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Low-Energy Photo-Ionization of the 1^1S and 2^1S States of He†

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The photo-ionization cross sections of the 1^1S and 2^1S states of He were evaluated in the energy regions 0.20–2.40 Ry and 3.15–3.30 Ry. The 56-term ^1S bound-state wave functions obtained by Pekeris were used for the initial states. An expansion into a complete discrete basis set (a modification of the close-coupling method used in electron-atom scattering) was carried out for the ^1P final-state continuum wave functions. Particular attention was given to the processes where the ejected photoelectron leaves the He^+ ion in an $n=2$ excited state. The results obtained from the length and velocity expressions for the photo-ionization cross sections show an agreement to within 1% in the lower-energy region. Good accuracy is achieved for the negative-power moments of the oscillator-strength distributions.

I. INTRODUCTION

Although the photo-ionization of He has been the subject of extensive theoretical investigations for over thirty years,[1] the emphasis in the earlier calculations[2–4] has been primarily on the ordinary photo-ionization process where the ejected photoelectron leaves the residual He^+ ion in its ground state. The availability of improved far-ultraviolet absorption-spectroscopy techniques enabled Madden and Codling[5,6] to make systematic observations of double-electron excitation processes in the continuous absorption spectrum of He. They identified several Rydberg series of ^1P doubly excited states which converge onto the $n=2$, 3, and 4 excitation thresholds of He^+ (ionization thresholds of He). These observations stimulated detailed theoretical calculations of the He photo-ionization spectrum below the $n=2$ threshold by Burke and McVicar[7] and by Altick and Moore.[8] Quite elaborate wave functions for both the initial and final states of the two-electron system were used in these calculations. The doubly excited (resonance) states of He below the $n=2$ excitation threshold of He^+ were thoroughly investigated. There is now renewed interest in the double-electron excitation processes just above the $n=2$ threshold as a result of Samson's recent measurement[9] of the partial photo-ionization cross section for the processes in which the residual He^+ ion is left in an $n=2$ excited state.

This paper presents some accurate calculations of the He photo-ionization cross sections for incident photon energies in the nonresonant regions below the $n=2$ threshold and between the $n=2$ and $n=3$ thresholds. The partial photo-ionization cross sections for the processes where the residual He^+ ion is left in the $1s$, $2s$, and $2p$ states are evaluated and compared with Samson's experimental results. Less accurate calculations are carried out at higher energies. These calculations are based on an independent-particle approximation for the continuum states, and they enable an evaluation of the oscillator-strength sum rules to be made.

We also consider the photo-ionization of the He 2^1S metastable state, where the partial photo-ionization cross sections for the transitions to the $n=2$ excited states of the ion are an order of magnitude larger than the partial photo-ionization cross section for the transition in which the ion is left in its ground state. No experimental results for the photo-ionization of He in the 2^1S state are available at the present time. Pearl,[10] however, has recently reported an experimental value of $(38 \pm 8) \times 10^{-3}$ sec for the lifetime of the He 2^1S state.

II. FINAL-STATE CONTINUUM WAVE FUNCTION

The major effort in our calculations is associated with the difficulty in obtaining accurate continuum wave functions for the final states of the two-electron system in the photo-ionization process. This task is simplified considerably by restricting our primary interest to an energy region where only a few singly ionized final states are energetically accessible. In this section, we focus our attention on the electron scattering by the residual He^+ ion. This scattering is described by the final states in the photo-ionization of He. Although the main emphasis in our discussion of e^-–He^+ scattering will be on the asymptotic region of the wave function, we are motivated by the need to obtain a reasonably accurate representation of the inner region of the wave function.

The ^1P two-electron states in the continuum can be expanded in a complete orthonormal basis $S_{nl_1}(r_1)$ with undetermined functions $F_{\mu\nu}(r_2)$ as expansion coefficients in the form

$$\psi_{\nu,E}(\vec{r}_1, \vec{r}_2) = \frac{(1+P_{12})}{\sqrt{2}} \sum_{\mu=nl_1l_2} \frac{S_{nl_1}(r_1)}{r_1} \frac{F_{\mu\nu}(r_2)}{r_2} \times \sum_{m_1m_2} \langle l_1 l_2 L M_L | l_1 m_1 l_2 m_2 \rangle Y_{l_1}^{m_1}(\hat{r}_1) Y_{l_2}^{m_2}(\hat{r}_2) , \tag{1}$$

where P_{12} interchanges the spatial coordinates of the two electrons. The index ν specifies the independent energetically accessible continuum states (open channels) at the given total energy E. We require only the continuum states with total orbital angular momentum $L = 1$ ($M_L = 0$), because only this single partial wave gives a nonvanishing contribution to the dipole photo-ionization cross sections of the ^1S states.

In electron-scattering calculations, the expansion basis is usually restricted to include only the first few discrete eigenstates of the target (He$^+$ ion in our discussion) Hamiltonian. This approach, originally introduced by Massey and Mohr,[11] goes under the name of "close-coupling" and has considerable intuitive appeal. However, extensive numerical calculations by Burke and his co-workers[12] have demonstrated that the expansion in target eigenstates is very slowly convergent, especially for excitation cross sections.[13] The slow convergence of the target eigenstate expansion is associated with the difficulty of representing the contributions from the continuum target eigenstates in a numerical calculation. In recent calculations of elastic positron-hydrogen scattering by Rotenberg[14] and Perkins,[15] and of elastic electron-hydrogen scattering by Burke, Gallaher, and Geltman,[16] only the first few bound target eigenstates were retained, while the remaining contributions were represented by states selected from a certain complete discrete basis set.

