Multichannel eikonal treatment of atomic collisions: The $2\,^1S$ and $2\,^1P$ inelastic scattering of electrons by helium*

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A multichannel eikonal treatment of atomic collisions is presented and applied to the excitation of atomic helium by electrons with incident energy E in the range $50 \le E \le 500$ eV. Two different sets of orthogonal wave functions are employed. A four-channel description yields differential- and total-excitation cross sections in satisfactory agreement with experiment.

I. INTRODUCTION

Apart from the application of the first and second Born approximations,[1-3] Ochkur modifications,[4] Glauber-type approaches,[5,6] and impact-parameter methods[7,8] to collisional excitation of atomic helium by incident electrons, theoretical knowledge of these collisions for low and intermediate impact energies beyond the inelastic thresholds is very limited. The experimental measurement of the vacuum-uv excitation functions is difficult[9-19] and requires high resolution, and full account must be taken of cascade and other well-identified problems. In order to provide absolute cross sections, the measurements must then be normalized to some high-energy theoretical cross section, and the energy-point of departure of the actual cross sections from the corresponding Born and Bethe values is extremely uncertain.

In an effort to obtain an accurate description of electron-(excited) atom collisions in the intermediate energy region, a multistate-eikonal treatment of atomic collisions has recently been developed.[20,21] The method achieved notable success for $e-\mathrm{H}(1s)$ excitation and the resulting differential and total cross sections agreed closely with experiment and with other refined treatments. Moreover, the basic formulae which acknowledged different speeds in various channels reduced upon successive approximation to those obtained previously by other authors.[5,22-24] In an effort to probe the further reliability of the present method, the $2\,^1S$ and the $2\,^1P$ excitations of atomic helium by electron impact are examined in this paper. The resulting total and differential cross sections are compared with previous treatments and with experiment.

II. THEORY

The scattering amplitude describing a transition between an initial channel i and a final channel f of the electron-helium collision system of reduced mass μ is, in the center-of-mass reference frame,

$$f_{if}(\theta,\varphi) = -(1/4\pi)(2\mu/\hbar^2) \times \langle \Psi_f(\vec{k}_f;\vec{r},\vec{R})|\,V(\vec{r},\vec{R})\,|\Psi_i^+(\vec{k}_i;\vec{r},\vec{R})\rangle_{\vec{r},\vec{R}} \tag{1}$$

where $V(\vec{r},\vec{R})$ is the instantaneous electrostatic interaction between the electron at $\vec{R}$ and the helium atom with internal electronic coordinates denoted collectively by $\vec{r}$, both vectors being relative to the helium nucleus as the origin. The wave numbers for the relative motion in the initial and final channels asymptotically ($\vec{R}\sim\infty$) tend to k_i and k_f, respectively, the final stationary state of the isolated atoms in channel f is Ψ_f, and Ψ_i^+ is the solution of the time-independent Schrödinger equation,

$$\left(-\frac{\hbar^2}{2\mu}\nabla_R^2 + H_e(\vec{r}) + V(\vec{r},\vec{R})\right)\Psi_i^+(\vec{r},\vec{R}) = E_i\Psi_i^+(\vec{r},\vec{R})\,, \tag{2}$$

solved subject to the asymptotic boundary condition

$$\Psi_i^+(\vec{r},\vec{R}) \xrightarrow{\text{large } R} \mathop{\mathrm{S}}_n \left(e^{i\vec{k}_n\cdot\vec{R}}\delta_n + f_{in}(\theta,\varphi)\frac{e^{ik_nR}}{R}\right) \times\varphi_n(\vec{r}_1,\vec{r}_2)\,, \tag{3}$$

in which $\varphi_n(\vec{r}_1,\vec{r}_2)$ are eigenfunctions of the Hamiltonian $H_e(\vec{r})$ for the isolated helium atom with internal electronic energy ϵ_n, such that the total energy E_i in channel i is $\epsilon_i + \hbar^2k_i^2/2\mu$, which is conserved throughout the collision. In the absence of the interaction the wave function for the system in the final channel is therefore $\varphi_f(\vec{r}_1,\vec{r}_2)\exp(i\vec{k}_f\cdot\vec{R})$.

The eikonal approximation to (2) writes the total wave function in the presence of the interaction as

$$\Psi_i^+(\vec{r},\vec{R}) = \mathop{\mathsf{S}}_n A_n(\vec{\rho},Z)\exp iS_n(\vec{\rho},Z)\varphi_n(\vec{r}_1,\vec{r}_2)\,, \tag{4}$$

where the e-ion separation $\vec{R} \equiv (R,\Theta,\Phi) \equiv (\rho,\Phi,Z)$ in spherical and cylindrical coordinate frames, respectively. The eikonal S_n in (4) is the characteristic-function solution of the classical Hamilton-Jacobi equation (i.e., the Schrödinger equation in the $\hbar \to 0$ limit) for the e – He relative motion under the static interaction $V_{nn}(\vec{R})$, and is therefore given by

$$S_n(\vec{\rho},Z) = k_n Z + \int_{-\infty}^{Z} [\kappa_n(\vec{R}) - k_n]\,dZ\,, \tag{5}$$

in which the local wave number of relative motion at $\vec{R}$ is

$$\kappa_n(\vec{R}) = [k_n^2 - (2\mu/\hbar^2)V_{nn}(\vec{R})]^{1/2}\,, \tag{6}$$

and where dZ is assumed to be an element of path length along the trajectory. The interaction matrix elements coupling the various atomic states are

$$V_{nm}(\vec{R}) = \langle\varphi_n(\vec{r}_1,\vec{r}_2)|\,V(\vec{r},\vec{R})|\,\varphi_m(\vec{r}_1,\vec{r}_2)\rangle\,. \tag{7}$$

