation relating $\Psi_j^{(-)}(\vec{X})$ to $\Psi_j(\vec{X})$ is

$$\Psi_i^{(-)}(\vec{X}) = \left(\frac{1}{\pi} \right)^{1/2} \sum_j \Psi_j(\vec{X}) (I + iK)_{ji}^{-1}. \tag{16}$$

In the calculations described in Sec. III, we will approximate $\Psi_j(\vec{X})$ by a close-coupling wave function. Now that we have established the connection between $\Psi_j^{(-)}(\vec{X})$ and $\Psi_j(\vec{X})$, we can evaluate the form factor of Eq. (7) and thus the triple differential cross section.

Substituting Eq. (8) into Eq. (7) and making use of conventional Racah algebra relations, we obtain the following expression for the triple differential ionization cross section:

$$\frac{d^3\sigma}{d\omega\, d\omega_E\, dE} = \frac{4k_f}{K^4 k_0}\frac{1}{2L_0+1}\frac{1}{\sqrt{4\pi}}\sum_{LS_0\pi}\sum_{L'S_0\pi'}\sum_{l_j l_j'}\sum_{\lambda\lambda' l}(2\lambda+1)(2\lambda'+1)Y_l^0(\hat{k})(-1)^{l_j+l_j'+L_0}$$
$$\times\left(\frac{(2L'+1)(2L+1)(2l_j+1)(2l_j'+1)}{2l+1}\right)^{1/2}C(l_jl_j'l;000)$$
$$\times\left\langle\Psi_j^{(-)}\middle\|\sum_q j_\lambda(Kr_q)C^\lambda(\hat{r}_q)\middle\|\Phi_0\right\rangle\left\langle\Phi_0\middle\|\sum_q j_{\lambda'}(Kr_q)C^{\lambda'}(\hat{r}_q)\middle\|\Psi_j'^{(-)}\right\rangle$$
$$\times W(L'Ll_j'l_j;lL_j)W(\lambda\lambda'LL';lL_0)C(\lambda\lambda'l;000). \tag{17}$$

This expression is identical to that derived by Jacobs[5]; however, we have retained explicitly the possibility of different residual ionic-state spins S_t in Eq. (12). Further, our notation is consistent with our generally available computer codes.[6,7] If we integrate Eq. (17) over the solid angles of the two continuum electrons we have the following expression for the differential cross section with respect to the ejected electron energy:

$$\frac{d\sigma}{dE} = \int_{K_{\min}}^{K_{\max}}\frac{8\pi dK}{K^3k_0^2}\sum_{LS_0\pi,l_j\lambda}\frac{2\lambda+1}{2L_0+1}$$
$$\times\left|\left\langle\Psi_j^{(-)}(E)\middle\|\sum_q j_\lambda(Kr_q)C^\lambda(\hat{r}_q)\middle\|\Phi_0\right\rangle\right|^2. \tag{18}$$

The values of $K_{\min}$ and $K_{\max}$ are defined by

$$K_{\min}=k_0-k_f\,,\quad K_{\max}=k_0+k_f\,, \tag{19}$$

where

$$k_f^2=k_0^2-I-E.$$

Again, the units of the cross section σ are a_0^2, E is the ejected electron energy in Rydbergs, and I is the ionization potential of the atom in Rydbergs. This expression integrated over the ejected electron energy yields the total cross section,

$$\sigma(k_0^2)=\frac{8\pi}{k_0^2}\int_0^{k_0^2-I}dE\int_{K_{\min}}^{K_{\max}}\frac{dK}{K^3}\sum_{LS_0\pi,l_j\lambda}\frac{2\lambda+1}{2L_0+1}$$
$$\times\left|\left\langle\Psi_j^{(-)}(E)\middle\|\sum_q j_\lambda(Kr_q)C^\lambda(\hat{r}_q)\middle\|\Phi_0\right\rangle\right|^2. \tag{20}$$

TABLE I. Continuum generalized oscillator strengths for helium $\Phi(1s^2)\to\Psi^-$ (static exchange) using calculated $E_{\text{ionization}}=0.75$ a.u. Results using identical wave functions and physical approximations, but completely different numerical techniques and independent computer codes: (a) R-matrix calculations; (b) NIEM calculations.