It is natural for the expansion Eq. (1) to contain the target eigenstates corresponding to the open channels.[17] This automatically ensures that the trial wave function will have the correct asymptotic behavior, provided the open-channel functions $F_{\mu\nu}(r_2)$ (for $k_\mu^2 > 0$) satisfy the boundary conditions

$$F_{\mu\nu}(r_2) \xrightarrow[r_2\to\infty]{} [1/(\pi k_\mu)^{1/2}](\sin\theta_\mu \delta_{\mu\nu} + \cos\theta_\mu K_{\mu\nu}) \quad , \tag{2}$$

where $K_{\mu\nu}$ is the reactance matrix.[13] The asymptotic phase θ_μ is given by

$$\theta_\mu = k_\mu r_2 - l_2\pi/2 + [(Z-1)/k_\mu]\ln 2k_\mu r_2 + \arg\{l_2 + 1 - i[(Z-1)/k_\mu]\} \ . \tag{3}$$

The nuclear charge Z equals 2 in the present case. k_μ is the wave number in the open channel $\mu = nl_1l_2$ and is defined by

$$k_\mu^2 \equiv 2E + Z^2/n^2 \ (E \text{ in a.u.}) \ . \tag{4}$$

We employ a modified expansion basis which includes only the He$^+$ eigenstates corresponding to open channels. Contributions from higher bound and continuum He$^+$ eigenstates are represented by independent functions selected from either of the two discrete radial basis sets $r^n e^{-\alpha r}$ and $r^{l_1+1}e^{-\alpha(n-l_1)r}$, which are complete for any value of the parameter α.[18] The desired complete discrete expansion basis $S_{nl_1}(r_1)$ is obtained by orthogonalizing the independent functions to each other and to the He$^+$ eigenstates included:

$$\int_0^\infty S_{nl_1}(r_1) S_{n'l_1}(r_1) dr_1 = \delta_{nn'} \quad . \tag{5}$$

In our calculations, $1s$, $\bar{2}s$, $\bar{2}p$ and $1s$, $2s$, $2p$, $\bar{3}s$, $\bar{3}p$ expansions were carried out for the energy regions below the $n = 2$ threshold and between the $n = 2$ and $n = 3$ thresholds, respectively. (The notation $\bar{n}l_1$ will be used throughout this paper to indicate the expansion states which are not He$^+$ eigenstates.) The independent function r^2e^{-Zr} was used to construct the $\bar{2}s$, $\bar{2}p$, $\bar{3}s$, and $\bar{3}p$ states. These closed-channel states are given in Table I. The $1s$ and $\bar{2}s$ (or $\bar{3}s$) states are members of the complete discrete basis set $r^n e^{-Zr}$, while the $2p$ and $\bar{3}p$ states are members of the complete discrete basis set $r^{l_1+1}e^{-0.5Z(n-l_1)r}$. Our choice for the $\bar{2}p$ state differs from that of Burke, Gallaher, and Geltman,[16] who follow the suggestion made by Damburg and Karule.[19] Their motivation was to take into account the fact that low-energy electron scattering is strongly influenced by the long-range polarization potential $\alpha_1 r^{-4}$. Their $\bar{2}p$ state gives the full dipole polarizability of the hydrogen atom ground state, replacing the infinite summation over intermediate p states in the expression for α_1.

Our computational procedures are identical to those used by Burke, Gallaher, and Geltman,[16] once the expansion basis $S_{nl_1}(r_1)$ has been selected. Our limited expansion basis automatically diagonalizes the matrix representation of the one-electron Hamiltonian:

$$\int_0^\infty S_{nl_1}(r_1)\left[\frac{d^2}{d^2r_1} - \frac{l_1(l_1+1)}{r_1^2} + \frac{2Z}{r_1}\right] S_{n'l_1}(r_1)dr_1 = -2\epsilon_{nl_1}\delta_{nn'} \quad . \tag{6}$$

TABLE I. Expansion states $S_{nl_1}(r)$ which are not eigenstates of the one-electron Hamiltonian.

$S_{nl_1}(r)$	$\epsilon_{nl_1}(Z=2)$ a.u.
$\bar{2}s = -4(Z^5/3)^{1/2}[r^2 - (3/2Z)r]e^{-Zr}$	0.666 667
$\bar{2}p = -2(Z^5/3)^{1/2} r^2 e^{-Zr}$	0
$\bar{3}s = -\{11664Z^5/[2187 - 8192 \times (1 - 8/3Z)^2]\}^{1/2}\{r^2e^{-Zr} - (3/2Z)re^{-Zr} - (16/81Z^2) \times (3Z-8)[r - (Z/2)r^2]e^{-Zr/2}\}$	1.498 39
$\bar{3}p = -[(78732Z^5/26281)]^{1/2}r^2 \times [e^{-Zr} - (32/243)e^{-Zr/2}]$	0.623 416

This simplifies the numerical procedures. The energies ϵ_{nl_1} equal $-Z^2/2n^2$ only for the He$^+$ eigenstates. The closed-channel functions $F_{\mu\nu}(r_2)$[corresponding to the expansion states $S_{nl_1}(r_1)$ which are not eigenstates of the one-electron Hamiltonian] are obtained subject to boundary conditions which represent exponentially decaying waves:

$$F_{\mu\nu}(r_2)\xrightarrow[r_2\to\infty]{}\exp\{-|k_\mu|r_2+[(Z-1)/|k_\mu|]\ln 2|k_\mu|r_2\} \quad . \tag{7}$$

The closed-channel states used in our calculations have effective energies ϵ_{nl_1} (see Table I) which satisfy the conditions

$$k_\mu^2\equiv 2(E-\epsilon_{nl_1})<0 \quad , \tag{8}$$

over the energy range of interest. The constraints given by Eq. (8) are required by the boundary conditions of Eq. (7).

The appropriate form of the Kohn variational principle is

$$\delta[\langle\psi_{\nu,E}|H-E|\psi_{\nu',E}\rangle-(K_{\nu\nu'}/2\pi)]=0 \quad , \tag{9}$$

where the variation δ is taken with respect to the expansion functions $F_{\mu\nu}(r_2)$, subject to the boundary conditions at infinity given by Eqs. (2) and (7) and the required behavior at the origin:

$$F_{\mu\nu}(r_2)\xrightarrow[r_2\to 0]{} r_2^{l_2+1} \quad (\text{for all } \mu) \quad . \tag{10}$$

Carrying out the indicated variation results in a set of coupled integrodifferential equations for the functions $F_{\mu\nu}(r_2)$:

$$\left(\frac{d^2}{dr_2^2}-\frac{l_2(l_2+1)}{r_2^2}+\frac{2Z}{r_2}+k_\mu^2\right)F_{\mu\nu}(r_2)$$
$$=\sum_{\mu'}\left[V_{\mu\mu'}(r_2)F_{\mu'\nu}(r_2)+\int_0^\infty W_{\mu\mu'}(r_2,r_2')F_{\mu'\nu}dr_2'\right] . \tag{11}$$

The quantities V and W are given in detail by Burke, Gallaher, and Geltman.[16] The functions $F_{\mu\nu}(r_2)$ were obtained using the computer code of Burke, which proceeds essentially according to the method described by Burke and Schey,[20] except that the exchange integral terms are represented by additional coupled differential equations which are solved simultaneously with those for the functions $F_{\mu\nu}(r_2)$.