By inserting Eq. (4) into (1), and with the aid of Eqs. (2)–(7), Flannery and McCann[21] have shown that the scattering amplitude then reduces to

$$f_{if}(\theta,\varphi) = -i^{\Delta+1}\int_0^\infty J_\Delta(K'\rho) \times [I_1(\rho,\theta) - iI_2(\rho,\theta)]\rho\,d\rho\,, \tag{8}$$

where K' is the XY component $k_f \sin\theta$ of $\vec{K}$ and where J_Δ are Bessel functions of integral order. Both the functions

$$I_1(\rho,\theta;\alpha) = \int_{-\infty}^{\infty} \kappa_f(\rho,Z)\left(\frac{\partial C_f(\rho,Z)}{\partial Z}\right)e^{i\alpha Z}\,dZ \tag{9}$$

and

$$I_2(\rho,\theta;\alpha) = \int_{-\infty}^{\infty}\left(\kappa_f(\kappa_f - k_f) + \frac{\mu}{\hbar^2}V_{ff}\right)C_f(\rho,Z) \times e^{i\alpha Z}\,dZ \tag{10}$$

depend on the scattering angle θ, via the parameter

$$\alpha = k_f(1-\cos\theta) = 2k_f\sin^2(\theta/2)\,, \tag{11}$$

the difference between the Z component of the momentum change $\vec{K}$ and the minimum momentum change $k_i - k_f$ in the collision. The transition amplitudes $C_f(\rho,Z)$ which are related to the original phase Φ-dependent coefficients $A_f(\vec{\rho},Z)$ by

$$C_f(\rho,Z) = A_f(\vec{\rho},Z) \times \exp\left(i\int_{-\infty}^{Z}(\kappa_f - k_f)\,dZ\right)\exp(-i\Delta\Phi), \tag{12}$$

where Δ is the change $M_i - M_f$ in the azimuthal quantum number of the atom, can be shown to satisfy the following set of N-coupled differential equations

$$\frac{i\hbar^2}{\mu}\kappa_f(\rho,Z)\frac{\partial C_f(\rho,Z)}{\partial Z} + \left(\frac{\hbar^2}{\mu}\kappa_f(\kappa_f - k_f) + V_{ff}(\rho,Z)\right)C_f(\rho,Z) = \sum_{n=1}^{N} C_n(\rho,Z)V_{fn}(\rho,Z)e^{i(k_n - k_f)Z}\,, \quad f = 1,2,\ldots N \tag{13}$$

to be solved subject to the boundary condition $C_f(\rho,-\infty) = \delta_{if}$. Equations (8)–(13) are basic to the present multichannel eikonal treatment and a variety of approximations readily follow. For example, in the absence of all couplings except that connecting the initial and final channels, i.e., $C_n = \delta_{ni}$ in (13), then (8) reduces to

$$f_{if}(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int V_{fi}(\vec{R})\exp(i\vec{K}\cdot\vec{R})\,d\vec{R}\,, \tag{14}$$

which is the Born-wave formula for the scattering amplitude.

When $\kappa_f(\vec{R})$ is approximated by $k_f - (\mu/\hbar^2 k_f)V_{ff}(\vec{R})$ then, with the aid of (6) for κ_f^2, both I_2 and the term within large parentheses of the left-hand side of (13) vanish identically to give

$$f_{if}^A(\theta,\varphi) = -i^{\Delta+1}\int_0^\infty J_\Delta(K'\rho)\rho\,d\rho \times \int_{-\infty}^{\infty}\kappa_f\left(\frac{\partial C_f^A}{\partial Z}\right)\exp(i\alpha Z)\,dZ\,, \tag{15}$$

an approximation A to the scattering amplitude, for which the N-coupled equations reduce to

$$\frac{i\hbar^2}{\mu}\kappa_f\frac{\partial C_f^A}{\partial Z} = \sum_{n=1}^{N} C_n^A(\rho,Z)V_{fn}(\rho,Z)e^{i(k_n - k_f)Z}\,, \quad f = 1,2\ldots,N\,. \tag{16}$$

If the local wave number κ_f in (15) and (16) is now replaced by its asymptotic value k_f, then a further approximation B is obtained. For a one-channel approximation B, $C_n^B = C_i^B\delta_{in}$ in (16) with

$\kappa_i = k_i$. After some analysis, the customary eikonal expression[22] for elastic scattering by a fixed potential $V_{ii}(\vec{R})$ is then recovered. Moreover, if the distorted wave for the final state

$$\Psi_f(\vec{r},\vec{R}) = \varphi_f(\vec{r}_1,\vec{r}_2)\exp i\left(\vec{k}_f\cdot\vec{R} - \frac{1}{\hbar v_f}\int_{+\infty}^{Z} V_{ff}\,dZ\right) \tag{17}$$

is used in (1), then the theory follows through as before, to give, in approximation B

$$f_{if}^{\mathrm{DW}}(\theta,\varphi) = -i^{\Delta+1}\int_0^\infty J_\Delta(K'\rho)\rho\,d\rho\int_{-\infty}^{\infty} k_f\left(\frac{\partial C_f^B}{\partial Z}\right)\times\exp i\left(\alpha Z + \frac{1}{\hbar v_f}\int_\infty^Z V_{ff}\,dZ'\right)dZ \tag{18}$$

where, C_f^B satisfies (16), with $\kappa_f = k_f$. Equation (18) represents the multichannel distorted-wave treatment. By setting $C_n^B = C_i^B\delta_{in}$ in a two-state treatment of (16), then, after some analysis, (18) reduces to

$$f_{if}^{DWB}(\theta,\varphi) = -\frac{i^\Delta\mu}{\hbar^2}\int_0^\infty J_\Delta(k_f\rho\sin\theta)\rho\,d\rho\int_{-\infty}^{\infty} V_{fi}(\rho,Z)\times\exp i\{[(k_i-k_f)+\alpha]Z + \delta\Phi(Z)\}\,dZ\ , \tag{19}$$

where

$$\delta\Phi(Z) = -\frac{1}{\hbar v_i}\int_{-\infty}^{Z} V_{ii}\,dZ - \left(\frac{1}{\hbar v_f}\right)\int_Z^\infty V_{ff}\,dZ\ , \tag{20}$$

formulas which are identical to the distorted Born-wave expressions of Chen *et al.*[23] for e-H collisions. Equations (19) and (20) have been used by Shields and Peacher[25] to evaluate differential cross sections for atom-atom collisions.

