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A Modified Optical Potential Approach To Low-energy Electron-Helium Scattering*

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ABSTRACT

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 second order optical potential without recourse to the usual adiabatic approximation. The diagramatic 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 energy range 1.2 ev. 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 second order optical potential, usually neglected in most calculations, was found to be very significant.

INTRODUCTION

In the theoretical calculation of electron-atom scatterings 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 Schrodinger equation such 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 exclusion 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 the polarization effect, arises from the distortion experienced by the atomic electrons in the presence of the incident electron's Coulomb field. The distortion or the 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 $-\frac{\alpha}{r^4}$ where α is the polarizability of the atom. This is the familiar adiabatic condition usually assumed for low energy scattering processes.[1] The validity of the adiabatic 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 such that it will 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 non-adiabatic effect will be considerable. The actual potential as seen by the scattering electron is therefore a very complicated non-local (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 non-adiabatic 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 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 non-adiabatic approach[7] which do take non-adiabatic 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 diagramatic approach

similar to the Bruckner-Goldstone's linked-cluster perturbation expansion[10] which was successfully applied by Kelly to the atomic correlation energy calculations.[11] Formally, this optical potential does contain all the non-adiabatic effects, as previously described, through the propagators which contains 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 Schrodinger 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 $-\frac{\alpha}{r^4}$ dipole polarization potential. To remedy the divergent behavior at small r, some ad hoc cut-off parameters must be introduced such as the parameter d, in the Buckingham type potential $-\frac{\alpha}{(r^2+d^2)^2}$. 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 solve the optical potential expression and then trying to solve the subsequent Schrodinger equation, we use the optical potential directly in a variational expression for the scattering phase shifts. The associated diagramatic 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 potential 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 be then 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 electron-helium scattering for energies from 1.2 ev. to 16.4 ev. with gratifying result.

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

Section 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 Green's function for the system. In the following brief review, we aim to give some plausibility argument for their final optical potential expression. To add some clarity, we have made a slight deviation by invoking the result from the Brueckner-Goldstone linked-cluster perturbation expansion.[10] For 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.

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

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.

$$E = \mathcal{E}_0 + \frac{k_0^2}{2m} \tag{2.4}$$

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 so that the total system is approximated by an unperturbed system Ψ_0 with a Hamiltonian

$$H_0 = \sum_{i=1}^{Z+1} (T_i + V_i^s)$$

$$H_0 \Psi_0 = E \Psi_0$$

$$H' = H - H_0 = \sum_{i>j}\sum v_{ij} - \sum_i V_i^s \tag{2.5}$$

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 condition makes 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 are used as the basis for perturbation expansion.

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

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

and

$$H' = \sum_{pqmn} \langle pq|v|mn\rangle \eta_p^+ \eta_q^+ \eta_m \eta_n - \sum_{p,m} \langle p|V^s|m\rangle \eta_p^+ \eta_m \qquad (2.7)$$

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

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

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

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 $\langle qp|v|nm\rangle$.

Let us designate $\Phi_0(Z)$ as the Hartree-Fock ground state of 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

$$\Psi_0 = \eta_{k_0}^+ |\Phi_0\rangle \qquad (2.8)$$

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

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

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

and
$$H'(t) = e^{iH_0 t} H' e^{-iH_0 t} e^{\alpha t}$$

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 as 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 2 z lines at the top, z particle lines and z hole lines.

Similarly the true solution for the entire scattering system is

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

The diagrams representing Ψ has 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 $\psi(k_0)$ we project $\Psi(Z+1)$ onto $\Phi(Z)$

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

In terms of diagrams, 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

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

Where the symbol LP means that one sum diagrams only 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. 3a is a proper diagram while the diagram Fig. 3b is not. The reason for the requirement of the "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 conventional optical potential formulation that the ground state of atom can not occur in the intermediate state.[8]

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

$$(T + V^s + \mathcal{V}_{op})\, \psi(k_0) = \frac{k_0^2}{2m} \psi(k_0)$$

or

$$\left(K + V^{nuclear} + V^{s} + \mathcal{V}_{op} \right) f(k_0) = \frac{k_0^2}{2m} f(k_0) \quad (2.14^1)$$

The total optical potential V_{op} is then

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

Choice of Single Particle Potential

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

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

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

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 equation (2.15). For example, we can write a more general expression,