The continuum states $\psi_{\nu,E}$, with functions $F_{\mu\nu}(r_2)$ having the asymptotic behavior given by Eq. (2), do not correspond to the correct physical final states in the photo-ionization process. Formal considerations have established that the final states should be represented by the incoming wave modification $\psi_{\nu,E}^{(-)}$.[21] The corresponding functions $\bar{F}_{\mu\nu}(r_2)$ have the asymptotic behavior

$$\bar{F}_{\mu\nu}(r_2)\xrightarrow[r_2\to\infty]{}[i/2(\pi k_\mu)^{1/2}[e^{-i\theta_\mu}S_{\mu\nu}^{+}-e^{i\theta_\mu}\delta_{\mu\nu}] \quad . \tag{12}$$

After introducing the real orthogonal matrix U which diagonalizes both the scattering matrix S and the reactance matrix K:

$$(U^TSU)_{\mu\nu}=e^{2i\eta_\mu}\delta_{\mu\nu} \quad , \tag{13}$$

$$(U^TKU)_{\mu\nu}=\tan\eta_\mu\delta_{\mu\nu} \quad , \tag{14}$$

the required states $\psi_{\nu,E}^{(-)}$ are obtained by transforming the functions $F_{\mu\nu}(r_2)$ according to

$$\bar{F}_{\mu\nu}(r_2)=\sum_{\alpha\beta}F_{\mu\alpha}(r_2)U_{\alpha\beta}e^{-i\eta_\beta}\cos\eta_\beta U_{\nu\beta} \quad . \tag{15}$$

The states $\psi_{\nu,E}^{(-)}$ now have the normalization per unit Ry energy adopted in the photo-ionization calculation:

$$\langle\psi_{\nu,E}^{(-)}|\psi_{\nu',E'}^{(-)}\rangle=\delta_{\nu\nu'}\delta(E-E') \quad . \tag{16}$$

The eigenphases η_μ, defined as the arctangents of the diagonalized K matrix, cannot be associated exclusively with any particular channel and have no direct physical meaning. It has been rigorously established[22–24] that these eigenphases increase monotonically toward their exact values with the successive enlargement of the expansion basis $S_{nl_1}(r_1)$, provided all target eigenstates corresponding to the open channels are included in the trial function. This minimum principle is of considerable practical importance in the numerical calculations, even though it does not provide any assurance that the cross sections of interest are improved with the addition of more expansion states.

The minimum principle is well illustrated by comparing our values for the P wave e^-–He$^+$ elastic scattering phase shift, evaluated with the $1s$, $\bar{2}s$, $\bar{2}p$ expansion, with the corresponding values obtained by Burke and McVicar[7] using a $1s$, $2s$, $2p$ target eigenstate expansion (see Table II). We conclude that the expansion states selected from a

TABLE II. P wave e^-–He$^+$ elastic scattering phase shift η evaluated in the nonresonant region below $n=2$ threshold using He$^+$ eigenstate expansion and complete discrete expansion.

k_1^2(Ry)	$\eta(1s, 2s, 2p)$(Ref. 7)	$\eta(1s, \bar{2}s, \bar{2}p)$
0.2	−0.0605	−0.0464
0.4	−0.0631	−0.0485
0.6	−0.0641	−0.0490
0.8	−0.0636	−0.0482
1.0	−0.0622	−0.0466
1.2	−0.0600	−0.0441
1.4	−0.0571	−0.0410
1.6	−0.0536	−0.0373
1.8	−0.0495	−0.0331
2.0	−0.0447	−0.0285
2.2	−0.0388	−0.0234
2.4	−0.0302	−0.0178

complete discrete basis led to a significant improvement over the results obtained with an equal number of bound target states, even in this very restricted calculation. Our 1s, $\bar{2}s$, $\bar{2}p$ phase shifts are 5–10% lower than the polarized orbital phase shifts presented by Sloan.[25] Unfortunately, no highly accurate variational calculations, similar to those done by Schwartz[26] ($L=0$) and by Armstead[27] ($L=1$) on e^-– H elastic scattering, are available for comparison. The eigenphases in the energy region between the $n=2$ and $n=3$ thresholds, evaluated with the 1s, 2s, 2p, $\bar{3}s$, $\bar{3}p$ expansion, are compared in Table III with the corresponding values obtained using a 1s, 2s, 2p target eigenstate expansion. We observe that one of the four eigenphases (η_2) has undergone an improvement comparable to that undergone by the elastic scattering phase shift. Perhaps this eigenphase is mainly associated with the elastic channel.

III. PHOTO-IONIZATION CROSS SECTIONS

We feel that the results presented in the preceding section indicate that good accuracy has been achieved for the final-state continuum wave functions in the asymptotic region. We now proceed with the calculation of the photo-ionization cross sections which depend on the inner region of the continuum wave functions. The results of this section are presented by giving the differential oscillator strengths corresponding to the energetically allowed transitions as a function of k_1^2, the kinetic energy in rydbergs of an ejected photoelectron which leaves the residual He$^+$ ion in its ground state. The incident photon wavelength is given by

$$\lambda = \frac{911.754}{k_1^2 + I}\ \text{Å} , \tag{17}$$

where I is the ionization potential of the initial (bound) state of the two-electron system measured in rydbergs.