	k^2						
K^2	0.05	0.2	0.6	1.0	2.0	4.0	6.0
0.01	(a)0.2866	0.3014	0.3176	0.3125	0.2624	0.1545	0.0893
	(b)0.2862	0.3005	0.3172	0.3128	0.2625	0.1546	0.0893
0.04	(a)0.2812	0.2966	0.3147	0.3112	0.2631	0.1559	0.0902
	(b)0.2808	0.2957	0.3143	0.3115	0.2633	0.1559	0.0902
0.09	(a)0.2723	0.2887	0.3098	0.3088	0.2642	0.1580	0.0917
	(b)0.2720	0.2879	0.3093	0.3090	0.2644	0.1581	0.0917
0.16	(a)0.2603	0.2779	0.3027	0.3052	0.2656	0.1610	0.0938
	(b)0.2601	0.2773	0.3024	0.3054	0.2658	0.1611	0.0939
0.25	(a)0.2456	0.2645	0.2935	0.3002	0.2669	0.1648	0.0965
	(b)0.2455	0.2640	0.2932	0.3003	0.2671	0.1648	0.0966
0.36	(a)0.2288	0.2488	0.2821	0.2936	0.2680	0.1693	0.0998
	(b)0.2287	0.2484	0.2820	0.2936	0.2681	0.1692	0.0999
0.49	(a)0.2104	0.2312	0.2686	0.2850	0.2684	0.1743	0.1037
	(b)0.2104	0.2309	0.2686	0.2850	0.2686	0.1743	0.1038
1.0	(a)0.1517	0.1726	0.2175	0.2474	0.2626	0.1913	0.1189
	(b)0.1518	0.1725	0.2179	0.2474	0.2627	0.1913	0.1190
4.0	(a)0.0272	0.0339	0.0539	0.0768	0.1323	0.1904	0.1737
	(b)0.0272	0.0339	0.0542	0.0768	0.1324	0.1904	0.1737

Finally we can write down the expression for the generalized oscillator strength to the continuum,

$$f(K)=\frac{I+E}{K^2}\sum_{LS_0\pi,l_j\lambda}\frac{2\lambda+1}{2L_0+1}\times\left|\left\langle\Psi_j^{(-)}(E)\right\|\sum_q j_\lambda(Kr_q)C^\lambda(\hat{r}_q)\left\|\Phi_0\right\rangle\right|^2. \quad (21)$$

III. RESULTS

The most complete theoretical study of electron-impact ionization for a target system in which approximate wave functions must be used has been for helium and heliumlike ions.[5,8-10] In addition, there are accurate experimental determinations of generalized oscillator strengths[11] for neutral helium.

So we propose to test our computer codes and choice of wave functions for the helium atom, since such rigorous comparison is available.

A. Static exchange plus crude closed-shell approximation

In this case we take the ground-state ^1S wave function for the helium atom to have the single-configuration representation of $1s^2$. Further, we take the radial orbital function $P_{1s}(r)$ to be that of He$^+$. This allows us to use the correct $e^-+\mathrm{He}^+(1s)$ static-exchange final-state wave function, and to easily maintain the orthonormality of the initial- and final-state wave functions. We have computed the generalized oscillator strength to the continuum, using Eq. (21), for a wide range of values of momentum transfer K and ejected electron energy k^2. Values obtained using both the NIEM and R-matrix codes are tabulated in Table I, and the excellent numerical agreement between them is obvious. Naturally, the results in this approximation are not expected to be good due to the crudeness of the target-state wave function, but it is useful to have an idea of the effect on the final results of using poor wave functions.

TABLE II. Overlap integrals for the S-wave continuum and bound-state wave functions.

k^2_{ejected}	$\langle\Phi_0\|\Psi_j(^1S)\rangle$
0.05	0.0201
0.20	0.0118
0.60	0.0294
1.00	0.0040
2.00	0.0042
4.00	0.0064
6.00	0.0033

B. Static exchange plus correlation and correlated atomic state

In this case we have used the four-configuration wave function of Burke and Robb[12] to describe the atomic ^1S state. This $\Phi_0(c_1 1s^2+c_2 1s\overline{2s}+c_3\overline{2s}^2+c_4\overline{2p}^2)$ function uses the He$^+$ $1s$ orbital and $\overline{2s}$ and $\overline{2p}$ orbitals which are optimized on the target-state energy. The continuum-state wave functions had the following static exchange plus correlation form:

$$\begin{aligned}\Psi_j(^1S)&=\mathcal{A}\phi(1s)\psi(k_js)+a_1\chi_1(1s^2)+a_2\chi_2(1s\overline{2s})\\&\quad+a_3\chi(\overline{2s^2})+a_4\chi(\overline{2p^2}),\\\Psi_j(^1P)&=\mathcal{A}\phi(1s)\psi(k_jp)+b_1\chi_1(1s\overline{2p})+b_2\chi_2(\overline{2s}\,\overline{2p}),\\\Psi_j(^1D)&=\mathcal{A}\phi(1s)\psi(k_jd)+c_1\chi_1(\overline{2p^2}),\\\Psi_j(^1F)&=\mathcal{A}\phi(1s)\psi(k_jf).\end{aligned} \quad (22)$$