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

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

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

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + \sum_{i=1}^{Z} \int d\underset{\sim}{r}'\, \varphi_i^*(\underset{\sim}{r}')\left(e^2/|\underset{\sim}{r}-\underset{\sim}{r}'|\right)\varphi_i(\underset{\sim}{r}')\, d\underset{\sim}{r}'\right\}\varphi_n(\underset{\sim}{r})$$

$$- \sum_{i=1}^{Z} \delta(m_{sn}, m_{si}) \int d\underset{\sim}{r}'\, \varphi_i^*(r')\left(e^2/|\underset{\sim}{r}-\underset{\sim}{r}'|\right)\varphi_n(\underset{\sim}{r}')\,\varphi_i(\underset{\sim}{r}) = \epsilon_n \varphi_n(\underset{\sim}{r}) \tag{2.17}$$

The Hartree-Fock orbitals of atomic ground state is generated since for i=n the direct and the exchange terms cancel so 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 a field of nucleus and N orbital electrons. From the works of Kelly for Be and O[11], one expects that no bound excited states. This was found to be true also for the Helium case here. We invoked the 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 $\epsilon_n = \frac{k_n^2}{2m}$ in equation (2.17). Since helium atom is close-shelled, we can assume spherical symmetry and write

$$\varphi(k,\ell,m,m_s) = \frac{R(k,\ell;r)}{r} Y_{\ell m}(\theta,\varphi) X_s(m_s) \tag{2.18}$$

where the $Y_{\ell m}(\theta,\varphi)$ is the usual spherical harmonics and $X_s(m_s)$ is the spin eigenfuctions. The radical function $R(k,\ell;r)$ satisfies the radical equation, $L_0 R(k,\ell;r) = k^2 R(k,\ell;r)$ where

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

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

$$R(k,\ell;r) \propto kr\left[\cos\delta_0(k,\ell)\, j_\ell(kr) - \sin\delta_0(k,\ell)\, N_\ell(kr)\right]$$

$$\sim \lim_{kr\to\infty} \cos\left(kr + \delta_0(k,\ell) - \frac{(\ell+1)}{2}\pi\right) \tag{2.20}$$

The $j_\ell(kr)$ and $N_\ell(kr)$ are the spherical Bessel and spherical Neumann functions respectively. We adopt the normalization given in equation (2.19). With the radial wave function $R(k,\ell;r)$ thus normalized it can be shown[11] that in calculations one may replace the summation over intermediate states φ_k by an investigation over k with a factor $\left(\frac{2}{\pi}\right)$, i.e.

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

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

Scattering Phase Shift

As mentioned before, it is impracticable to solve the Schrodinger

equation of the scattering electron since it will then be necessary to make the adiabatic approximation of the optical potential V_{op}. To avoid this dilemma, we shall instead obtain phase shift through a variational expression.[13] (Normalization convention (2.20) is imposed here.)

$$\delta_{exact}(k,\ell) = \delta_0(k,\ell) - \frac{1}{k_0}\int_0^\infty R^*(k,\ell;r)\,(L-k_0^2)\,R(k,\ell;r)\,dr \tag{2.22}$$

where $L = \left(-\frac{d^2}{dr} + \frac{2m}{\hbar^2}V_{op} + \frac{\ell(\ell+1)}{r^2}\right)$. But the radial function $R(k,\ell;r)$ satisfies the radial equation (2.19), we thus have.

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

The correction to zeroth order phase shift is,

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

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

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

$$\delta_{exchange}(k_0, \ell)$$

$$= -\left(\frac{1}{k_0}\right)\left(\frac{2m}{\hbar^2}\right)\left(\frac{2}{\pi}\right)^2 \sum_{n=1}^{Z} \delta(m_{sn}, m_{sk_0}) \iint \frac{\langle k_0 n | V | k' k'' \rangle \langle k' k'' | V | n k_0 \rangle}{\epsilon_n + \frac{1}{2m}(k_0^2 - k'^2 - k''^2)} dk' dk'' \quad (2.26)$$