TABLE III. P wave e^-–He$^+$ scattering eigenphases η_μ evaluated in the nonresonant region between $n=2$ and $n=3$ thresholds using 1s, 2s, 2p and 1s, 2s, 2p, $\bar{3}s$, $\bar{3}p$ expansions.

k_1^2(Ry)	η_1	η_2	η_3	η_4
			1s, 2s, 2p expansion	
3.15	0.447	−0.0501	−0.639	−1.38
3.20	0.449	−0.0499	−0.609	−1.44
3.25	0.452	−0.0497	−0.584	−1.50
3.30	0.451	−0.0493	−0.560	−1.54
			1s, 2s, 2p, $\bar{3}s$, $\bar{3}p$ expansion	
3.15	0.461	−0.0268	−0.630	−1.37
3.20	0.465	−0.0264	−0.600	−1.44
3.25	0.470	−0.0258	−0.575	−1.49
3.30	0.475	−0.0250	−0.553	−1.54

Chandrasekhar[28] gives three alternative expressions for the dipole photo-ionization cross sections which would give identical results if they could be evaluated using exact wave functions for the initial and final states. The dipole length and dipole velocity expressions have been found to give the best results when approximate wave functions are used, and a close agreement between the results obtained using these two expressions usually gives a certain confidence in the accuracy of the wave functions. We do not evaluate the dipole acceleration expression, because it usually gives disappointing results compared with the other two expressions due to its emphasis on the region near the nucleus where the bound-state wave functions are known to be not so well represented. We can write, for the length and velocity partial photoionization cross sections when the residual He$^+$ ion is left in the nl_1 state:

$$\sigma^L_{nl_1}(k_1^2) = 4\pi^2\alpha(I + k_1^2)\sum_{l_2} \left| \langle \psi^{(-)}_{nl_1l_2,E} | z_1 + z_2 | \psi_B \rangle \right|^2 a_0^2 , \tag{18}$$

$$\sigma^V_{nl_1}(k_1^2) = 16\pi^2\alpha(I + k_1^2)^{-1} \times \sum_{l_2} \left| \left\langle \psi^{(-)}_{nl_1l_2,E} \left| \frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2} \right| \psi_B \right\rangle \right|^2 a_0^2 , \tag{19}$$

where α is the fine structure constant. ψ_B is a ^1S bound-state wave function. $\psi^{(-)}_{nl_1l_2,E}$ is a ^1P continuum wave function defined with the asymptotic form given by Eq. (12), which represents an outgoing spherical wave in the channel nl_1l_2 and incoming spherical waves in all other open channels. The photoelectron is ejected with kinetic energy $k^2_{nl_1} = k_1^2 - Z^2(1 - n^{-2})$ Ry and relative orbital angular momentum l_2. The total photo-ionization cross section is obtained by summing over all energetically accessible states of the residual ion:

$$\sigma_T(k_1^2) = \sum_{nl_1} \sigma_{nl_1}(k_1^2) . \tag{20}$$

The ^1S bound-state wave functions obtained by Pekeris[29,30] can be rearranged in the form

$$\psi_B = N(1 + P_{12})e^{-ar_1 - br_2} \sum_{ijk} C_{ijk} r_1^i r_2^j r_{12}^k , \tag{21}$$

where N is defined by the condition that ψ_B be normalized to unity. In the 1^1S ground-state wave function, $a = b = (-E_B)^{1/2}$, where $-E_B$ is the binding energy in a.u. In the 2^1S metastable-state wave function, $a = Z$, while b was optimized to obtain the best energy eigenvalue with a given number of terms in the expansion.[31] We feel that the 56-term expansions used in our computations were entirely adequate. The use of larger bound-state expansions should probably be deferred until a more accurate continuum wave function is obtained.

For an efficient evaluation of the integrals in Eqs. (18) and (19), we employ the following techniques. First we expand each power of r_{12} in the form

$$r_{12}^k = \sum [(\sum_m C_{kl2m}(r_<^{2m+l}/r_>^{2m+l-k})]P_l(\cos\theta_{12}) \quad . \tag{22}$$

It turns out that only the $l = 0$, 1, and 2 terms give nonvanishing contributions when the continuum expansions are restricted to s and p states. The coefficients are most easily evaluated using the recurrence relation derived by Sack[32]:

$$\begin{aligned} C_{klm+2} &= [(k-2l-m)/(m+2)] \\ &\quad \times [(k-m+1)/(2l+m+3)]C_{klm} \; , \\ C_{kl0} &= [\Gamma(-\tfrac{1}{2}k+l)/\Gamma(\tfrac{1}{2}+l)][\Gamma(\tfrac{1}{2})/\Gamma(-\tfrac{1}{2}k)] \; . \end{aligned} \tag{23}$$

The summation over m is finite for all positive integral powers of r_{12}, and only such terms occur in the bound-state wave functions obtained by Pekeris. The angular integrations and one of the two remaining radial integrations can be done analytically by well-known techniques.

The oscillator strength per unit rydberg energy in the continuum is given by

$$\frac{df_{nl_1}}{dE} = \frac{\sigma_{nl_1}(k_1^2)}{4\pi^2\alpha} \quad , \tag{24}$$

corresponding to the transition in which the He^+ ion is left in the state nl_1. After all the algebraic reductions have been completed, the dipole-length and dipole-velocity expressions can be written

$$\left(\frac{df_{nl_1}}{dE}\right)_L = \frac{32\pi^2}{3}(I+k_1^2) \times \sum_{l_2} \left| \sum_{\mu=n'l_1'l_2'} \int_0^\infty W_\mu^L(r)\bar{F}_{\mu\nu}(r)\,dr \right|^2 \; , \tag{25}$$

$$\left(\frac{df_{nl_1}}{dE}\right)_V = \frac{128\pi^2}{3}(I+k_1^2)^{-1} \times \sum_{l_2} \left| \sum_{\mu=n'l_1'l_2'} \int_0^\infty W_\mu^V(r)\bar{F}_{\mu\nu}(r)\,dr \right|^2 \; , \tag{26}$$

where $\nu = nl_1l_2$. Similar expressions have been given by Burke and McVicar[7] and by Macek.[33]

We have utilized the recurrence relation Eq. (23) in writing a computer code which gives the weight functions $W_\mu(r)$ in the convenient form

$$W_\mu(r) = \sum_{ij} \omega_{ij}^\mu r^i e^{-\gamma_j r} \quad , \tag{27}$$

where $\gamma_1 = a$, $\gamma_2 = b$, and $\gamma_j = a + b + \alpha_{j-2}$ $(j \geqslant 3)$ for each different exponential parameter α_j which occurs in the continuum expansion basis $S_{nl_1}(r_1)$. Although the finite summation over the integer i begins with a negative value in some cases, all the weight functions $W_\mu(r)$ can be shown to be finite at $r = 0$. The He 1^1S weight functions obtained using the 1s, $\bar{2}s$, $\bar{2}p$ continuum expansion are illustrated in Fig. 1. The weight functions $W_{101}(r)$ were found to be practically the same as those obtained by Burke and McVicar,[7] apart from a normalization constant. It can be noted that the length and velocity weight functions emphasize the regions of space at large and at intermediate distances from the nucleus, respectively.