In (22) the $\psi(k_jl)$ are continuum orbitals which are orthogonal to the $1s$, $\overline{2s}$, and $\overline{2p}$ orbitals for $l=0$ and 1, respectively. Further, the coefficients a_i, $i=1,4$ of $\Psi_j(^1S)$ are obtained in the solution of the close-coupling equation and subsequently adjusted by Schmidt orthogonalization to ensure that

$$\langle\Psi_j(^1S)|\Phi_0(^1S)\rangle=0. \quad (23)$$

As an illustration of the size of the S-wave overlap before Schmidt orthogonalization, we give values for various k_j^2 in Table II.

In Table III we present the values of the general-

TABLE III. Continuum generalized oscillator strengths for helium $\Phi(c_1 1s^2+c_2 1s\overline{2s}+c_3\overline{2s}^2+c_4\overline{2p}^2)\rightarrow\Psi$ (static exchange plus some correlation) using exact $E_{\mathrm{ionization}}=0.904\,85$ a.u., NIEM calculations.

	k^2						
K^2	0.05	0.2	0.6	1.0	2.0	4.0	6.0
0.01	0.9070	0.8633	0.6078	0.4219	0.2100	0.0854	0.0310
0.04	0.8843	0.8478	0.6123	0.4297	0.2145	0.0843	0.0317
0.09	0.8481	0.8221	0.6176	0.4416	0.2223	0.0866	0.0329
0.16	0.8002	0.7864	0.6204	0.4555	0.2334	0.0904	0.0346
0.25	0.7428	0.7417	0.6178	0.4691	0.2477	0.0954	0.0368
0.36	0.6785	0.6897	0.6073	0.4800	0.2649	0.1016	0.0397
0.49	0.6097	0.6321	0.5879	0.4858	0.2842	0.1091	0.0431
1.0	0.4009	0.4445	0.4817	0.4585	0.3396	0.1412	0.0571
4.0	0.0447	0.0565	0.0852	0.1134	0.1943	0.2578	0.1405

TABLE IV. Reduced-matrix elements, static exchange plus four-correlation terms, and four-term CI initial state.

		k^2							
		0.05		1.0		4.0		6.0	
K^2		Reβ [a]	Imβ	Reβ	Imβ	Reβ	Imβ	Reβ	Imβ
0.01	*s*	0.0019	−0.0008	0.0005	−0.0002	0.0017	−0.0023	0.0002	0.0000
	p	0.0402	0.0030	0.0222	0.0017	0.0068	0.0000	0.0024	0.0027
	d	0.0012	0.0000	0.0012	0.0000	0.0003	0.0000	0.0002	0.0000
	f	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.09	*s*	0.0239	−0.0099	0.0105	−0.0039	0.0030	−0.0041	0.0014	−0.0004
	p	0.1150	0.0085	0.0668	0.0052	0.0206	0.0001	0.0074	0.0082
	d	0.0102	0.0000	0.0106	0.0000	0.0028	−0.0000	0.0014	0.0000
	f	0.0003	0.0000	0.0013	0.0000	0.0003	0.0000	0.0001	0.0000
0.25	*s*	0.0623	−0.0258	0.0307	−0.0114	0.0059	−0.0080	0.0038	−0.0010
	p	0.1748	0.0128	0.1104	0.0085	0.0351	0.0002	0.0126	0.0141
	d	0.0251	0.0000	0.0272	0.0001	0.0076	0.0000	0.0041	−0.0001
	f	0.0014	0.0000	0.0053	0.0000	0.0015	0.0000	0.0007	0.0000
0.49	*s*	0.1085	−0.0449	0.0599	−0.0222	0.0105	−0.0144	0.0076	−0.0020
	p	0.2142	0.0157	0.1504	0.0116	0.0506	0.0004	0.0183	0.0205
	d	0.0497	0.0001	0.0476	0.0002	0.0148	−0.0001	0.0083	0.0002
	f	0.0036	0.0000	0.0121	0.0000	0.0039	0.0000	0.0019	0.0000
1.00	*s*	0.1733	−0.0717	0.1139	−0.0422	0.0214	−0.0292	0.0162	−0.0043
	p	0.2333	0.0172	0.1955	0.0151	0.0761	0.0005	0.0279	0.0312
	d	0.0561	0.0000	0.0762	0.0003	0.0308	−0.0002	0.0175	−0.0005
	f	0.0075	0.0000	0.0243	0.0000	0.0112	0.0000	0.0058	0.0000
4.00	*s*	0.2061	−0.0852	0.2114	−0.0784	0.1003	−0.1369	0.0802	−0.0212
	p	0.1181	0.0087	0.1625	0.0126	0.1616	0.0011	0.0602	0.0673
	d	0.0291	0.0000	0.0720	0.0003	0.0989	−0.0005	0.0744	−0.0020
	f	0.0042	0.0000	0.0266	0.0000	0.0553	0.0001	0.0430	0.0001

