provides for neither the low-energy nor the high-energy fine structure.

Since the spectrum shows a line structure superimposed on a continuum, it is likely that there are at least two mechanisms operating. The line spectrum seems to result quite naturally from the Fano-Lichten model of electron promotion. The continuum is reasonably well fitted in the case of H^+-H_2 and H^+-He collisions[12] by scaling from calculations made on the Born approximation assuming Coulomb interactions and using hydrogen wave functions. It is likely that this collisional ionization is the mechanism for the continuum in the argon spectra as well.

The various theoretical treatments[3–5] concern themselves only with small impact-parameter (violent) collisions and the total cross section for such collisions is only a small fraction (perhaps a few percent) of the total cross section for ionization.[13] Therefore, it is difficult to determine whether the violent collisions contribute anything to the cross section in the continuum as envisioned in the statistical theory or whether such collisions populate only the fine-structure regions. Presumably, this question could be settled by counting only electrons which are in coincidence with projectile particles which had been deflected appreciably by the collision. We are presently pursuing this approach.

ACKNOWLEDGMENTS

We wish to thank Professor Everhart and Professor Fano for stimulating and helpful discussions and Alan Edwards for assistance in taking the cross-section data. Some of the data reported here were taken at Concordia College, Moorhead, Minnesota while one of us (M.E.R.) was on the staff there.

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[13] We wish to thank Professor Everhart for clarifying this point for us and for supplying data from which this estimate was made.

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Modified Optical-Potential Approach to Low-Energy Electron-Helium Scattering*

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A modified optical-potential approach is introduced for electron-atom scattering at low energies whereby the formal optical potential is used directly in a variational expression for scattering phase shifts. This approach has the advantage that one may include the effect of the second-order optical potential without recourse to the usual adiabatic approximation. The diagrammatic approach associated with the present method makes it possible to identify different contributing terms with different physical effects, and thus to assess the relative importance of various physical effects involved in the scattering process. To test the approach as a practical method for low-energy electron-atom scattering, we applied it to the case of electron-helium scattering for the energy range 1.2 to 16.4 eV. Good agreement with available experimental data has been obtained. The contributions of various multipole components in the second-order optical potential are examined. In particular, the effect of exchange in the second-order optical potential, neglected in most calculations, was found to be very significant.

INTRODUCTION

In the theoretical calculation of electron-atom scattering at low energies, the difficulty is well-known to be one of complexity. That is, the problem one faces is to make suitable approximations to the solution of the complicated, but known, many-body Schrödinger equation so that good results may be obtained with reasonable effort. From a physical point of view, the approximation scheme must take into account two important physical effects, the exchange effect and the distortion effect. The exchange effect arises from the Pauli principle between the incident electron and the atomic electrons. In general, this is taken into account in theoretical calculations by explicitly antisymmetrizing the trial solution. The distortion effect, or polarization effect, arises from the distortion experienced by the atomic electrons in the presence of the incident electron's Coulomb field. The distortion or polarization of the target atom in turn produces a potential on the scattering electron. When the scattering electron is stationary, or moving slowly, the atomic electrons will polarize and adjust adiabatically to the position of the scattering electron. At large distances the dominant polarization potential is the dipole potential $-\alpha/r^4$, where 2α is the polarizability of the atom. This is the familiar adiabatic condition usually assumed for low-energy scattering processes.[1] The validity of the adia-

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batic condition for low-energy electron-atom scattering is rather dubious. It has been shown[2] that in the case of electron-hydrogen atom scattering the incident electron, given to be at rest at infinity, would be accelerated by the attractive adiabatic potential so that it would acquire speeds comparable to that of the atomic electrons while still several atomic distances away from the target atom. For atoms such as alkali atoms, where the polarizability is large, the validity of adiabaticity can be expected to be even worse. The nonadiabatic effect will be considerable. The actual potential as seen by the scattering electron is therefore a very complicated nonlocal (velocity-dependent) one. In practice the conventional theoretical methods are less able to cope with the above-mentioned distortion effect. The familiar close-coupling method[3] does include some nonadiabatic effects, but the complexity of the resulting close-coupled integro-differential equations severely limits the number of atomic states one is able to close-couple. This in turn will give wrong asymptotic values for the effective potential.[4] In addition, the close-coupling method as applied to e-H scattering showed that the convergence is poor as the number of close-coupled states is increased.[5] A more serious practical difficulty associated with the close-coupling approximation is the fact that it requires a knowledge of the wave functions of the excited atomic states. This makes the method much less general in practice than it appears. There are other methods, such as the variational approach[6] and Temkin's nonadiabatic approach,[7] which do take nonadiabatic effects into account more completely. But these methods are either developed for special cases or become difficult for complex-atom cases and are therefore restrictive in their practical applications.

Another general approach is the optical-potential method, where the effect of the target atom on the scattering particle is represented by an equivalent one-body potential. The optical-potential approach was first applied to atomic-scattering problems by Mittleman and Watson,[8] and others. The Pauli-principle effect for the cases where the incident particle is an electron introduces some additional complications. This was set on a more rigorous basis by Bell and Squires,[9] who used basis wave functions and a diagrammatic approach similar to the Brueckner-Goldstone linked-cluster perturbation expansion,[10] which was successfully applied by Kelly to atomic correlation energy calculations.[11] Formally, this optical potential does contain all the nonadiabatic effects, as previously described, through the propagators which contain operators for the scattering electron. Conventionally, after obtaining the formal optical-potential expression, one proceeds to calculate the scattering wave function by solving the one-body Schrödinger equation with the appropriate optical potential. However, the fact that operators for the scattering electrons are contained in the propagator makes the optical potential extremely difficult to evaluate, and one is forced to make the adiabatic approximation. Moreover, even the adiabatically approximated second-order optical potential can only be evaluated in its asymptotic region, yielding the expected dominant $-\alpha/r^4$ dipole polarization potential. To remedy the divergent behavior at small r, some *ad hoc* cutoff parameters must be introduced, such as the parameter d, in the Buckingham-type potential $-\alpha/(r^2+d^2)^2$. Unfortunately, there is no consistant criterion for choosing the parameter d.[12]