The angular momentum indices of k_0, k', k'' states have been suppressed in equations (2.25) and (2.26). The integrations over k' and k'' are used since we have adopted the normalization as given in equation (2.20). The atomic state n for helium is in $1S$ state. Both orbital electrons in helium contributes to the direct part, while only one orbital electron contributes to the exchange part. When angular momentum indices are specified, we can further identify the contributions from various multipole components. For example, let k_o be in S-state, then for k' and K" both in S-state we have the monopole component while dipole contribution comes from k' and k" both in P-state. We shall use the notation $\ell_{k_0} \ell_n \ell_{k'} \ell_{k''}$ to denote these multipole contributions. For helium, where the atomic orbital state is S-state $\ell_n = S$, the matrix element for monopole component for S-wave is denoted (SSSS) and the dipole component comes from matrix element type (SSPP), etc. For P-wave, the monopole component matrix element is (PSPS) while the dipole component comes from (PSSP) and (PSDP) matrix elements, etc.

Section III: NUMERICAL PROCEDURE

In this calculation the ground state helium wave function were 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 is integrated out from origin to $R=10A_o$ (unit is Bohr radius). Iterative procedure is used and convergence criterion is satisfied when successive values of the integral

$\int_0^\infty R^*_{1s}(r)\left(\frac{1}{r^{\ell+1}}\right)R(k,\ell;r)\,dr$ differ by less than 0.0001. We have used a mesh size 0.01 A_o throughout. Zeroth order phase shift $\delta_0(k,\ell)$ and the normalization were computed by fitting the wave function at two points in the asymptotic region, usually $R=9.5A_o$ and $R=10A_o$.

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

Section IV: RESULTS AND DISCUSSIONS

In Table 1 we have tabulated the phase shift values from the present calculation for $\ell = 0$ and $\ell = 1$ partial waves in energy range 1.2 ev. to 16.4 ev. Also presented there are our zeroth order phase shifts. To compare with other theoretical calculations, these are plotted in Figures 6a and 6b. 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 P-wave, the energy difference term vanishes and indeed our zeroth order result agrees 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 seem, our result lies between that of LaBahn and Callaway and that of Morse and Allis. It 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 non-adiabatic effect. At higher energies we expect our result 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 non-adiabatic effect is still appreciable and the adiabatic condition can be valid only at very low energy regions. For more polarizable atoms such as the alkali atoms, one may have to take into account the non-adiabatic 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 with the experimental result of Golden and Bandel at higher energies but diverges to infinity at low energy, is not displayed 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 offers 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 that 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 diagramatic 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 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 they cancel each other. So the net contribution (except for Fig. 10a) from each multipole is the difference between the direct (D) and the exchange (E) curves in Figs. 9 and 10.

For S-wave phase shift, as seen from Figs. 9abc, 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 quadrupole, the exchange part is about 40% of the direct one although both are small.

For 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. 10a) is the sum of the

two curves. The dipole contribution for P-wave comes from two types of matrix elements, the PSSP and the PSDP type. Their exchange contribution is identical to the P-wave monopole exchange (Fig. 10a) and the quadrupole exchange (Fig. 10c) values respectively and thus are not individually drawn there. Since these two exchange contributions have opposite signs, the net dipole exchange contribution for 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, one concludes 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.

In a recent dynamic-exchange calculation[22], LaBahn and Callaway 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. 9a) turns out to be nearly

equal to the exchange part of the dipole contribution (Fig. 9b). The neglect of the second order exchange contribution and the omission of the monopole contribution thus balances each other and gives 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 their calculation, 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 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 and as the one in equation (2.16) with V_p equal to some commonly used polarization potential such as the Buckingham potential or the type of potential given by Bethe[23] and Callaway-Temkin.[24] The zeroth order phase shift then includes already the effect of adiabatic polarization. The first order optical potential will not in general vanish. The first and the second order optical potential will carry a much lighter load of describing only the non-adiabatic corrections. The flexibility of the choice

in V^S should enable one to use this approach in a wide range of energies.

Section V: CONCLUSION

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 orders optical potential can be included in systematic manner and the Pauli principle is preserved in each order. From the results of our application to the 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 the 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 contributes to phase shifts in a straight-forward 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 cut-off 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 scatterings.