Table IV presents the differential oscillator strength for the He 1^1S state evaluated in the nonresonant energy region below the $n = 2$ threshold. The length and velocity results obtained using the 1s, $\bar{2}s$, $\bar{2}p$ expansion agree within 1%, whereas for the 1s, 2s, 2p expansion the agreement is only to within 2%. As expected, our 1s, 2s, 2p values, especially those obtained from the velocity expression, do not differ significantly from the results reported by Burke and McVicar[7] using a different but equally sophisticated bound-state wave function. Bell and Kingston[34] have evaluated df/dE for the He 1^1S state using the polarized orbital continuum wave function described by Sloan.[25] For the lower

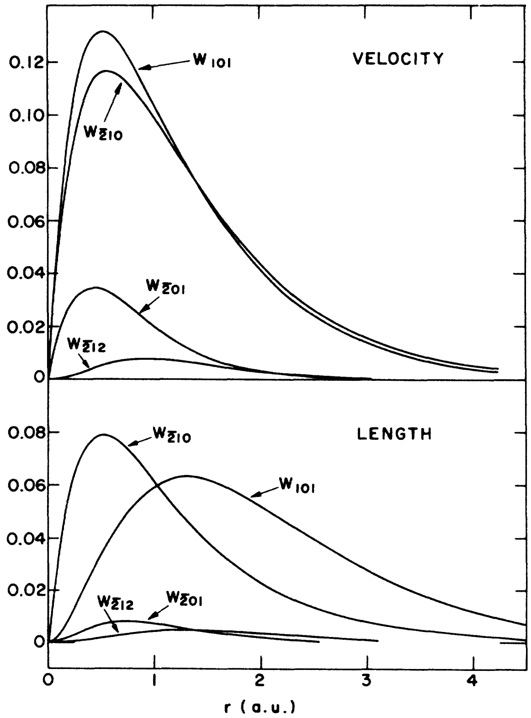

FIG. 1. Length and velocity weight functions occurring in expressions for photo-ionization cross sections, evaluated with the 1^1S bound-state wave function of Pekeris and the 1s, $\bar{2}s$, $\bar{2}p$ continuum expansion.

energies their length results are as much as 4% higher than our length results, whereas for the higher energies their results approach ours to within 1%. Table V presents the differential oscillator strength for the He 2^1S state below the $n = 2$ threshold. Whereas the $1s$, $\bar{2}s$, $\bar{2}p$ expansion yields results for the 2^1S state which are as good as those for the 1^1S state, the $1s$, $2s$, $2p$ expansion gives disappointing values at the higher energies. Huang[3] carried out calculations for the He 1^1S and 2^1S states using a bound-state wave function containing the r_{12} variable, and a product of hydrogenic wave functions for the continuum. Our 1^1S results are in good agreement with those of Huang, but our 2^1S results are substantially different from his.

Although the major contributions to the photoionization cross sections come from the region of space near the nucleus, the He 2^1S weight functions were found to have appreciable amplitudes at distances as large as $r = 20$ a.u. Therefore, it was necessary to evaluate the asymptotic expansions for the functions $F_{\mu\nu}(r)$ to obtain the values at large distances. These asymptotic expansions, which are used by Burke's code, have the form

$$F_{\mu\nu}(r) = \sum_{\lambda=1}^{m_a} \left[\sin\left(k_\lambda r + \frac{(Z-1)}{k_\lambda} \ln 2k_\lambda r \right) \sum_{P=0}^{\infty} \alpha_{P\lambda}^{\mu\nu} r^{-P} + \cos\left(k_\lambda r + \frac{(Z-1)}{k_\lambda} \ln 2k_\lambda r \right) \sum_{P=0}^{\infty} \beta_{P\lambda}^{\mu\nu} r^{-P} \right] + \sum_{\lambda=1}^{m_b} \exp\left(-|k_\lambda| r + \frac{(Z-1)}{|k_\lambda|} \ln 2|k_\lambda| r \right) \sum_{P=0}^{\infty} \gamma_{P\lambda}^{\mu\nu} r^{-P}, \tag{28}$$

where there are m_a and m_b different independent wave numbers k_λ above and below threshold, respectively. The coefficients are determined by the recurrence relations derived by Burke and Schey,[20] except for a modification subsequently made by Burke[7] to account for the residual Coulombic interaction for $Z \neq 1$. This procedure is clearly more economical than that of enlarging the region of space in which the coupled equations are solved beyond the limit where the solutions are obtained with significantly greater precision.

TABLE IV. Oscillator strength df/dE for He 1^1S ground state evaluated in the nonresonant energy region below $n = 2$ threshold using $1s, 2s, 2p$ and $1s, \bar{2}s, \bar{2}p$ expansions.

	$1s, 2s, 2p$ expansion		$1s, \bar{2}s, \bar{2}p$ expansion	
k_1^2 (Ry)	$\left(\frac{df}{dE}\right)_L$	$\left(\frac{df}{dE}\right)_V$	$\left(\frac{df}{dE}\right)_L$	$\left(\frac{df}{dE}\right)_V$
0.2	0.7796	0.7625	0.7830	0.7748
0.4	0.6655	0.6525	0.6669	0.6621
0.6	0.5719	0.5619	0.5716	0.5690
0.8	0.4950	0.4867	0.4937	0.4923
1.0	0.4316	0.4243	0.4298	0.4288
1.2	0.3791	0.3722	0.3769	0.3758
1.4	0.3352	0.3284	0.3327	0.3314
1.6	0.2982	0.2915	0.2955	0.2939
1.8	0.2668	0.2603	0.2639	0.2621
2.0	0.2404	0.2339	0.2370	0.2350
2.2	0.2184	0.2121	0.2139	0.2118
2.4	0.2018	0.1957	0.1942	0.1921

TABLE V. Oscillator strength df/dE for He 2^1S metastable state evaluated in the nonresonant energy region below $n = 2$ threshold using $1s, 2s, 2p$ and $1s, \bar{2}s, \bar{2}p$ expansions.