To avoid this difficulty, we suggest a modification of the conventional optical-potential approach. Instead of trying to determine the optical-potential expression and then trying to solve the subsequent Schrödinger equation, we use the optical potential directly in a variational expression for the scattering phase shifts. The associated diagrammatic approach in enumerating different perturbation terms in the optical-potential expression has two advantages. First, it enables one to improve the phase shift as one includes higher order optical potentials in a systematic and tractable fashion. Secondly, it is possible to associate different physical effects with different diagrams. Thus one is able to evaluate the individual contributions of the direct and the exchange part of the optical potential for each multipole component

Of course, our main aim is to obtain a general method that is also practical. As in common with any perturbational approach, the convergence of the optical-potential expression depends on the basis wave functions one uses, which in turn depend on the "single-particle potential" one chooses to generate them. For a well-chosen single particle V^s, one hopes to obtain good results with the inclusion of only up to the second-order optical potential. The second-order optical-potential contribution to the phase shift can then be evaluated without recourse to adiabatic approximations or the introduction of any *ad hoc* parameters. In this paper we have adopted the above procedure in a calculation of

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electron-helium scattering for energies from 1.2 to 16.4 eV with gratifying results.

In Sec. II we review the single-particle potential and the results for the formal optical potential, first derived by Bell and Squires. The variational expression for the phase shifts in terms of the optical potential is given. The application to e-He scattering is carried out with a numerical procedure described in Sec. III. Results and discussion are presented in Sec. IV. Concluding remarks are given in Sec. V.

II. REVIEW OF THE FORMAL OPTICAL POTENTIAL

The formal optical potential for a system of identical fermions was first derived by Bell and Squires[9] in the context of nuclear-scattering problems. The result is of course applicable to electron-atom scatterings as well. In their treatment, Bell and Squires obtained the formal optical potential through the construction of the Green's function for the system. In the following brief review, we aim to give some plausibility arguments for their final optical-potential expression. To add clarity, we have made a slight deviation by invoking the result from the Brueckner-Goldstone linked-cluster perturbation expansion.[10] For the detailed derivation we refer readers to the original papers by Bell and Squires.[9]

The system we are considering is the scattering of an electron by a neutral atom with Z atomic electrons. The total Hamiltonian for the system, neglecting the motion of the heavy atomic nucleus, is

$$H=\sum_{i=1}^{Z+1} T_i+\sum\sum_{i>j}^{Z+1} v_{ij}\,, \tag{2.1}$$

where the symbol T_i is the sum of the kinetic energy for the electron and the nuclear Coulomb interaction acting on it,

$$T_i=K_i+V_i^{\text{nuclear}}\,, \tag{2.2}$$

and v_{ij} is the mutual Coulomb interaction between the ith and the jth electron.

The scattering equation we are interested in solving is

$$H\Psi(Z+1)=E\Psi(Z+1)\,, \tag{2.3}$$

where E is the total energy of the system,

$$E=\epsilon_0+k_0^2/2m\,, \tag{2.4}$$

i.e., the sum of the energy of the initial neutral atom ϵ_0 and the initial kinetic energy of the incident electron $k_0^2/2m$.

To construct a basis from which a perturbational expansion for the solution Ψ can be obtained, we first approximate the effect of the interacting particles by a single-particle potential V^s such that the total system is approximated by an unperturbed system Ψ_0 with a Hamiltonian

$$\begin{aligned} H_0&=\sum_{i=1}^{Z+1}(T_i+V_i^s)\,,\\ H_0\Psi_0&=E\Psi_0\,,\\ H'&=H-H_0=\sum\sum_{i>j} v_{ij}-\sum_i V_i^s\,. \end{aligned} \tag{2.5}$$

The choice of the single-particle potential V^s, at this point, is completely arbitrary, except that it should be Hermitian so that the single-particle wave functions φ_n satisfying

$$(T+V^s)\varphi_n=\epsilon_n\varphi_n \tag{2.6}$$

form a complete orthonormal set. The unperturbed $(Z+1)$-particle wave function Ψ_0 is a Slater determinant formed from $(Z+1)$ single-particle states φ_n. Physical conditions make it desirable that Z states in Ψ_0 should represent the ground state of the atom. This demands that the V^s should generate a complete set of φ_n's such that the lowest Z states coincide with the Hartree-Fock states of the ground-state atom. The complete set of φ_n's is used as the basis for the perturbation expansion.

In treating a system of identical fermions, it is desirable to use the second-quantization formalism since the commutation relations of the creation and destruction operators for single-particle states automatically take care of the Pauli principle between electrons. Using the basis just defined, Eqs. (2.5) become, in the second-quantization formalism,

$$H_0=\sum_n \epsilon_n\eta_n^\dagger\eta_n$$

and

$$H'=\sum_{pqmn}\langle pq|v|mn\rangle\eta_p^\dagger\eta_q^\dagger\eta_m\eta_n -\sum_{p,m}\langle p|V^s|m\rangle\eta_p^\dagger\eta_m\,. \tag{2.7}$$

The $\eta_n^\dagger$ and η_n are the usual creation and destruction operators for the single-particle state φ_n. They obey the Fermi-Dirac anticommutation relations. The exact expressions for the matrix elements $\langle pq|v|mn\rangle$ and $\langle p|V^s|m\rangle$ are

$$\langle pq|v|mn\rangle=\int\int\varphi_p^*(\mathbf{r})\varphi_q^*(\mathbf{r}')\times\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\varphi_m(\mathbf{r})\varphi_n(\mathbf{r}')d\mathbf{r}d\mathbf{r}'\,,$$

$$\langle p|V^s|m\rangle=\int\varphi_p^*(\mathbf{r})V^s(\mathbf{r})\varphi_m(\mathbf{r})d\mathbf{r}\,.$$

The summation of the matrix elements is over distinct elements only, e.g., $\langle pq|v|mn\rangle$ is not distinct from the matrix element $\langle qp|v|nm\rangle$.