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TABLE 1

S-WAVE AND P-WAVE PHASE SHIFTS

(δ^s s ARE THE CORRESPONDING ZEROTH ORDER VALUES)

		S-WAVE		P-WAVE	
E (eV)	k	δ_0^s	δ_0	δ_1^s	δ_1
1.224	.3	2.7048	2.7391	0.0105	0.0242
2.175	.4	2.5672	2.6058	0.0233	0.0455
3.399	.5	2.4356	2.4781	0.0422	0.0732
4.894	.6	2.3111	2.3555	0.0663	0.1060
6.662	.7	2.1942	2.2415	0.0943	0.1417
8.701	.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

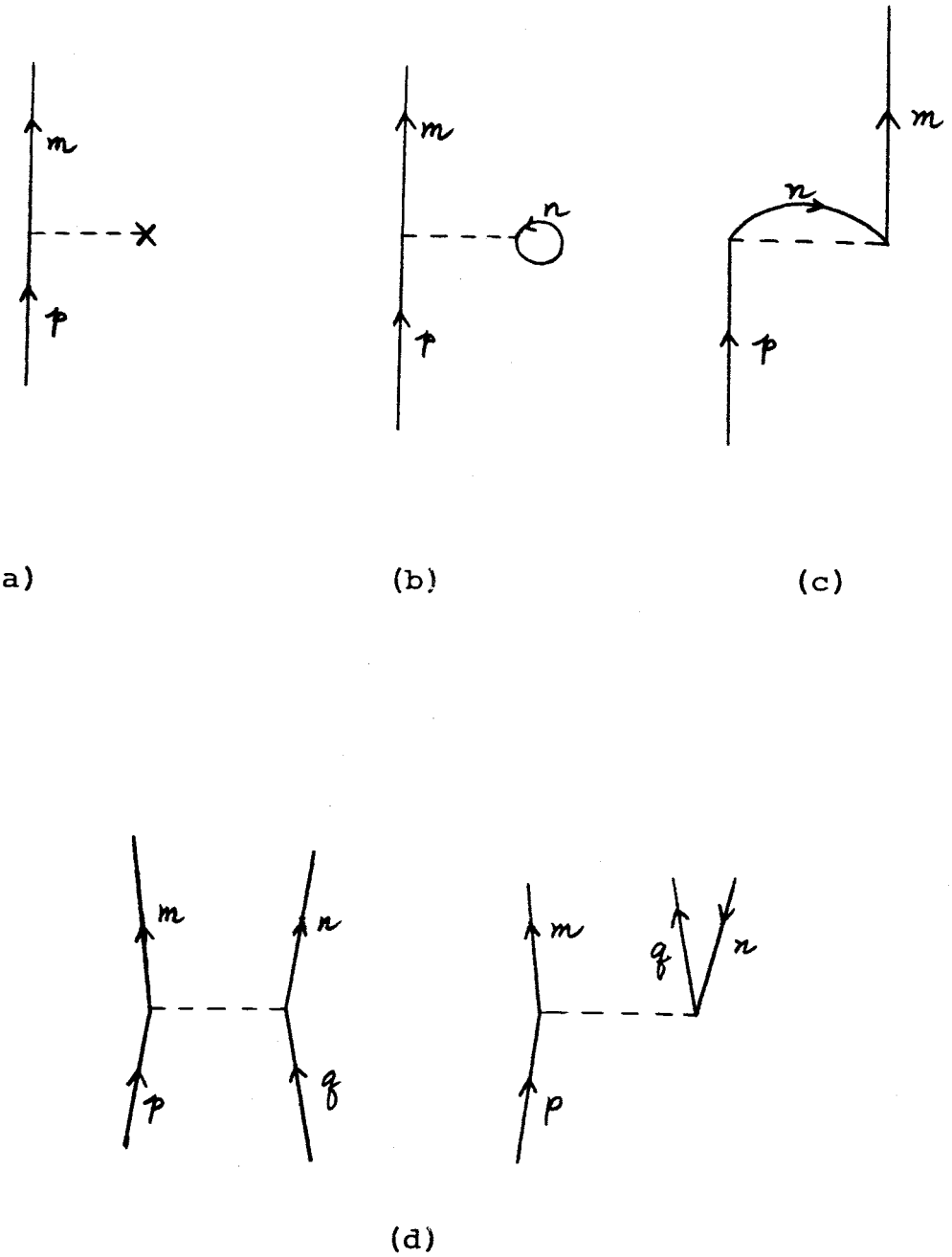


Figure 1. Diagrams representing various interaction matrix elements:

(a) Single particle potential,

(b) Direct interaction with hole state n,

(c) Exchange interaction with hole state n.