	$1s, 2s, 2p$ expansion		$1s, \bar{2}s, \bar{2}p$ expansion	
k_1^2 (Ry)	$\left(\frac{df}{dE}\right)_L$	$\left(\frac{df}{dE}\right)_V$	$\left(\frac{df}{dE}\right)_L$	$\left(\frac{df}{dE}\right)_V$
0.2	0.472 6	0.478 6	0.476 9	0.483 2
0.4	0.257 2	0.251 9	0.258 6	0.254 3
0.6	0.152 3	0.150 1	0.152 7	0.152 1
0.8	0.098 75	0.097 17	0.099 09	0.099 12
1.0	0.067 65	0.066 35	0.068 06	0.068 41
1.2	0.047 85	0.046 95	0.049 06	0.049 12
1.4	0.035 62	0.033 98	0.036 45	0.036 28
1.6	0.026 34	0.024 80	0.027 47	0.027 28
1.8	0.019 08	0.017 96	0.020 62	0.020 71
2.0	0.016 72	0.015 03	0.015 91	0.015 75
2.2	0.013 72	0.012 53	0.012 16	0.011 84
2.4	0.008 809	0.007 697	0.008 726	0.008 615

In the energy region between the $n = 2$ and $n = 3$ thresholds, a photoelectron can be ejected from He with kinetic energy k_1^2 leaving the residual He$^+$ ion in its ground state, or it can be ejected with kinetic energy $k_1^2 - 3$ leaving the ion in an $n = 2$ excited state. Samson[9] observed that 0.08 ± 0.02 of the total number of photoelectrons detected at $k_1^2 = 3.088$ Ry were ejected with the lower energy. In his experiment, it was not possible to distinguish between the transition to the $2s$ state of the ion and the transition to the $2p$ state of the ion. From our results for the oscillator strengths for the He 1^1S state presented in Table VI, we obtain 0.095 (L) and 0.094 (V) at $k_1^2 = 3.20$ Ry, and 0.093 (L) and 0.092 (V) at $k_1^2 = 3.15$ Ry for this ratio. These values seem to extrapolate within the error limits of Samson's experimental value. Brown[35] carried out calculations using a product of hydrogenic wave functions for the final state. He obtained results of the correct order of magnitude for this ratio, but his df/dE values for the transitions to the $n = 2$ excited states of the ion are quite different from ours. The success, in certain situations, of the treatment using a product of hydrogenic wave functions for the final state may be attributed to the dominance of the nonvanishing centrifugal potential $l_2(l_2+1)/r^2$ near the nucleus, where the photo-ionization process mainly occurs. This point has

TABLE VI. Oscillator strengths for the He 1^1S ground state, corresponding to transitions in which the He^+ ion is left in $1s, 2s$, and $2p$ states, evaluated in the nonresonant region between $n=2$ and $n=3$ thresholds.

k_1^2 (Ry)	$\left(\frac{df_{1s}}{dE}\right)_L$	$\left(\frac{df_{1s}}{dE}\right)_V$	$\left(\frac{df_{2s}}{dE}\right)_L$	$\left(\frac{df_{2s}}{dE}\right)_V$	$\left(\frac{df_{2p}}{dE}\right)_L$	$\left(\frac{df_{2p}}{dE}\right)_V$
			$1s, 2s, 2p$ expansion			
3.15	0.1312	0.1263	0.003 375	0.003 376	0.010 48	0.010 53
3.20	0.1278	0.1230	0.003 485	0.003 485	0.010 46	0.010 51
3.25	0.1244	0.1197	0.003 570	0.003 571	0.010 44	0.010 47
3.30	0.1213	0.1167	0.003 638	0.003 643	0.010 42	0.010 33
			$1s, 2s, 2p, \bar{3}s, \bar{3}p$ expansion			
3.15	0.1296	0.1278	0.003 321	0.003 246	0.009 891	0.009 606
3.20	0.1262	0.1245	0.003 429	0.003 350	0.009 839	0.009 542
3.25	0.1229	0.1212	0.003 509	0.003 426	0.009 763	0.009 455
3.30	0.1197	0.1181	0.003 566	0.003 481	0.009 674	0.009 355

been stressed by Massey and Bates.[36]

Table VII presents our results for the He 2^1S metastable state in the energy region between the $n=2$ and $n=3$ thresholds. Our values of the oscillator strengths for the transitions to the s states of the He^+ ion are significantly different from those obtained by Suh and Zaidi.[37] Their procedures for the continuum are based on the numerical solution of the Hartree differential equations.

For He 2^1S, we find that the oscillator strengths for the transitions to the $n=2$ excited states of the ion are an order of magnitude larger than the oscillator strength for the transition in which the ion is left in its ground state. This is explained by noting that the $1s$ amplitude is larger than that of the $2s$ near the nucleus, where the photo-ionization process mainly occurs.

Figure 2 presents the photo-ionization cross sections for the 1^1S and 2^1S states, obtained from the velocity expression. Calculations could not be carried out for energies less than 0.15 Ry above threshold, because for very small values of k_μ^2 the asymptotic expansions Eq. (28) provide a good representation of the wave function only for very large values of r.