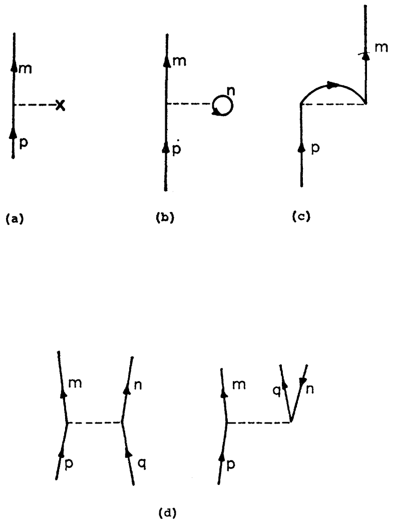

FIG. 1. Diagrams representing various interaction matrix elements. (a) Single-particle potential. (b) Direct interaction with hole state n. (c) Exchange interaction with hole state n. (d) General interaction matrix element.

Let us designate $\Phi_0(Z)$ as the Hartree-Fock ground state of the atom. The number Z is used to remind us that the wave function is a Z-electron function. Following Goldstone,[10] the single-particle states occupied in $\Phi_0(Z)$ are called unexcited states, while the rest φ_n's are called excited states. An unoccupied unexcited state is called a hole, and an occupied excited state is called a particle. The unperturbed scattering system $\Psi_0(Z+1)$ is

$$\Psi_0=\eta_{k_0}{}^{\dagger}|\Phi_0\rangle. \tag{2.8}$$

Goldstone[10] showed that the true ground state of the atom Φ is

$$\Phi=\lim_{\alpha\to 0}\frac{U_\alpha(0)|\Phi_0\rangle}{\langle\Phi_0|U_\alpha(0)|\Phi_0\rangle}, \tag{2.9}$$

where

$$U_\alpha(t)=\sum_{n=0}^{\infty}(-i)^n\int_{t>t_1\cdots>t_n}H'(t)\cdots \times H'(t_n)dt_1\cdots dt_n, \tag{2.10}$$

and

$$H'(t)=e^{iH_0t}H'e^{-iH_0t}e^{\alpha t}.$$

The true ground state Φ, through Wick's theorem, may be represented by a sum of distinct diagrams where a "particle" is represented by a line directed upwards while a "hole" is represented by a line directed downwards. The unperturbed ground-state Hartree-Fock atom is the "vacuum" state. The matrix elements $\langle pq|v|mn\rangle$ and $\langle p|V^s|m\rangle$ are represented by the graphs shown in Fig. 1. Carrying out the time integration, one obtains

$$\Phi=\sum_{\substack{n=0\\L}}^{\infty}\left(\frac{1}{E_0-H_0}H'\right)^n\Phi_0, \tag{2.11}$$

where the sum is over linked diagrams only. In general, the diagrams representing Φ has no particle or hole lines at the bottom but has a maximum of $2Z$ lines at the top, Z particle lines, and Z hole lines.

Similarly, the true solution for the entire scattering system is

$$\Psi=\sum_{\substack{n=0\\L}}^{\infty}\left(\frac{1}{E-H_0+i\epsilon}H'\right)^n\Psi_0$$
$$=\sum_{\substack{n=0\\L}}^{\infty}\left(\frac{1}{E-H_0+i\epsilon}H'\right)^n\eta_{k_0}{}^{\dagger}|\Phi_0\rangle. \tag{2.12}$$

The diagrams representing Ψ have only one particle line at the bottom (incoming electron k_0) and a maximum of $2Z+1$ lines at the top, $Z+1$ particle lines, and Z hole lines.

To obtain the true scattering electron wave function $\chi(k_0)$ we project $\Psi(Z+1)$ onto $\Phi_0(Z)$,

$$\chi(k_0)=\langle\Phi_0(Z)|\Psi(Z+1)\rangle$$
$$=\sum_{\substack{n=0\\L}}^{\infty}\left(\frac{1}{E-H_0+i\epsilon}H'\right)^n\varphi_{k_0}. \tag{2.13}$$

In terms of diagrams, χ is the sum of all linked diagrams where a particle line of k_0 is directed upward at the bottom and only one "particle" line at the top, as illustrated in Fig. 2. The optical potential for this particle, as first derived by Bell and Squires, is then

$$\mathcal{V}_{\text{op}}=\sum_{\substack{n=0\\LP}}^{\infty}H'\left(\frac{1}{E-H_0+i\epsilon}H'\right)^n, \tag{2.14}$$

where the symbol LP means that one sums only diagrams that are linked and proper, using the designation of Bell and Squires.[9] By "proper" they mean those linked diagrams which are not linked by one particle line at any intermediate state. The diagram Fig. 3(a) is a proper diagram, while the diagram Fig. 3(b) is not.

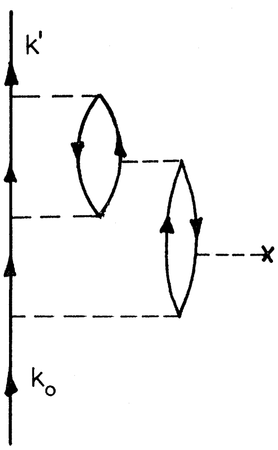

FIG. 2. A general diagram for χ.