(d) General interaction matrix elements

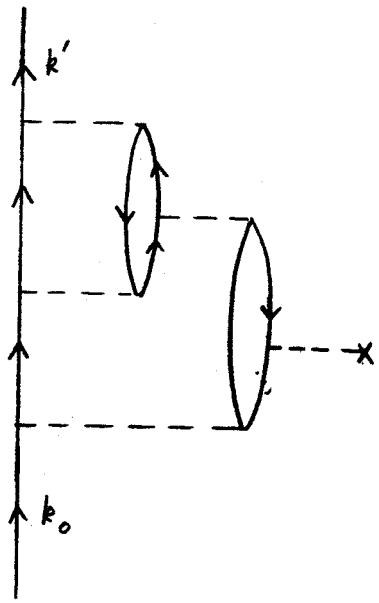
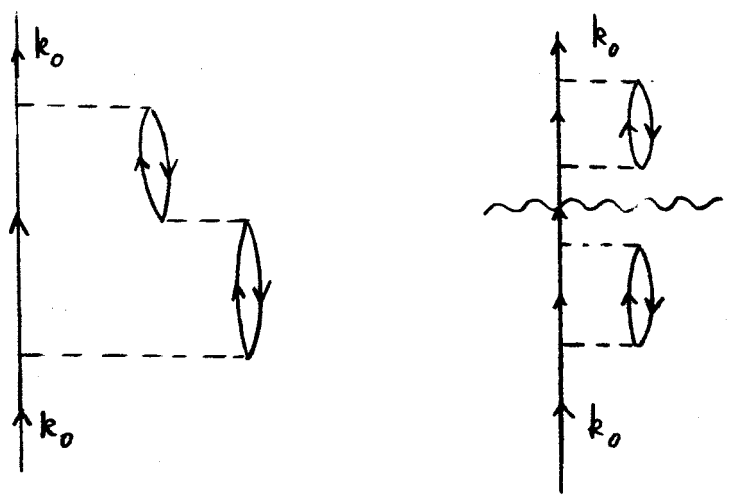


Figure 2. A general diagram for



(a) (b)

Figure 3.

(a) A linked and proper diagram.

(b) An improper linked diagram where a single particle line occurs in intermediate state.

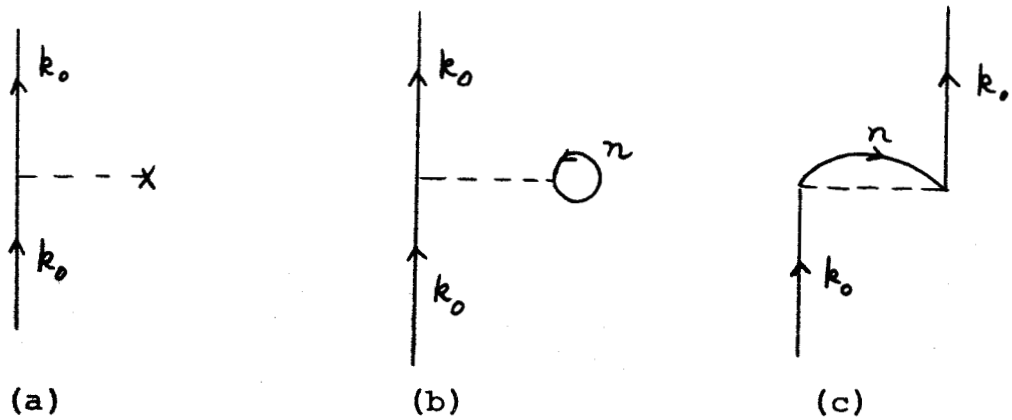


Figure 4. Phase shift corrections from the first order optical potential diagrams.