In the heavy-particle or high-energy limit, the asymptotic wave numbers k_f in approximation B can be replaced by

$$k_f = k_i - (\epsilon_{fi}/\hbar v_i)[1 + (\epsilon_{fi}/2\mu v_i^2) + \cdots],\quad \epsilon_{fi} = \epsilon_f - \epsilon_i\ , \tag{21}$$

and a third approximation $C(\alpha)$ follows by setting all the individual k_n in approximation B equal to k_i, and any difference $k_n - k_f = \epsilon_{fn}/v_i$. Hence

$$f_{if}^c(\theta,\varphi) = -i^{\Delta+1}k_i\int_0^\infty J_\Delta(K'\rho)\times\left(\int_{-\infty}^{\infty}\frac{\partial C_f^c(\rho,Z)}{dZ}\exp(i\alpha Z)\,dZ\right)\rho\,d\rho,$$
$$\alpha = K_Z - \epsilon_{fi}/\hbar v_i\ . \tag{22}$$

In addition, for small-angle scattering at high energies $\alpha\approx 0$ from (11) and the Z-integration above can therefore be performed so that a further approximation $C(\alpha=0)$ is characterized by

$$f_{if}^{c(0)}(\theta,\varphi) = -i^{\Delta+1}k_i\times\int_0^\infty J_\Delta(K'\rho)(C_f^c(\rho,\infty) - \delta_{if})\rho\,d\rho \tag{23}$$

where $K'^2 = K^2 - \epsilon_{fi}^2/\hbar^2 v_i^2$, and the amplitudes C_f^c satisfy

$$i\hbar v_i\frac{\partial C_f^c}{\partial Z} = \sum_{n=1}^{N} C_n^c(\rho,Z)V_{fn}(\rho,Z)\exp\left(\frac{i\epsilon_{fn}Z}{\hbar v_i}\right)\ , \tag{24}$$

in which $v_i = \hbar k_i/\mu$, for $n = 1, 2, \ldots, N$, is the incident speed. Equations (22)–(24) are simply those derived previously[26] for the differential cross sections in the multistate impact parameter description of heavy particle collisions. They have recently been applied to various atom-atom and ion-atom collisions.[27] Equation (22) has previously been obtained by Byron[5] who subsequently applied (23) and (24) to e – H(1s) collisions. In order to acknowledge polarization of the initial state due to the incident electron, Bransden and Coleman[24] modified (24) and used (23) with $K' = 2k_i\sin\frac{1}{2}\theta$. The above derivation, however, demonstrates that the validity of the impact parameter equations (22)–(24) is confined only to the heavy-particle or high-energy limit of atomic collisions when $k_i\approx k_f$ and the scattering is mainly in the forward direction.

The Glauber approximation which follows by neglecting the exponential term in (24), and by inserting the exact solution C_f of the resulting equations in (23), is also a heavy-particle–high-energy approximation and one in which no account is taken of the different relative momenta in the various channels. In spite of this, however, it is apparently remarkably successful.

III. RESULTS AND DISCUSSION

The full multichannel eikonal theory, as represented by Eq. (8)–(13), is now applied to the examination of differential and total cross sections for the excitation processes

$$e + \mathrm{He}(1\,^1S) \to e + \mathrm{He}(2\,^1S, 2\,^1P) \tag{25}$$

in which the four-channels $e - (1\,^1S, 2\,^1S, 2\,^1P_{0,\pm1})$ of the e-He system are closely coupled. For this investigation two relevant orthogonal sets of wave functions were adopted. The first set includes the normalized Hartree-Fock ground-state function of

Byron and Joachain,[28]

$$\varphi_{1s,1s}(\vec{r}_1,\vec{r}_2)=(1.6966/\pi)(e^{-1.4r_1}+0.799e^{-2.61r_1})\times(e^{-1.4r_2}+0.799e^{-2.61r_2}), \quad (26)$$

the $2\,^1P$ function of Goldberg and Clogston,[29]

$$\varphi_{1s,2pm}(\vec{r}_1,\vec{r}_2)=(0.37831/\pi^{1/2})[r_1 e^{-(0.485r_1+2r_2)}Y_{1m}(\hat{\vec{r}}_1)+r_2 e^{-(0.485r_2+2r_1)}Y_{1m}(\hat{\vec{r}}_2)], \quad (27)$$

and the $2\,^1S$ function of Flannery[7]

$$\varphi_{1s,2s}(\vec{r}_1,\vec{r}_2)=\frac{0.706\,40}{\pi(1+\Delta^2)^{1/2}}[e^{-2r_2}(e^{-\lambda r_1}-cr_1e^{-\mu r_1})+e^{-2r_1}(e^{-\lambda r_2}-cr_2e^{-\mu r_2})], \quad (28)$$

in which the parameters $\lambda=1.1946$, $\mu=0.4733$, $c=0.268\,32$, and $\Delta=0.007\,322$, which ensured orthogonality with (26), were chosen so as to provide a simple curve fit to the multi-parameter function of Cohen and McEachran.[30] With the aid of standard integral techniques, the interaction potentials (7), deduced from the above set of wave functions (26)–(28), can be expressed as analytic functions of $\vec{R}$.