The reason for the requirement of "proper" diagrams in the optical-potential expression can be explained as follows. If there is only one "particle" line at some intermediate state of the diagram, it means that out of the $(Z+1)$-electron system there are Z electrons in the unexcited states, i.e., the atom is in its ground state. Thus the restriction on "proper" diagrams is equivalent to the restriction in the conventional optical-potential formulation that the ground state of the atom cannot occur in the intermediate state.[8]

Since the optical potential $\mathcal{V}_{\text{op}}$ is defined for the basis states φ_n, the scattering electron satisfies the one-particle Schrödinger equation:

$$(T+V^s+\mathcal{V}_{\text{op}})\chi(k_0)=(k_0^2/2m)\chi(k_0)\,,$$

or

$$(K+V^{\text{nuclear}}+V^s+\mathcal{V}_{\text{op}})\chi(k_0)=(k_0^2/2m)\chi(k_0)\,. \qquad (2.14')$$

The total optical potential V_{op} is then

$$V_{\text{op}}=V^{\text{nuclear}}+V^s+\mathcal{V}_{\text{op}}\,.$$

Choice of Single-Particle Potential

The general optical potential in Eq. (2.14) yields, in first order, three different diagrams, as shown in Figs. 4(a), 4(b), and 4(c). If one chooses the single-particle V^s to be the Hartree-Fock potential V_{HF} defined by its matrix element, then

$$\langle i|\,V_{\text{HF}}\,|j\rangle=\sum_{n=1}^{Z}\left(\langle in|v|jn\rangle-\langle in|v|nj\rangle\right), \qquad (2.15)$$

where the summation is over all the Hartree-Fock orbitals of the ground-state atom. The potential in Fig. 4(c) cancels exactly the terms shown in Figs. 4(a) and 4(b). The first-order optical potential vanishes exactly and the leading terms are the second-order optical potentials, direct and exchange, as shown in Figs. 5(a) and 5(b). These are the terms we shall retain in our calculation.

As mentioned before, the closer one chooses the single-particle potential V^s to resemble the actual scattering situation, the better the convergence. A close examination shows that the single-particle states one generates with V_{HF} are, except for the constant energy-difference term, equal to the usual static approximation with exchange.[3] Thus, even in zero order we have a phase-shift value which is expected to be correct at high energies.

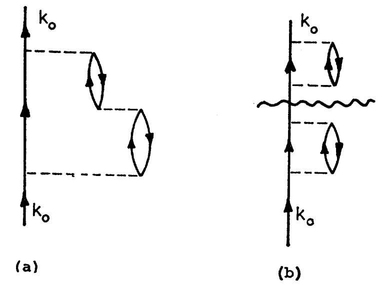

FIG. 3. (a) A "linked and proper" diagram. (b) An improper linked diagram where a single-particle line occurs in intermediate state.

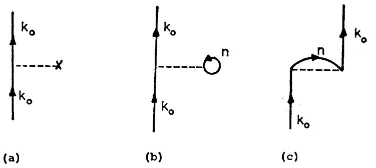

FIG. 4. Phase-shift corrections from the first-order optical-potential diagrams.

Another remark can be made about the choice of V^s. The choice of V^s is by no means limited to the one in Eq. (2.15). For example, we can write a more general expression[9]

$$\langle i|\,V^s\,|j\rangle=\sum_{n=1}^{Z}\left(\langle in|v|jn\rangle-\langle in|v|nj\rangle\right)+\Big(I-\sum_{n=1}^{Z}\Pi_n\Big)V_p\Big(I-\sum_{n=1}^{Z}\Pi_n\Big)\,. \qquad (2.16)$$

The projection operator Π_n projects out the nth Hartree-Fock atomic state orbital; V_p is some arbitrary potential that one may wish to introduce. The expression in Eq. (2.16) will always satisfy the condition that it generates the Hartree-Fock ground states of the atom. We shall return to Eq. (2.16) later in the discussion.

When we choose $V^s=V_{\text{HF}}$, the single-particle equation (2.6) in configuration space is, more explicitly,

$$\left\{-\frac{\hbar^2}{2m}\nabla^2-\frac{Ze^2}{r}+\sum_{i=1}^{Z}\int d\mathbf{r}'\,\varphi_i^*(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\varphi_i(\mathbf{r}')d\mathbf{r}'\right\}\varphi_n(\mathbf{r})-\sum_{i=1}^{Z}\delta(m_{sn},m_{si})\int d\mathbf{r}'\,\varphi_i^*(r')\times\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\varphi_n(\mathbf{r}')\varphi_i(\mathbf{r})=\epsilon_n\varphi_n(\mathbf{r})\,. \qquad (2.17)$$

The Hartree-Fock orbitals of the atomic ground state are generated, since for $i=n$ the direct and the exchange terms cancel, so that the state n sees a potential due to the nucleus and $(N-1)$ other orbital electrons. For excited states, no such complete cancellation occurs, so the state n sees the field of the nucleus and N orbital electrons. From the work of Kelly[11] for Be and O, one expects no bound excited states. This was found to be true also for the helium case here. We invoked Levinson's theorem and looked for other bound excited states, but none were found.

The continuum single-particle state $\varphi(k,l,m,m_s)$ is determined by letting $\epsilon_n=k_n^2/2m$ in Eq. (2.17). Since the helium atom is close-shelled, we can assume spherical symmetry and write

$$\varphi(k,l,m,m_s)=[R(k,l;r)/r]Y_{lm}(\theta,\varphi)X_s(m_s)\,, \qquad (2.18)$$

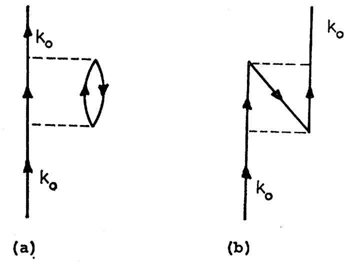

FIG. 5. Phase-shift corrections due to the second-order optical-potential diagrams. (a) Direct terms. (b) Exchange terms.

where the $Y_{lm}(\theta,\varphi)$'s are the usual spherical harmonics and $X_s(m_s)$ is the spin eigenfunction. The radial function $R(k,l;r)$ satisfies the radial equation, $L_0R(k,l;r) = k^2R(k,l;r)$, where

$$L_0=\left[-\frac{d^2}{dr^2}+\frac{2m}{\hbar^2}(V^{\text{nuclear}}+V^s)+\frac{l(l+1)}{r^2}\right]. \tag{2.19}$$

At large distances from the atom, where the potential is effectively zero, $R(k,l;r)$ becomes

$$\begin{aligned} R(k,l;r) &\propto kr[\cos\delta_0(k,l)j_l(kr)-\sin\delta_0(k,l)n_l(kr)] \\ &\sim \lim_{kr\to\infty} \cos(kr+\delta_0(k,l)-\tfrac{1}{2}(l+1)\pi). \end{aligned} \tag{2.20}$$

The $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and spherical Neumann functions, respectively. We adopt the normalization given in Eq. (2.19). With the radial wave function $R(k,l;r)$ thus normalized, it can be shown[11] that in calculations one may replace the summation over intermediate states φ_k by an integration over k with a factor $(2/\pi)$, i.e.,

$$\sum_k=\left(\frac{2}{\pi}\right)\int dk. \tag{2.21}$$

The $\delta_0(k,l)$ is the zeroth-order scattering phase shift, which is very similar to the result of the static approximation with exchange.