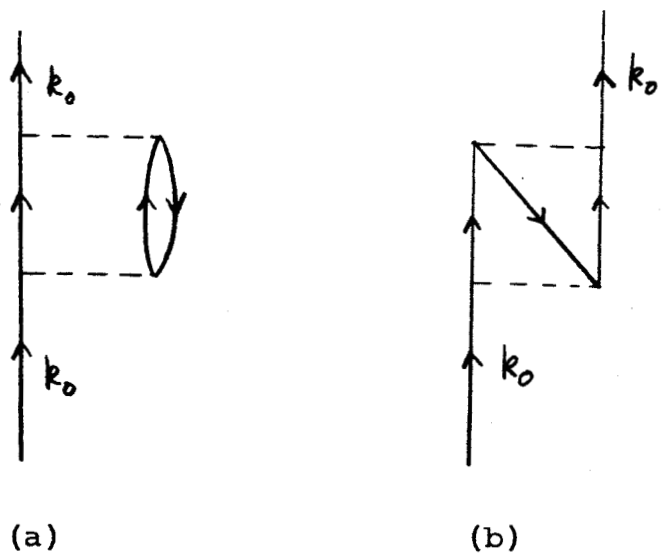


Figure 5. Phase shift corrections due to the second order optical potential diagrams.

(a) Direct term.

(b) Exchange term.