[a] $\beta \equiv \langle \Psi_j^{(-)}(E) || \sum_q j_\lambda (K r_q) C^\lambda (\hat{r}_q) || \Psi_0 \rangle$.

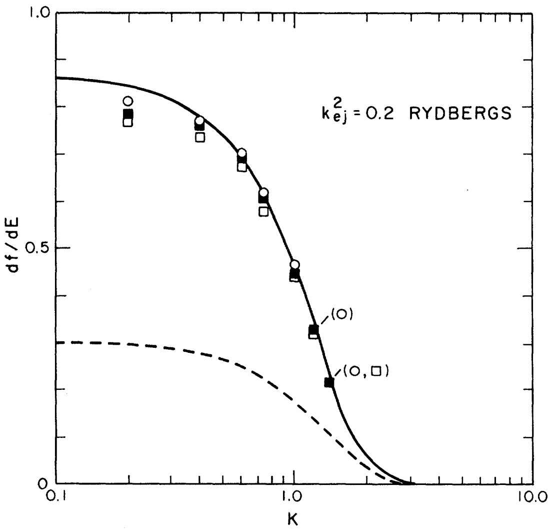

FIG. 1. Continuum generalized oscillator strength for helium vs momentum transfer for ejected electron energy equal to 0.2 Ry. Solid curve, present work, Φ_0(CI); dashed curve, present work $\Phi_0(1s^2)$; □ values, Jacobs (Ref. 5); ■ values, interpolated from Oldham (Ref. 8); O values, interpolated from Bell and Kingston (Ref. 9).

ized oscillator strengths in this approximation. All of these numbers were obtained from the NIEM code, since the numerical quality of $\Psi_j(^1P)$ was poor for the R-matrix method. Computer resources did not allow us to improve this calculation. However, the R-matrix and NIEM values of the $\pi L S_0 = {}^1S^e$, ${}^1D^e$, ${}^1F^o$ contributions to the summation in Eq. (21) were in agreement to better than

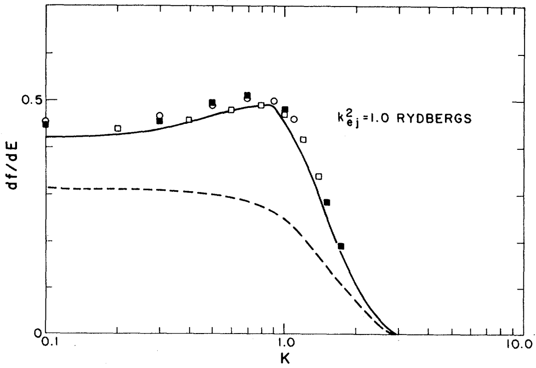

FIG. 2. Same as Fig. 1 except that the ejected electron energy is 1.0 Ry.

TABLE V. Triple differential cross section for ionization of helium.