Scattering Phase Shift

As mentioned before, it is impracticable to solve the Schrödinger equation of the scattering electron since it will then be necessary to make an adiabatic approximation to the optical potential V_{op}. To avoid this dilemma, we shall instead obtain the phase shifts through a variational expression.[13] [The normalization convention (2.20) is imposed here.]

$$\begin{aligned} \delta_{\text{corrected}}(k_0,l) = \delta_0(k_0,l)-\frac{1}{k_0}\int_0^\infty & R^*(k_0,l;r) \\ &\times(L-k_0^2)R(k_0,l;r)dr, \end{aligned} \tag{2.22}$$

where

$$L=\left(-\frac{d^2}{dr}+\frac{2m}{\hbar^2}V_{\text{op}}+\frac{l(l+1)}{r^2}\right).$$

But the radial function $R(k,l;r)$ satisfies the radial equation (2.19). We thus have

$$\begin{aligned} \delta_{\text{corrected}}(k_0,l) &= \delta_0(k_0,l)-\frac{1}{k_0}\int_0^\infty R^*(k_0,l;r) \\ &\qquad\times(L-L_0)R(k_0,l;r)dr \\ &= \delta_0(k_0,l)-\frac{1}{k_0}\left(\frac{2m}{\hbar^2}\right) \\ &\qquad\times\int_0^\infty R^*(k_0,l;r)\mathcal{V}_{\text{op}}R(k_0,l;r)dr. \end{aligned} \tag{2.23}$$

The correction to the zeroth order phase shift is

$$\begin{aligned} \Delta\delta(k_0,l) &= \delta_{\text{corrected}}(k_0,l)-\delta_0(k_0,l) \\ &= -\left(\frac{2m}{k_0\hbar^2}\right)\int_0^\infty R^*(k_0,l;r)\mathcal{V}_{\text{op}}R(k_0,l;r)dr. \end{aligned} \tag{2.24}$$

In the present calculation, we shall retain only the contribution due to the second-order optical potential corresponding to Figs. 5(a) and 5(b). The direct and the exchange potentials contribute, respectively,

$$\begin{aligned} \Delta\delta_{\text{direct}}(k_0,l) &= -\sum_{n=1}^{Z}\frac{1}{k_0}\left(\frac{2m}{\hbar^2}\right)\sum_{k',k''}\frac{\langle k_0,n|v|k',k''\rangle^2}{\epsilon_n+k_0^2\hbar^2/2m-k'^2\hbar^2/2m-k''^2\hbar^2/2m} \\ &= -\left(\frac{1}{k_0}\right)\left(\frac{2m}{\hbar^2}\right)\left(\frac{2}{\pi}\right)^2\sum_{n=1}^{Z}\int\int\frac{\langle k_0n|v|k'k''\rangle^2}{\epsilon_n+(\hbar^2/2m)(k_0^2-k'^2-k''^2)}dk'dk'', \end{aligned} \tag{2.25}$$

$$\delta_{\text{exchange}}(k_0,l) = +\left(\frac{1}{k_0}\right)\left(\frac{2m}{\hbar^2}\right)\left(\frac{2}{\pi}\right)^2\sum_{n=1}^{Z}\delta(m_{sn},m_{sk_0})\int\int\frac{\langle k_0n|v|k'k''\rangle\langle k'k''|v|nk_0\rangle}{\epsilon_n+(\hbar^2/2m)(k_0^2-k'^2-k''^2)}dk'dk''. \tag{2.26}$$

The angular momentum indices of the k_0, k', k'' states have been suppressed in Eqs. (2.25) and (2.26). The integrations over k' and k'' are used since we have adopted the normalization as given in Eq. (2.20). The atomic state n for helium is the $1s$ state. Both orbital electrons in helium contribute to the direct part, while only one orbital electron contributes to the exchange part. When the angular momentum indices are specified,

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[13] T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962), p. 59.

we can further identify the contributions from the various multipole components. For example, let k_0 be in the s state; then for k' and k'' both in the s state we have the monopole component, while the dipole contribution comes from k' and k'' both in the p state. We shall use the notation $l_{k_0}l_nl_{k'}l_{k''}$ to denote these multipole contributions. For helium, where the atomic orbital state is an s state, $l_n=s$; the matrix element for the monopole component for the S wave is denoted ($ssss$), and the dipole component comes from matrix elements of the type ($sspp$), etc. For the P wave, the monopole-component matrix element is ($psps$), while the dipole component comes from ($pssp$) and ($psdp$) matrix elements, etc.