The second choice of wave functions are the actual analytical multi-parameter Hartree-Fock frozen-core set of McEachran and Cohen[31] and of Crothers and McEachran,[32] which yield very accurate eigenenergies. The set is written

$$\Psi_{1s,nlm}(\vec{r}_1,\vec{r}_2)=N_{nl}[\varphi_0(\vec{r}_1)\varphi_{nlm}(\vec{r}_2)+\varphi_0(\vec{r}_2)\varphi_{nlm}(\vec{r}_1)], \quad (29a)$$

where the normalized function representing the frozen 1s orbital is

$$\varphi_0(\vec{r})=2^{5/2}e^{-2r}\,Y_{00}(\hat{\vec{r}}), \quad (29b)$$

and where the unnormalized orbital for the second electron in state (nlm) is, in atomic units,

$$\varphi_{nlm}(\vec{r})=\sum_{j=2l+1}^{J=10}a_j^{nl}(2r)^l e^{-\beta r}L_j^{2l+1}(2\beta r)Y_{lm}(\hat{\vec{r}}),\qquad \beta=\frac{2}{n}, \quad (29c)$$

where the coefficients a_j^{nl} of the associated Laguerre polynomials

$$L_j^{\lambda}(x)=\sum_{k=0}^{j-\lambda}\frac{(-1)^{k+1}(j!)^2x^k}{k!(j-k-\lambda)!(k+\lambda)!} \quad (29d)$$

have been tabulated[30-32] for various states of helium. In order to evaluate the interaction matrix elements (7) as analytic functions of $\vec{R}$, it is convenient to express (29c), with the aid of (29d), as

$$\varphi_{nlm}(\vec{r})=\sum_{N=l+1}^{J-l}B_N^{nl}e^{-\beta r}r^{N-1}Y_{lm}(\hat{\vec{r}}), \quad (30a)$$

with coefficients given by

$$B_N^{nl}=\sum_{j=N+l}^{J}\frac{(-1)^{N-l}a_j^{nl}2^l(j!)^2(2\beta)^{N-l-1}}{(n-l-1)!(j-N-l)!(N+l)!}, \quad (30b)$$

which are tabulated in Table I for the $1\,^1S$, $2\,^1S$ and $2\,^1P$ states of interest. The overall normalization factor in (29a) is $N_{nl}=[2(H_{nl}+G_{nl}^2)]^{-1/2}$, where

$$H_{nl}=\sum_{N=l+1}^{J-l}\sum_{N'=l+1}^{J-l}B_N^{nl}B_{N'}^{nl}\frac{(N+N')!}{(2\beta)^{N+N'+1}} \quad (30c)$$

and

$$G_{nl}=2^{5/2}\delta_{l0}\sum_{N=1}^{J}B_N^{nl}\frac{(N+1)!}{(\beta+2)^{N+2}}, \quad (30d)$$

and is also given in Table I. With the aid of (30a) and (30b), and standard integrals, the interaction matrix elements can be expressed in the form

$$V_{nlm,n'l'm'}(\vec{R})=\sum_{L=|l-l'|,|l-l'+2|}^{|l+l'|}\left(-\frac{a_{-t}}{R^t}+\sum_{i=1}^{2}e^{-\alpha_i R}\sum_{s=-t}^{16}a_sR^s\right)Y_{LM}(\vec{R}). \quad (31)$$

The tabulation of the coefficients a_m for the various $\alpha_i=4$, $(1/n+1/n')$, and L values is extensive and

TABLE I. Coefficients B_N^{nl}, parameters β, normalization factors N_{nl}, and eigenenergies ϵ_n (a.u.) given by the Hartree-Fock frozen-core set of wave functions (29a)–(30a) for helium.

N \ nl	1s	2s	2p
1	−1.8385(0)[a]	−5.5677(−1)	0.0000
2	2.9332(−2)	5.2732(−1)	−1.2768(−1)
3	−1.2332(0)	−4.1053(−1)	−5.8948(−2)
4	−4.7143(−3)	3.1444(−1)	−1.5165(−2)
5	1.0769(−1)	−9.0158(−2)	−1.3793(−2)
6	−7.9926(−2)	1.7266(−2)	4.9854(−3)
7	2.0400(−2)	−1.5858(−3)	−1.2073(−3)
8	−2.6249(−3)	7.3009(−5)	1.1661(−4)
9	1.2433(−4)	−3.0679(−7)	−5.2312(−6)
β	2.0	1.0	1.0
N_{nl}	2.2745	9.1927(−2)	3.6218(−2)
ϵ_n (calc)	−0.8725	−0.1434	−0.1224
ϵ_n (expt)	−0.9036	−0.1460	−0.1238

[a] Numbers in parentheses indicate the power of 10 by which the entry is to be multiplied.

is available upon request. With a knowledge of the interaction matrices (31), the appropriate set of coupled differential equations (13) can be solved for the real and imaginary parts of C_i by standard numerical procedures.