IV. OSCILLATOR-STRENGTH SUMS

In the preceding section, the agreement between the results obtained from the length and velocity expressions has served as a criterion for judging the accuracy of our computed values for the oscillator strengths df/dE. An additional check on our computed df/dE values is provided by an evaluation of the oscillator-strength sums. The various moments of the oscillator-strength distribution can be defined as

$$S(k)=\sum_n (E_n-E_0)^k f_{n0}+\int_{k_1^2=0}^{\infty}(E-E_0)^k\left(\frac{df}{dE}\right)dE\ , \tag{29}$$

where E_0, E_n, and E denote the energies in rydbergs of a ^1S initial state, a (^1P-n)th discrete state, and a ^1P continuum state, respectively, and $E=I+k_1^2$. Some of these moments are related to properties of the He atom in the initial state by the following oscillator-strength sum rules:

TABLE VII. Oscillator strengths for the He 2^1S metastable state, corresponding to transitions in which the He^+ ion is left in $1s, 2s$, and $2p$ states, evaluated in the nonresonant region between $n=2$ and $n=3$ thresholds.

k_1^2 (Ry)	$\left(\frac{df_{1s}}{dE}\right)_L$	$\left(\frac{df_{1s}}{dE}\right)_V$	$\left(\frac{df_{2s}}{dE}\right)_L$	$\left(\frac{df_{2s}}{dE}\right)_V$	$\left(\frac{df_{2p}}{dE}\right)_L$	$\left(\frac{df_{2p}}{dE}\right)_V$
			$1s, 2s, 2p$ expansion			
3.15	0.007 167	0.006 218	0.069 19	0.067 30	0.070 05	0.067 58
3.20	0.006 863	0.005 949	0.062 90	0.061 08	0.067 26	0.064 72
3.25	0.006 629	0.005 754	0.059 15	0.057 45	0.063 40	0.061 92
3.30	0.006 434	0.005 600	0.057 26	0.055 67	0.062 56	0.060 11
			$1s, 2s, 2p, 3\bar{s}, 3\bar{p}$ expansion			
3.15	0.007 629	0.007 429	0.071 42	0.070 20	0.071 25	0.070 03
3.20	0.007 374	0.007 198	0.065 56	0.064 53	0.068 97	0.068 69
3.25	0.007 201	0.007 051	0.062 26	0.061 50	0.066 38	0.065 30
3.30	0.007 081	0.006 961	0.060 76	0.060 29	0.064 14	0.063 39

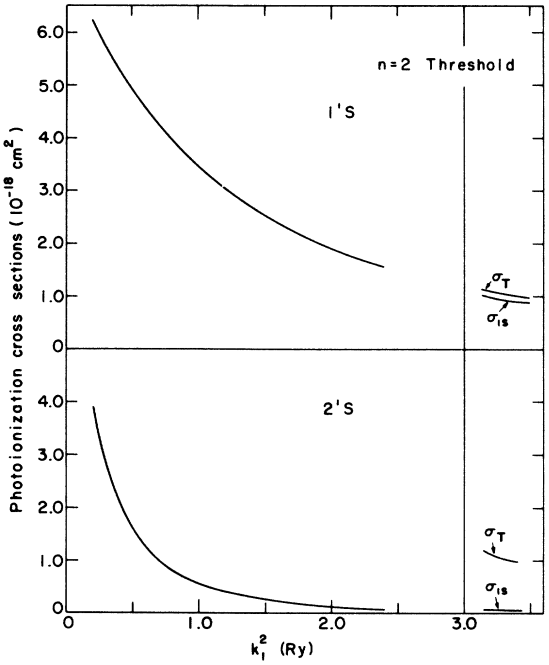

FIG. 2. Velocity results for photo-ionization cross sections of He. k_1^2 is energy of an ejected photoelectron which leaves He$^+$ ion in its ground state.

$$S(-3)=\tfrac{1}{4}\beta_1\ , \tag{30}$$

$$S(-2)=\tfrac{1}{4}\alpha_1\ , \tag{31}$$

$$S(-1)=\tfrac{1}{3}\langle 0|(\vec{r}_1+\vec{r}_2)^2|0\rangle\ , \tag{32}$$

$$S(0)=2\ , \tag{33}$$

$$S(1)=\tfrac{4}{3}(-E_0+2\langle 0|\vec{P}_1\cdot\vec{P}_2|0\rangle)\ , \tag{34}$$

$$S(2)=\tfrac{16}{3}\pi Z\langle 0|\delta^{(3)}(\vec{r}_1)+\delta^{(3)}(\vec{r}_2)|0\rangle\ . \tag{35}$$

$\vec{P}_i$ is the momentum of the ith electron, and α_1 is the dipole polarizability of the initial state of He measured in units of a_0^2. In the sum rule given by Eq. (30), β_1 is the coefficient of the nonadiabatic contribution of order r^{-6} in the asymptotic expansion for the potential experienced by an electron incident upon the initial state of He. This sum rule has been recently derived[38]; the others are well known.[39]

A highly accurate computation of the expectation values which occur in the expressions for $S(-1)$, $S(1)$, and $S(2)$ has been carried out by Pekeris.[30,40] This enables a precise evaluation of these sums to be made for the 1^1S and 2^1S states. Victor, Dalgarno, and Taylor[41] have recently computed $S(-3)$, $S(-2)$, and $S(-1)$ for these states by replacing the infinite summations over the intermediate states (including the integrations over the continua) by finite summations over the eigenvectors of the Hamiltonian matrix in a Hylleraas basis. This procedure is expected to give accurate results for those sums $S(k)$ which weight heavily the lower-energy part of the oscillator-strength distribution.

Our evaluation of the sums $S(k)$, which is summarized in Table VIII, utilizes the accurate f values obtained by Schiff, Accad, and Pekeris[42] for the dipole transitions to the lowest four discrete ^1P states. In order to estimate the contributions from the remaining discrete states, we have used the asymptotic result[43,44]

$$f_{n0}\xrightarrow[n\to\infty]{}\frac{2(Z-1)^2}{n^3}\left(\frac{df}{dE}\right)_{k_1^2=0}\ . \tag{36}$$

TABLE VIII. Various contributions to the sums $S(k)$.