III. NUMERICAL PROCEDURE

In this calculation, the ground-state helium wave function was taken as the "compromise wave function" of Roothaan, Sachs, and Weiss.[14] The integro-differential equation (2.17) for the radial function of the continuum states was solved by Numerov's method.[15] The solution was integrated out from the origin to $R=10a_0$ (where a_0 is the Bohr radius). An iterative procedure was used and the convergence criterion was satisfied when successive values of the integral

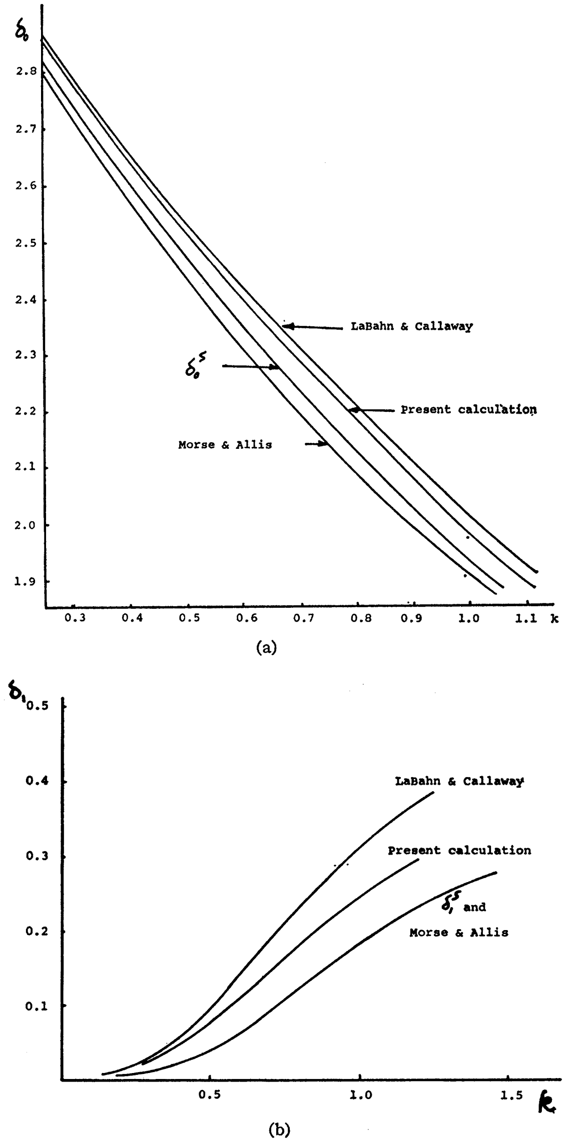
$$\int_0^\infty R_{1s}^*(r)\left(\frac{1}{r^{l+1}}\right)R(k,l;r)dr$$

differed by less than 0.0001. We used a mesh size $0.01a_0$ throughout. The zeroth-order phase shift $\delta_0(k,l)$ and the normalization were computed by fitting the wave function at two points in the asymptotic region, usually $R=9.5a_0$ and $R=10a_0$.

In evaluating all the integrals or matrix elements, Simpson rules or modified Simpson rules were used. In the integration over k' and k'' we used the limit k' and $k''=10$. The higher k', k'' region gives negligible contributions.

TABLE I. S-wave and P-wave phase shifts. (The δ^s's are the corresponding zeroth-order values.)

		S wave		P wave	
E (eV)	k	$\delta_0{}^s$	δ_0	$\delta_1{}^s$	δ_1
1.224	0.3	2.7048	2.7391	0.0105	0.0242
2.175	0.4	2.5672	2.6058	0.0233	0.0455
3.399	0.5	2.4356	2.4781	0.0422	0.0732
4.894	0.6	2.3111	2.3555	0.0663	0.1060
6.662	0.7	2.1942	2.2415	0.0943	0.1417
8.701	0.8	2.0850	2.1331	0.1243	0.1778
13.595	1.0	1.8900	1.9412	0.1831	0.2449
16.450	1.1	1.8036	1.8570	0.2096	0.2732



(a)

(b)

FIG. 6. (a) S-wave phase shifts. The momentum k is in atomic units. $E=\frac{1}{2}k^2$, where the unit of energy E is equivalent to 27.2 eV. (b) P-wave phase shifts. The momentum k is in atomic units. $E=\frac{1}{2}k^2$, where the unit of energy E is equivalent to 27.2 eV.

IV. RESULTS AND DISCUSSION

In Table I we have tabulated the phase-shift values from the present calculation for $l=0$ and $l=1$ partial waves in the energy range 1.2 to 16.4 eV. Also presented there are our zeroth-order phase shifts. To compare with other theoretical calculations, these are plotted in Figs. 6(a) and 6(b). For S-wave phase shifts, the static approximation with exchange of Morse and Allis[16] differs from our zeroth-order values through the energy difference term. For the P wave, the energy-difference term vanishes and indeed our zeroth-order result agrees

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[14] C. C. J. Roothaan, L. M. Sachs, and A. W. Weiss, Rev. Mod. Phys. 32, 186 (1960).

[15] M. G. Salvadori and M. L. Baron, *Numerical Methods in Engineering* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1961).

[16] P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933).

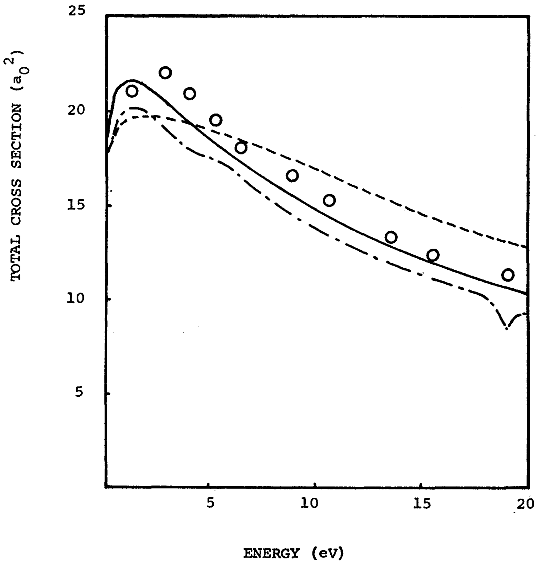

FIG. 7. Total cross section (in units of a_0^2) as a function of energy. The dashed curve represents the theoretical calculation of LaBahn and Callaway (Ref. 17); the solid curve is our present calculation. The circles and dot-dash curves represent, respectively, the experimental results of Ramsauer and Kollath (Ref. 18), and Golden and Bandel (Ref. 19).

well with that of Morse and Allis. The calculation of LaBahn and Callaway[17] takes into account the distortion effect (dipole component only) but employs the adiabatic approximation. As can be seen, our result lies between that of LaBahn and Callaway and that of Morse and Allis. This is not too surprising, since the adiabatic-exchange calculation of LaBahn and Callaway in general tends to overestimate the polarization effect, while the static approximation with exchange of Morse and Allis completely neglects it. It is interesting to observe that at low energies our results are closer to the results of LaBahn and Callaway, but move toward the values of Morse and Allis as the energy of the scattering electron increases, indicating the growing importance of the nonadiabatic effect. At higher energies we expect our results to approach that of our zeroth-order phase shift. It seems that even in this application, where the polarizability of helium is relatively small, the nonadiabatic effect is still appreciable and the adiabatic condition can be valid only in very low energy regions. For more polarizable atoms, such as the alkali atoms, one may have to take into account the nonadiabatic effect even at zero energy.