In Figs. 1 and 2, the resulting differential cross sections,

$$\frac{d\sigma}{d\Omega}=\frac{k_f}{k_i}\,|f_{if}(\theta,\varphi)|^2 \qquad (32)$$

computed from (8)–(13) as a function of scattering angle θ are displayed as solid and double-dashed curves [labeled FE1 and FE2 associated with the first and second choices (26)–(28) and (29a)–(29d) for the wave functions, respectively] at two representative electron-impact energies E_i of 50 eV and 100 eV. Use of the more refined set of wave functions (29a)–(29d) causes the scattering to be increased only in the forward direction ($\theta \lesssim 20°$) in the case of $2\,{}^1P$ excitation, and into all angles for the $2\,{}^1S$ collision. This amount of enhancement decreases with energy increase. Also shown are recent results labeled S, single-dashed curves, obtained by Berrington *et al.*[33] who used the first set of orthogonal wave functions (26)–(28) in the second-order potential theory of Bransden and Coleman,[24] i.e. Eq. (23) with $K' = 2k_i \sin\frac{1}{2}\theta$ and Eq. (24), suitably modified so as to acknowledge polarization of the initial state. While the long-range polarization is expected to be more effective for small-angle scattering (i.e., distant encounters), Berrington *et al.*[33] have shown that the resulting reduction in $d\sigma/d\Omega$ is nonetheless relatively small at small θ and vanishes for larger θ and/or E_i. Figure 1(a) and 1(b) show that the present treatment causes a further reduction both at small and large scattering angles for the $2\,{}^1P$ excitation. In Figs. 2(a) and 2(b) the effect is reversed for the $2\,{}^1S$ excitation. These effects can be attributed to the presence in (9) and (10) of α which tends to reduce all the cross sections particularly at the larger scattering angles and to the more important inclusion in the various channels of the different local momenta $\kappa_n(\vec{R})$ which tend to enhance[21] the $2\,{}^1S$ excitation at the expense of the $2\,{}^1P$ excitation at energies $\gtrsim 50$ eV.

The $2\,{}^1S$ Glauber cross sections of Yates and Tenney[34] and of Chan and Chen,[35] shown as crosses in Fig. 2, agree closely with the Glauber results of Franco[37] who used the same $2\,{}^1S$ wave functions as in FE1. The corresponding $2\,{}^1P$ cross sections[36] are in harmony with the present calculations in the angular range 5°–10°, but are larger for scattering in the forward direction.

The $2\,{}^1P$ and $2\,{}^1S$ differential cross sections measured by various groups[4,15–19] are also displayed in Figs. 1 and 2 for comparison purposes.

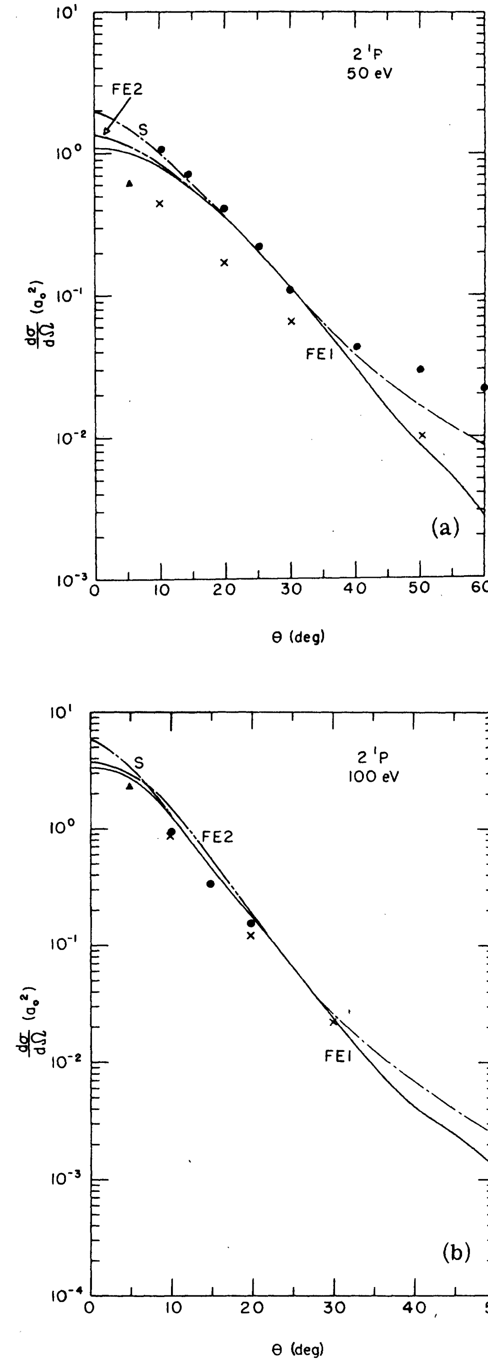

FIG. 1. Differential cross sections for the process $e + \mathrm{He}(1\,{}^1S) \rightarrow e + \mathrm{He}(2\,{}^1P)$ at incident electron energy (a) 50 eV and (b) 100 eV. Theory: FE1, Four-channel eikonal treatment with first set of atomic wave functions (26)–(28); FE2, four-channel eikonal treatment with second set of atomic wave functions (29); S, second-order potential method with first set of atomic wave functions [Berrington *et al.* (Ref. 33)]. Experiment: ▲, Chamberlain *et al.* (Ref. 17), ×, Crooks and Rudd (Ref. 18), ●, Truhlar *et al.* (Ref. 19) at 55.5 eV and Vriens *et al.* (Ref. 15) at 100 eV.