Single configuration—static exchange				Four configuration—static exchange plus correlation			
θ (deg)	$\frac{d^3\sigma}{d\omega d\omega_E dE}$	θ (deg)	$\frac{d^3\sigma}{d\omega d\omega_E dE}$	θ (deg)	$\frac{d^3\sigma}{d\omega d\omega_E dE}$	θ (deg)	$\frac{d^3\sigma}{d\omega d\omega_E dE}$
0	0.331	180	0.540	0	0.646	180	1.382
10	0.217	190	0.312	10	0.456	190	0.760
20	0.114	200	0.141	20	0.262	200	0.317
30	0.037	210	0.037	30	0.099	210	0.072
40	0.001	220	0.007	40	0.008	220	0.003
50	0.022	230	0.024	50	0.041	230	0.069
60	0.110	240	0.093	60	0.242	240	0.220
70	0.267	250	0.192	70	0.639	250	0.410
80	0.483	260	0.304	80	1.223	260	0.603
90	0.737	270	0.416	90	1.946	270	0.777
100	0.997	280	0.516	100	2.713	280	0.919
110	1.226	290	0.594	110	3.405	290	1.022
120	1.386	300	0.646	120	3.900	300	1.086
130	1.451	310	0.666	130	4.104	310	1.110
140	1.410	320	0.653	140	3.976	320	1.095
150	1.270	330	0.609	150	3.543	330	1.040
160	1.055	340	0.536	160	2.886	340	0.946
170	0.798	350	0.441	170	2.125	350	0.814

1%. In Table IV we give the partial-wave contributions to the reduced-matrix element in Eq. (21) for a range of momentum transfer and ejected electron energy.

In Figs. 1 and 2 we plot the present results against previous calculations, for ejected electron energies of $k_j^2=0.2$ and 1.0 Ry. Oldham[8] used a Hartree-Fock-type wave function for the atomic state, while Bell and Kingston[9] and Jacobs[5] used elaborate Hylleraas-type wave functions. It is interesting to note the severe error in the final result when one uses a really crude target-state wave function. We would expect that our correlated calculation would lie closest to the calculation of Jacobs.[5] This is indeed so, although all of these calculations agree extremely well. For $k_j^2=0.2$ Ry (Fig. 1) there is a significant difference between our results and Jacobs for low momentum transfer. This is probably due to the combined effect of the lack of orthogonality of Jacobs's S-wave functions and the slightly inferior nature of our $\Phi_0(c_1 1s^2+c_2 1s\overline{2s}+c_3\overline{2s}^2+c_4\overline{2p}^2)$ function.

Finally, in Fig. 3 we compare our triple differential cross section with that of Jacobs. Also shown in this plot are the experimental data of Ehrhardt *et al.*[13] For completeness we present our numerical values, for both calculations, in Table V. In the momentum-transfer direction our results are in good agreement with Jacobs, but the agreement is poor about the recoil peak. This discrepancy is due to a combination of the following facts: (i) In lieu of orthogonalizing the continuum s state to the initial target state, Jacobs includes the nuclear potential term. The corresponding states in the present work are constrained to be orthogonal. (ii) The initial-state wave function used by Jacobs is better than ours; however, our final-state wave function gives better $e^-+\mathrm{He}^+$

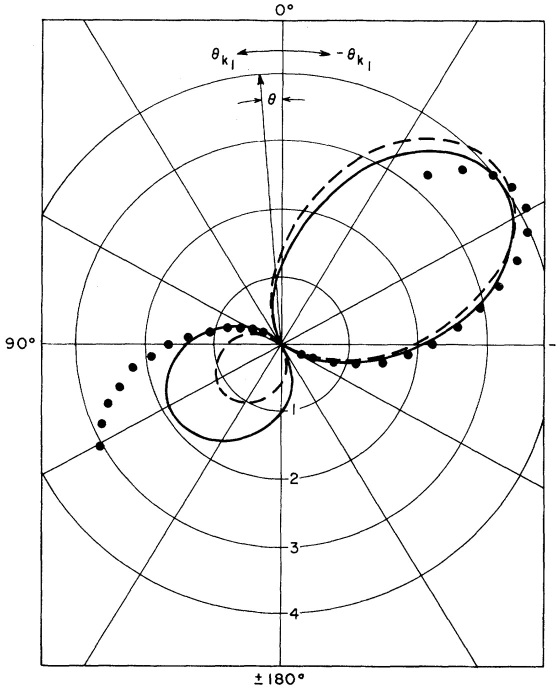

FIG. 3. Triple differential cross section for helium for a 256.5-eV incident electron energy, a scattering angle $\theta=4°$, and an ejected electron energy of 3.0 eV. Solid curve, Jacobs (Ref. 5); dots, experimental results of Ehrhardt *et al.* (Ref. 13); dashed line, present work with Φ_0(CI).

scattering phase shifts than his. (iii) There is no guarantee that the triple differential cross section will get better with improvement of the wave functions. This last point is clearly demonstrated by the fact that our single-configuration–static-exchange calculation gives a poor generalized oscillator strength, but gives a forward-peak–to–backward-peak ratio (see Table V) for the corresponding triple differential cross section which is in better agreement with experiment than the ratio obtained by Jacobs.

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