The total cross section is plotted in Fig. 7 along with the theoretical calculation of LaBahn and Callaway[17] and two experimental results, one by Ramsauer and Kollath[18] and the more recent one by Golden and Bandel.[19] The result of Morse and Allis,[16] which follows closely the experimental result of Golden and Bandel at higher energies but diverges to infinity at low energy, is not shown in Fig. 7. We have extended our curve below 1.2 eV by extrapolating our phase shift values below $k=0.3$. Our result is very good and lies, in general, between the two experimental results. In particular, the shape of our curve is remarkably similar to that of Golden and Bandel.

The momentum-transfer cross-section data offer another comparison. This is shown in Fig. 8. Again our result gives much better agreement with the experimental data of Crompton and Jory[20] and those of Frost and Phelps.[21] Thus the result of this calculation indicates that the present approach, with the inclusion of second-order optical potential, is sufficient to yield good results for electron-atom scatterings.

The diagrammatic approach of the present method, as mentioned earlier, offers the possibility of assessing the contribution of different physical effects. There are two questions of interest we can explore with regard to the contribution of the second-order optical potential to scattering phase shifts. The first one concerns the exchange contribution of the second-order optical potential. The second one concerns the relative importance of different multipole components in the second-order optical potential.

Calculations to date usually include the adiabatically approximated direct effect to the second order while retaining only the first-order exchange effect. In Figs. 9 and 10 we have plotted the monopole, dipole, and quadrupole components of the second-order direct and exchange contribution to the S-wave and P-wave phase

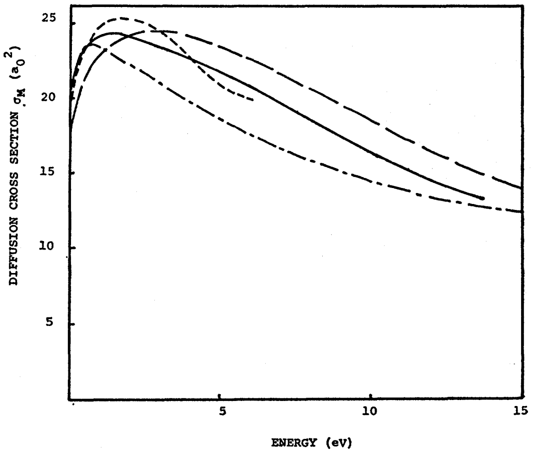

FIG. 8. Momentum-transfer cross-section data. Long-dash curve is that of LaBahn and Callaway (Ref. 17), the solid curve is our present calculation. The short-dash and dot-dash curves are the experimental results, respectively, of Crompton and Jory (Ref. 20), and Frost and Phelps (Ref. 21).

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[17] R. LaBahn and J. Callaway, Phys. Rev. **135**, A1539 (1964).

[18] C. Ramsauer and R. Kollath, Ann. Physik **3**, 536 (1929); **12**, 529 (1932).

[19] D. E. Golden and H. W. Bandel, Phys. Rev. **138**, A14 (1965).

[20] R. W. Crompton and R. L. Jory, in *Abstracts of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, 1965* (Science Bookcrafters, Hastings-on-Hudson, New York, 1965), p. 118.

[21] L. S. Frost and A. V. Phelps, Phys. Rev. **136**, A1538 (1964).

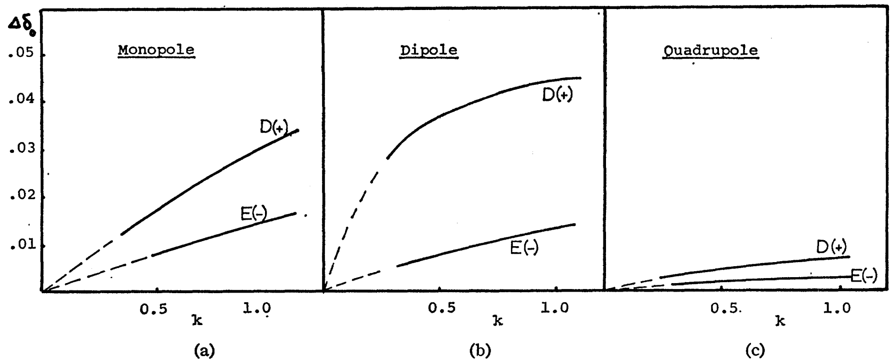

FIG. 9. Contributions to the S-wave phase shifts from multipole components. D = direct part; E = exchange part; ($\pm$) denotes the sign of the contribution.

shifts, respectively. The direct contribution comes from both orbital electrons, while only one orbital electron of parallel spin contributes to the exchange term. In most cases, the direct and the exchange contributions have opposite signs and therefore counteract each other. So the net contribution [except for Fig. 10(a)] from each multipole is the difference between the direct (D) and the exchange (E) curves in Figs. 9 and 10.

For the S-wave phase shift, as seen from Figs. 9(a), 9(b), and 9(c), the exchange contribution from the monopole component is very large, being nearly half that of the direct one. In the dipole part, the exchange contribution is less, but is still about 20–30% of the larger direct contribution. For the quadrupole, the exchange part is about 40% of the direct one, although both are small.