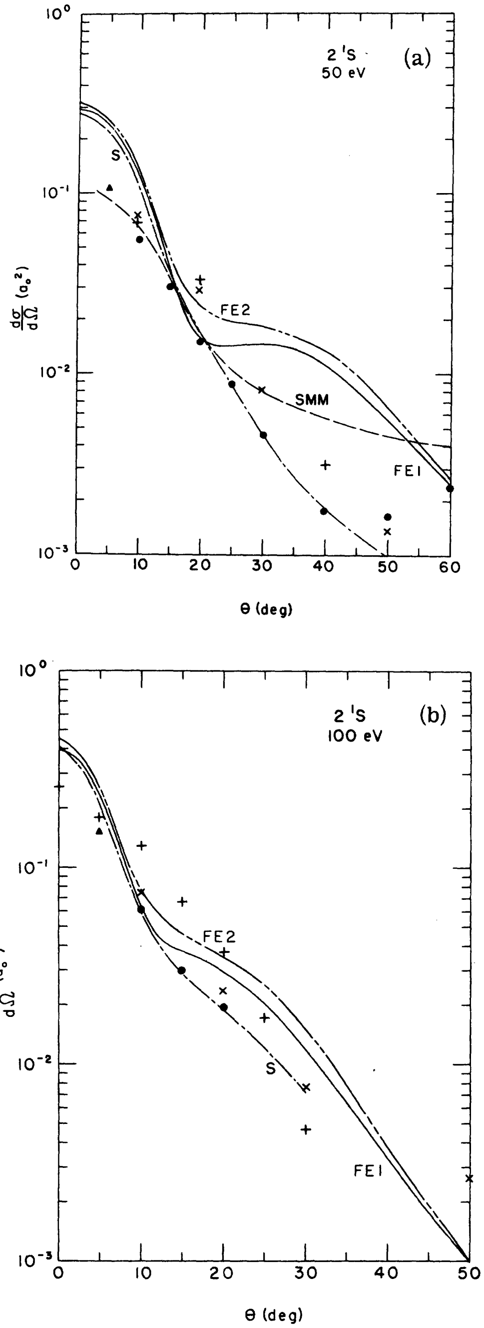

FIG. 2. Differential cross sections for the process $e + \mathrm{He}(1\,^1S) \rightarrow e + \mathrm{He}(2\,^1S)$ at incident electron energy. (a) 50 eV and (b) 100 eV. Theory: FE1, Four-channel eikonal treatment with first set of atomic wave functions (26)–(28); FE2, four-channel eikonal treatment with second set of atomic wave functions **(29)**; S, second-order potential method with first set of atomic wave functions [Berrington *et al.* (Ref. 33)]; +: Glauber approximation (Refs. 34 and 35). Experiment: SMM, Simpson *et al.* (Ref. 16); ▲, Chamberlain *et al.* (Ref. 17); ×, Crooks and Rudd (Ref. 18); ●, Rice *et al.* (Ref. 4) at 55.5 eV and Vriens *et al.* (Ref. 15) at 100 eV.

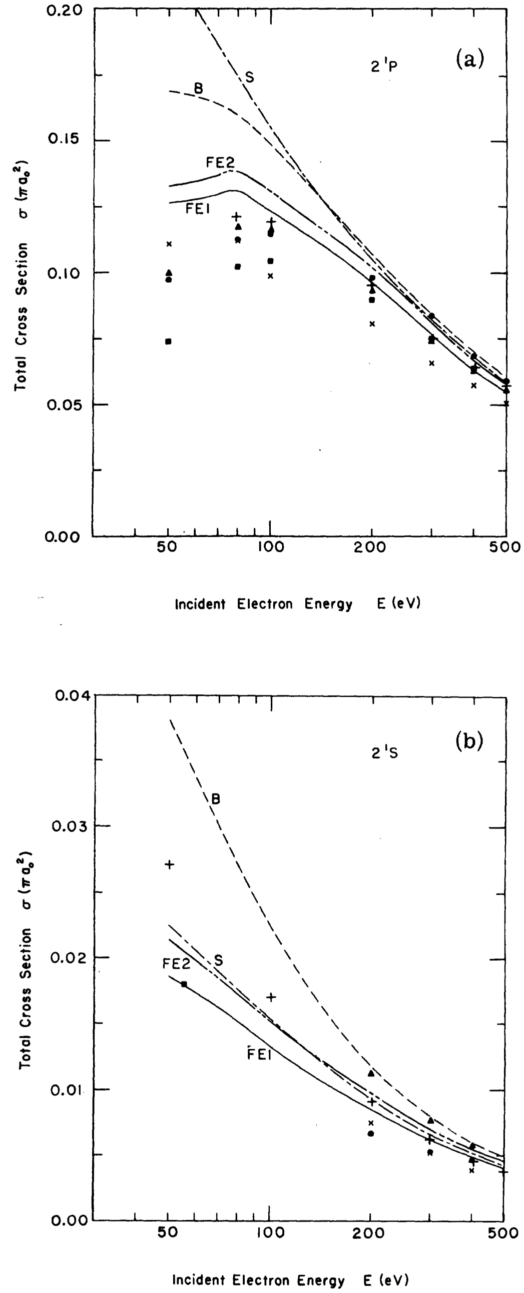

FIG. 3. Total cross sections for (a) the $2\,^1P$ and (b) the $2\,^1S$ excitations of $\mathrm{He}(1\,^1S)$ by electron impact. Theory: FE1, Four-channel eikonal treatment with first set of atomic wave functions (26)–(28); FE2, four-channel eikonal treatment with second set of atomic wave functions **(29)**; S, second-order potential method with first set of atomic wave functions [Berrington *et al.* (Ref. 33)]; B, Born-approximation (Ref. 2); +: Glauber approximation (Refs. 35 and 36). Experiment: ($2\,^1P$), ▲, Donaldson *et al.* (Ref. 9); ■, Jobe and St. John (Ref. 10); ×, Moustafa-Moussa (Ref. 11); ●, van Eck and de Jongh (Ref. 12); ($2\,^1S$), ▲, Lassettre *et al.* (Ref. 13); ×, Miller *et al.* (Ref. 14); O, Vriens *et al.* (Ref. 15).

Although large discrepancies do exist between the measured values, particularly for scattering at all angles for 50 eV, and for large-angle scattering, in general, the over-all agreement with theory is satisfactory only for scattering into small and intermediate angles $\lesssim 50°$.