$S(k)$	$\sum_{n=2}^{5}(E_n-E_0)^k f_{n0}$	$\sum_{n=6}^{\infty}(E_n-E_0)^k f_{n0}$	$\int_{k_1^2=0}^{2.4}(E-E_0)^k \times\left(\frac{df}{dE}\right)dE$	$\int_{k_1^2=2.4}^{\infty}(E-E_0)^k \times\left(\frac{df}{dE}\right)dE$	Total	Exact values	Previous evaluations
				He 1^1S			
$S(-3)$	0.096 11	0.005 14	0.073 44	0.002 50	0.1772	...	0.1766[a]
$S(-2)$	0.153 6	0.009 21	0.169 0	0.013 5	0.3453	...	0.3455[a]
$S(-1)$	0.245 9	0.016 5	0.407 5	0.079 9	0.7498	0.752 50[b]	0.7520[a]
$S(0)$	0.394 4	0.029 5	1.037	0.514	1.975	2	2.054[c]
$S(1)$	0.633 9	0.052 9	2.795	4.542	8.025	8.167 5[b]	7.923[c]
$S(2)$	1.021	0.094 8	7.997	110.5	119.6	121.34[b]	117.7[d]
				He 2^1S			
$S(-3)$	4372	1.90	5.558	0.004 9	4380	...	4397[a]
$S(-2)$	198.0	0.530	1.899	0.019 7	200.5	...	200.6[a]
$S(-1)$	9.640	0.141	0.736 6	0.122 9	10.64	10.685[d]	10.70[a]
$S(0)$	0.599 2	0.038 8	0.357 0	0.683 6	1.679	2	2.036[e]
$S(1)$	0.061 07	0.010 6	0.243 4	4.423	4.738	5.773 3[d]	5.642[e]
$S(2)$	0.009 745	0.002 94	0.245 8	84.64	84.90	87.761[d]	88.07[e]

[a] See Ref. 41. [b] See Ref. 40. [c] See Ref. 46. [d] See Ref. 30. [e] See Ref. 37.

Since we were unable to obtain the threshold values of df/dE from our computations, we have taken for the 1^1S state the value 0.900 (halfway between the length and velocity results of Stewart and Webb[4]), and for the 2^1S state we have chosen the value 1.125 (used by Dalgarno and Kingston[45]). These numbers are unlikely to be in error by more than 2%.

The main purpose of our evaluation of the sums $S(k)$ is to check our computed values of df/dE in the energy range $0.2 \leq k_1^2 \leq 2.4$. Although the major interest of this paper is in double-electron excitations, we have obtained reliable results for these processes only over an energy range which makes insignificant contributions to the sums $S(k)$. Lacking a more satisfactory approach for higher energies in the continuum, we have adopted the procedures used by Salpeter and Zaidi[46] and Suh and Zaidi[37] in order to estimate the contributions from the continua for $k_1^2 \geq 2.4$. As expected, we obtain good accuracy for the sums $S(-3)$, $S(-2)$, and $S(-1)$, which weight most heavily the lower energy part of the oscillator strength distribution. Our estimates of the sums $S(0)$, $S(1)$, and $S(2)$ for the 2^1S metastable state are quite poor compared with those for the 1^1S state, most probably because the double-electron excitations which are inadequately treated by the independent-particle approximation are of much greater importance in the 2^1S continuous absorption spectrum. These considerations would be of great importance in an accurate evaluation of the Lamb-shift mean-excitation energy of the 2^1S metastable state.

V. CONCLUSIONS

We have been able to obtain significantly improved results for photo-ionization processes at low energies before exceeding the limits of our computing facilities. A more detailed experimental investigation of the double-electron excitation processes just above the $n = 2$ threshold would be of great help in judging the accuracy of our results. Should greater precision be warranted, it would probably be best to abandon the expansion in product functions and include the r_{12} variable in the continuum trial wave function.

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*Weizmann Fellow.

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Infinite-Channel Close-Coupling Theory in the Second Born Approximation. I. Charge Polarization in the Elastic Electron Scattering from H and He† *

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One of the oldest methods suggested for treating the effect of charge polarization on elastic scattering is revived by the use of certain physically reasonable assumptions, and is shown to lead to results, in the limit of small scattering angles and high incident energies, which are in quantitative agreement with experimental and theoretical expectations. The theory is worked out in detail for one- and two-electron atoms, and the extension to more complex systems is also discussed. The effect of charge polarization on the elastic differential cross section for 500-eV incident electrons on He is calculated and compared with the experimental results of Bromberg and the theoretical results of LaBahn and Callaway. The agreement is good over the angular range $0° \leq \theta < 6°$ if exchange scattering contributions are included.

I. INTRODUCTION

Numerous treatments of charge polarization or charge distortion of the target on scattering by charged particles have been considered.[1] These methods can be put into two classifications. The first will consist of the so-called rigorous methods which are designed for use in the region of low incident energy of the bombarding charged particle. Such methods, in the case of electron scattering from atoms and molecules, become computationally messy at energies above 100 eV because of the proliferation of open excitation channels. The second class of methods, generally more empirical in nature, either simplify rigorous theory by the use of approximations or use parametrized models to represent the polarizing process.

One of the oldest methods of the second type, which is here called "the infinite-channel close-coupling theory in the second Born approximation," was first suggested by Massey and Mohr[2] and is the method to be dealt with in this paper. It simply consists of writing the coupled-channel differential equations, neglecting exchange and relativistic effects, in the form

$$
\begin{aligned}
(\nabla^2+k^2)f_0(\vec{r}) &= \sum_{l=0}^{\infty} U_{0l}(\vec{r})f_l(\vec{r}) \ , \\
(\nabla^2+k_1^2)f_1(\vec{r}) &= \sum_{l=0}^{\infty} U_{1l}(\vec{r})f_l(\vec{r}) \ , \\
&\vdots \\
(\nabla^2+k_n^2)f_n(\vec{r}) &= \sum_{l=0}^{\infty} U_{nl}(\vec{r})f_l(\vec{r}) \ ,
\end{aligned}
\qquad (1)
$$

where k^2 is the incident energy, $k_n^2 = k^2 - \Delta E_{0n}$ is the scattered energy after exciting the target to the state n, and $f_n(\vec{r})$ is the wave function for the scattering process where the scatterer is initially in its ground state and is left in its nth excited state. The interaction potential $U_{nl}(\vec{r})$ is given as

$$
U_{nl}(\vec{r}) = \frac{2m}{m_0}\left\langle \psi_n(\vec{r}_1, \ldots, \vec{r}_N) \right| -\frac{z}{r} + \sum_{i=1}^{N} \frac{1}{|\vec{r}-\vec{r}_i|} \left| \psi_l(\vec{r}_1, \ldots, \vec{r}_N) \right\rangle \ , \qquad (2)
$$

where m/m_0 is the electron mass ratio $(1 - v^2/c^2)^{-1/2}$ introduced to provide the main relativistic effects on the scattered electron in the forward scattering direction with incident energies less than 50 keV.