For the P-wave phase shift, the monopole component of the exchange part surprisingly has the same sign as the direct one. The total monopole contribution in this case [Fig. 10(a)] is the sum of the two curves. The dipole contribution for the P wave comes from two types of matrix elements, the *pssp* and the *psdp* types. Their exchange contributions are identical to the P-wave monopole exchange [Fig. 10(a)] and the quadrupole exchange [Fig. 10(c)] values, respectively, and thus are not individually drawn there. Since these two exchange contributions have opposite signs, the net dipole exchange contribution for the P wave is small. For the quadrupole contribution we have calculated the matrix element of *pspd* type. The exchange contribution is slightly larger in magnitude than the direct part.

The curves in Figs. 9 and 10 also show the relative importance of different multipole contributions to the phase shift. In general, as expected, the net dipole contribution is indeed dominant, since the long-range polarization effect comes from here. However, the net monopole contribution is quite sizable, especially for the s-wave case, being in general about 50% of the dipole contribution. The net quadrupole contribution is in general much smaller. Higher multipole contributions are expected to be small and therefore are not included.

From these results, we conclude that in general the exchange contribution of the second-order optical potential is very significant and must be properly included along with the direct part. It should be pointed out that the present approach does not treat completely the effect of the second-order optical potential. However, the conclusions we draw should be valid in general.

In a recent dynamic-exchange calculation, LaBahn and Callaway[22] observed that a better result can be obtained when they included only the dipole-contribution component while neglecting the monopole component. In the light of the present calculation this may be explained as follows. In their calculation, as in most calculations made to date, the second-order exchange effect is neglected. For the most important S-wave phase shift, our present calculation shows that the net monopole contribution [see Fig. 9(a)] turns out to be nearly equal to the exchange part of the dipole contribution [Fig. 9(b)]. The neglect of the second-order exchange contribution and the omission of the monopole contribution thus balance each other and give a result very close to the correct one. On the other hand, if both the direct-dipole and monopole contributions are included, but with their respective exchange parts neglected, as in the calculation of LaBahn and Callaway, the total contribution becomes larger than the true one by almost a factor of two. Since this near-cancellation is purely coincidental, both the exchange effect and the monopole contribution should be properly included in any calculation.

In this application we have not calculated phase shifts for energies below 1.2 eV. The single-particle potential V^s we have used for this calculation is the Hartree-Fock potential V_{HF}. The zeroth-order phase shift is essentially the result of the static approximation with exchange. In this sense, the present calculation is expected to be more accurate as energy increases. The second-order optical potential contribution then carries the load of describing the entire distortion effect.

For extremely low energy regions, where the polarization effect is most important and the adiabatic approximation is most likely to be useful, one may choose a slightly different single-particle potential V^s, such as the one in Eq. (2.16), with V_p equal to some commonly used

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[22] R. W. LaBahn and J. Callaway (private communication) and Phys. Rev. **147**, 28 (1966). Their result is very close to the result of the present calculation.

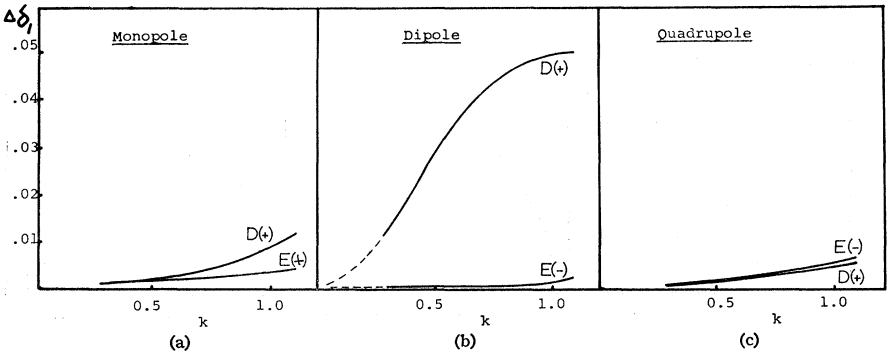

FIG. 10. Contributions to the P-wave phase shifts from multipole components. D = direct part; E = exchange part; $(\pm)$ denotes the sign of the contribution.

polarization potential such as the Buckingham potential or the type of potential given by Bethe,[23] and Callaway and Temkin.[24] The zeroth-order phase shift then already includes the effect of adiabatic polarization. The first-order optical potential will not in general vanish. The first- and second-order optical potentials will carry the much lighter load of describing only the nonadiabatic corrections. The flexibility of the choice in V^s should enable one to use this approach in a wide range of energies.

V. CONCLUSIONS

In this paper we have introduced a modified optical-potential approach for the calculation of elastic electron-atom scattering at low energies. The method is general and in principle can be readily applied to cases where the target atom is more complex. Corrections to the elastic phase shift by higher order optical potentials can be included in a systematic manner and the Pauli principle is preserved in each order. From the results of our application to e-He scattering in this paper, the approach is shown to be able to yield excellent results with the inclusion of only up to the second-order optical potential. This important feature makes the present approach not only general but also practical. The freedom in choosing the single-particle potential V^s gives the method an additional degree of flexibility. Another feature associated with the method is the fact that one may study the influence of various physical effects in detail. Thus in the e-He case we found that the effect of exchange in the second-order optical potential is actually very significant. Higher order diagrams, for example, can yield information on the influence of many-body correlation effects on the scattering process.

Perhaps the most appealing feature of the present approach is its simplicity. Once the single-particle potential V^s is chosen, one can simply generate the complete set of single-particle wave functions and compute the second-order optical potential contributions to the phase shifts in a straightforward manner. There is no need for the dubious adiabatic approximation, with its usual problems such as the determination of the dipole polarizability value α, or the uncertainty of the choice of *ad hoc* cutoff parameters.

The modified optical-potential approach is now being applied to other more complex scattering situations. These investigations are necessary to further assess the usefulness and limitations of the present method as a practical approach for general electron-atom elastic scattering.

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[23] H. A. Bethe, *Handbook of Physics* (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943), Vol. 24, Part 1, p. 339 ff.

[24] J. Callaway, Phys. Rev. **106**, 868 (1957); A. Temkin, *ibid.* **107**, 1004 (1957).