While the present treatment includes several important effects, e.g., the $2\,^1P - 2\,^1S$ coupling and the different relative local momenta in the various channels, it ignores both electron-exchange and that additional part of the polarization-interaction in the incident channel not included via the four-state treatment. Electron-exchange is mainly effective at the large scattering angles (i.e., close encounters) while the long-range polarization attraction mainly effects elastic scattering in the forward direction. For e-H(1s) excitation at 50 eV, Chen *et al.*[23] have shown the exchange effect to be small for $\theta \lesssim 30°$, an effect which is entirely dominated by the more important $2p$-$2s$ coupling included by Flannery and McCann,[21] but neglected in the treatment of Chen *et al.*[23] According to Berrington *et al.*,[33] the neglect of the additional amount of polarization in the incident channel introduces relatively small error[33] for e-He inelastic scattering in the forward direction. The present theoretical formulation is however amenable to the inclusion of both electron-exchange and the full polarization interaction.

However, both polarization in the incident channel and electron-exchange are significantly more important for elastic scattering than for inelastic scattering. Flannery and McCann[21] have shown that inclusion of these effects causes an overall increase in the total cross section for e-H(1s) elastic scattering, polarization being mainly responsible for enhancement in the forward direction while electron-exchange is needed to properly describe intermediate and large-angle scattering.

In Figs. 3(a)–3(b) are displayed the theoretical cross sections together with other theoretical values and the measurements for the total $2\,^1P$ excitations, Refs. 9–12, and for the $2\,^1S$ excitations, Refs. 13–15. Donaldson *et al.*[9] normalized their experimental data to the Born cross sections at 2000 eV. As exhibited in the figures, the present theory represents considerable improvement over the Born B and the second-order potential treatments, although a great deal of scatter still exists in the experimental data. The theoretical prediction of a peak in the $2\,^1P$ excitation around 80 eV is consistent with the experimental data. The use of the less accurate wave functions (26)–(28) reduces the $2\,^1P$ and $2\,^1S$ (FE2) cross sections by 6 and 12%, respectively. Comparison of FE1 and S in Fig. 3(b) shows that the additional physical effects acknowledged by the present treatment for the $2\,^1S$ excitation has introduced closer accord with experiment, while comparison between FE2 and FE1 demonstrate the need for using wave functions as accurate as possible.

Note that Berrington *et al.*[33] obtained their total cross sections by integrating the computed transition probabilities over impact parameter ρ, a procedure which, in general, overestimates the cross section calculated by integrating (32) directly over all solid angles. It is worth noting that the present Hartree-Fock frozen-core set of wave functions are the most accurate employed to date in a collision description more refined than the Born approximation.

The Glauber cross sections[35,36] are in accord with the present FE1 results for impact energy $E_i > 100$ eV, for the $2\,^1P$ excitation, and $E_i > 200$, for the $2\,^1S$ excitation. The $2\,^1P$ wave function used[36] was the same as in FE1 while the $2\,^1S$ wave function[35] differed.

TABLE II. Inelastic cross sections (πa_0^2) for the process $e + \mathrm{He}(1\,^1S) \rightarrow e + \mathrm{He}(2\,^1P)$.

	FE^a					2^1P	
E_i(eV)	2^1P_0	$2^1P_{\pm1}$	2^1P	P^b	S^c	IP^d	Born^e
50	0.0732	0.0600	0.1332	41.9	0.215	0.232	0.1694
80	0.0637	0.0750	0.1387	25.9	•••	•••	0.1596
100	0.0547	0.0759	0.1306	18.1	0.155	0.161	0.1485
200	0.0347	0.0671	0.1018	1.7	0.105	0.107	0.1069
300	0.0237	0.0577	0.0814	−9.8	0.0822	0.083	0.0841
400	0.0173	0.0500	0.0673	−18.2	0.0681	0.069	0.0700
500	0.0120	0.0466	0.0586	−32.0	0.0581	0.058	0.0602

[a] Present four-channel eikonal treatment (refined set of wave functions, Eqs. (29a)–(29d).
[b] Percentage polarization of emitted radiation.
[c] Second-order potential method [Berrington *et al.* (Ref. 33)].
[d] Impact-parameter method [Berrington *et al.* (Ref. 33)].
[e] Born approximation [Bell *et al.* (Ref. 2)].

TABLE III. Inelastic cross sections (πa_0^2) for the process $e + \mathrm{He}(1^1S) \to e + \mathrm{He}(2^1S)$.

E_i (eV)	FE[a]	S[b]	IP[c]	Born[d]
50	0.0215	0.0225	0.031	0.0390
80	0.0175	···	···	0.0270
100	0.0153	0.0154	0.0182	0.0222
200	0.0096	0.0093	0.0102	0.0118
300	0.0070	0.0066	0.0071	0.0080
400	0.0054	0.0052	0.0054	0.0060
500	0.0045	0.0042	0.0044	0.0048

[a] Present four-channel treatment [refined set of wave functions, Eqs. (29a)–(29d)].
[b] Second-order potential method [Berrington *et al.* (Ref. 33)].
[c] Impact-parameter method [Berrington *et al.* (Ref. 33)].
[d] Born approximation [Bell *et al.* (Ref. 2)].

In Tables II and III are displayed the actual numerical 2 $^1P_{0,\pm1}$ and 2 ^1S excitation cross sections FE2, together with those given by Born's approximation B, the four-state impact treatment IP and the second-order potential method S. For the 2 ^1P excitation at impact energies $E_i \lesssim 200$ eV, IP and S are higher than B which at 50 eV is, in turn, higher than the present four-state eikonal results FE2 by 34%. For the 2 ^1S excitation all the cross sections are lower than Born's approximation and the use of the more accurate second set of wave functions (29a) has resulted in (fortuitous) closer accord with IP and S which were determined from wave functions (26)–(28). At 500 eV, the Born cross sections are 3 and 6% higher than the FE2 results for the 2 ^1P and 2 ^1S excitations, respectively.

Also tabulated in Table II is the percentage polarization P of the radiation emitted from the 2 ^1P level obtained from the formula[38]

$$P = 100(\sigma_0 - \sigma_1)/(\sigma_0 + \sigma_1) \ , \qquad (33)$$

where σ_m is the cross section for excitation of a particular substate m. Direct measurement of P for a vacuum uv emission is extremely difficult.

In conclusion, the theoretical acknowledgment of the different local wave numbers $\kappa_n(\vec{R})$ [Eq. (6)] of relative motion in various channels, the important 2 ^1P – 2 ^1S dipole coupling, the momentum parameter α[Eq. (11)], and various distortion effects within a multichannel eikonal treatment of atomic collisions has introduced closer accord with experiment for e-He collisions and, in particular, has produced a theoretical peak given also by Glauber's approximation but absent in previous theoretical treatments of the 2 ^1P cross section. The effect of including these physical effects can, however, be rendered null for the 2 ^1S excitation by an inappropriate choice of wave functions, i.e., the inclusion of refinements to the collision theory should be preferably accompanied, whenever possible, by a choice of accurate He wave functions. The present agreement for e-He($1s^2$) collisions taken together with the previous[21] agreement for e-H($1s$) collisions is encouraging and represents the status of the present multichannel eikonal approximation. In particular, this theoretical model finds ready application over a large impact energy range to e-excited atom and e-complex atom collisions, instances for which application of the full wave treatment is prohibitively difficult.

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[1]Y. K. Kim and M. Inokuti, Phys. Rev. 175, 176 (1968).
[2]K. L. Bell, D. J. Kennedy, and A. E. Kingston, J. Phys. B 2, 26 (1969).
[3]A. R. Holt, J. Hunt, and B. L. Moiseiwitsch, J. Phys. B 4, 1318 (1971).
[4]J. R. Rice, D. G. Truhlar, D. C. Cartwright, and S. Trajmar, Phys. Rev. A 5, 1 (1972).
[5]F. W. Byron, Phys. Rev. A 4, 1907 (1971).
[6]V. Franco, Phys. Rev. A 8, 2927 (1973).
[7]M. R. Flannery, J. Phys. B 3, 306 (1970).
[8]K. A. Berrington, B. H. Bransden, and J. P. Coleman, J. Phys. B 6, 436 (1973).
[9]F. G. Donaldson, M. A. Hender, and J. W. McConkey, J. Phys. B 5, 1192 (1972).
[10]J. E. Jobe and R. M. St. John, Phys. Rev. 164, 117 (1967).
[11]H. R. Moustafa-Moussa, F. J. de Heer, and J. Schulten, Physica (Utr.) 40, 517 (1969).
[12]J. van Eck and J. P. de Jongh, Physica (Utr.) 47, 141 (1970).
[13]E. N. Lassettre, A. Skerbele, and M. A. Dillon, J. Chem. Phys. 52, 2797 (1970).
[14]K. J. Miller, S. R. Mielczarek, and M. Krauss, J. Chem. Phys. 51, 945 (1968).
[15]L. Vriens, C. E. Kuyatt, and S. R. Mielczarek, Phys. Rev. 165, 7 (1968).
[16]J. A. Simpson, M. G. Menendez, and S. R. Mielczarek, Phys. Rev. 150, 76 (1966).
[17]G. E. Chamberlain, S. R. Mielczarek, and C. E. Kuyatt, Phys. Rev. A 2, 1905 (1970).
[18]G. B. Crooks and M. E. Rudd, Ph.D. thesis (University of Nebraska, 1972) (unpublished).
[19]D. G. Truhlar, J. K. Rice, A. Kuppermann, S. Trajmar, and D. C. Cartwright, Phys. Rev. A 5, 762 (1972).
[20]M. R. Flannery and K. J. McCann, J. Phys. B 7, L223 (1974).
[21]M. R. Flannery and K. J. McCann, J. Phys. B (to be

published).
[22]R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959), Vol. 1, p. 369.
[23]J. C. Y. Chen, C. J. Joachain, and K. M. Watson, Phys. Rev. A 5, 2460 (1972).
[24]B. H. Bransden and J. P. Coleman, J. Phys. B 5, 537 (1972).
[25]R. H. Shields and J. L. Peacher, Phys. Rev. A 9, 743 (1974).
[26]M. R. Flannery and K. J. McCann, Phys. Rev. A 8, 2915 (1973).
[27]M. R. Flannery and K. J. McCann, Phys. Rev. A 10, 1947 (1974); M. R. Flannery and K. J. McCann, J. Phys. B 7, 840, 1349, 1558 (1974).
[28]F. W. Byron and C. J. Joachain, Phys. Rev. 146, 1 (1966).
[29]L. Goldberg and A. M. Clogston, Phys. Rev. 56, 696 (1939).
[30]M. Cohen and R. P. McEachran, Proc. Phys. Soc. Lond. 92, 37 (1967). Note that hydrogenic orbitals contain $L_{n+l}^{2l+1}(2/nr)$.
[31]R. P. McEachran and M. Cohen, J. Phys. B 2, 1271 (1969).
[32]D. S. F. Crothers and R. P. McEachran, J. Phys. B 3, 976 (1970).
[33]K. A. Berrington, B. H. Bransden, and J. P. Coleman, J. Phys. B 6, 436 (1973).
[34]A. C. Yates and A. Tenney, Phys. Rev. A 6, 1451 (1972).
[35]F. T. Chan and S. T. Chen, Phys. Rev. A 8, 2191 (1973).
[36]F. T. Chan and S. T. Chen, Phys. Rev. A 9, 2393 (1974).
[37]V. Franco, Phys. Rev. A 8, 2927 (1974).
[38]I. C. Percival and M. J. Seaton, Philos. Trans. R. Soc. Lond. A 251, 113 (1958).