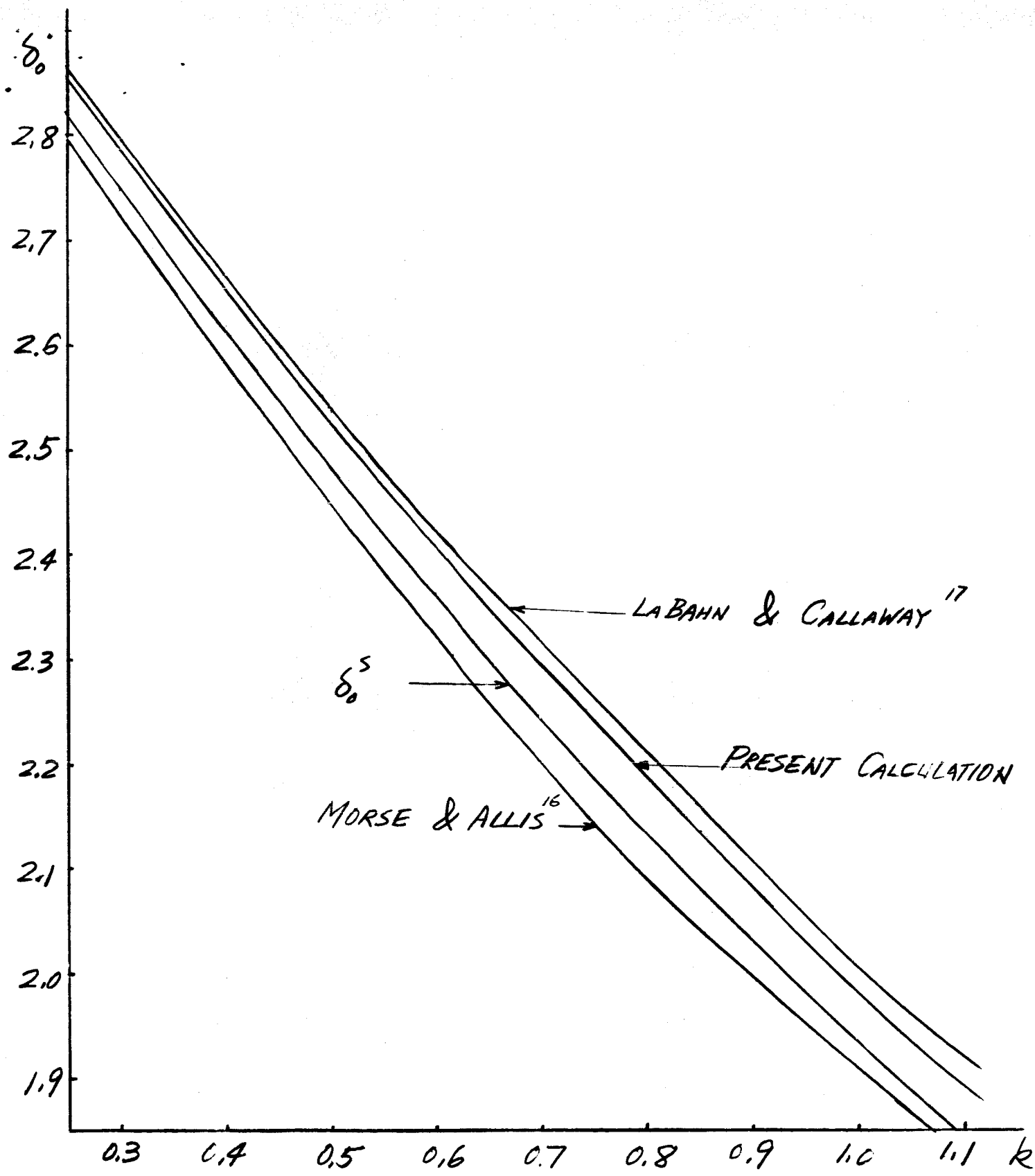


FIG. 6a

S-WAVE PHASE SHIFTS

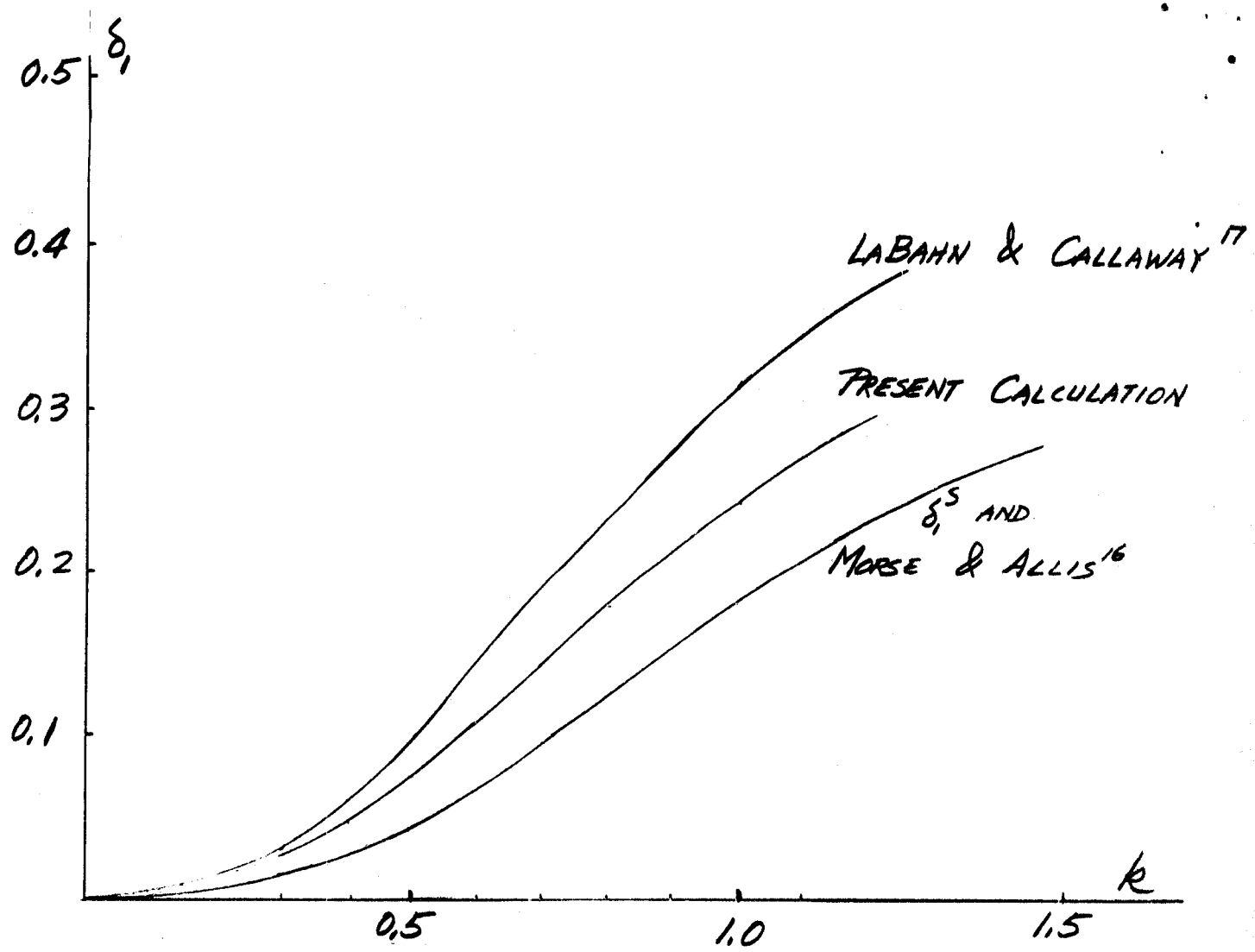


FIG. 6b

P-WAVE PHASE SHIFTS

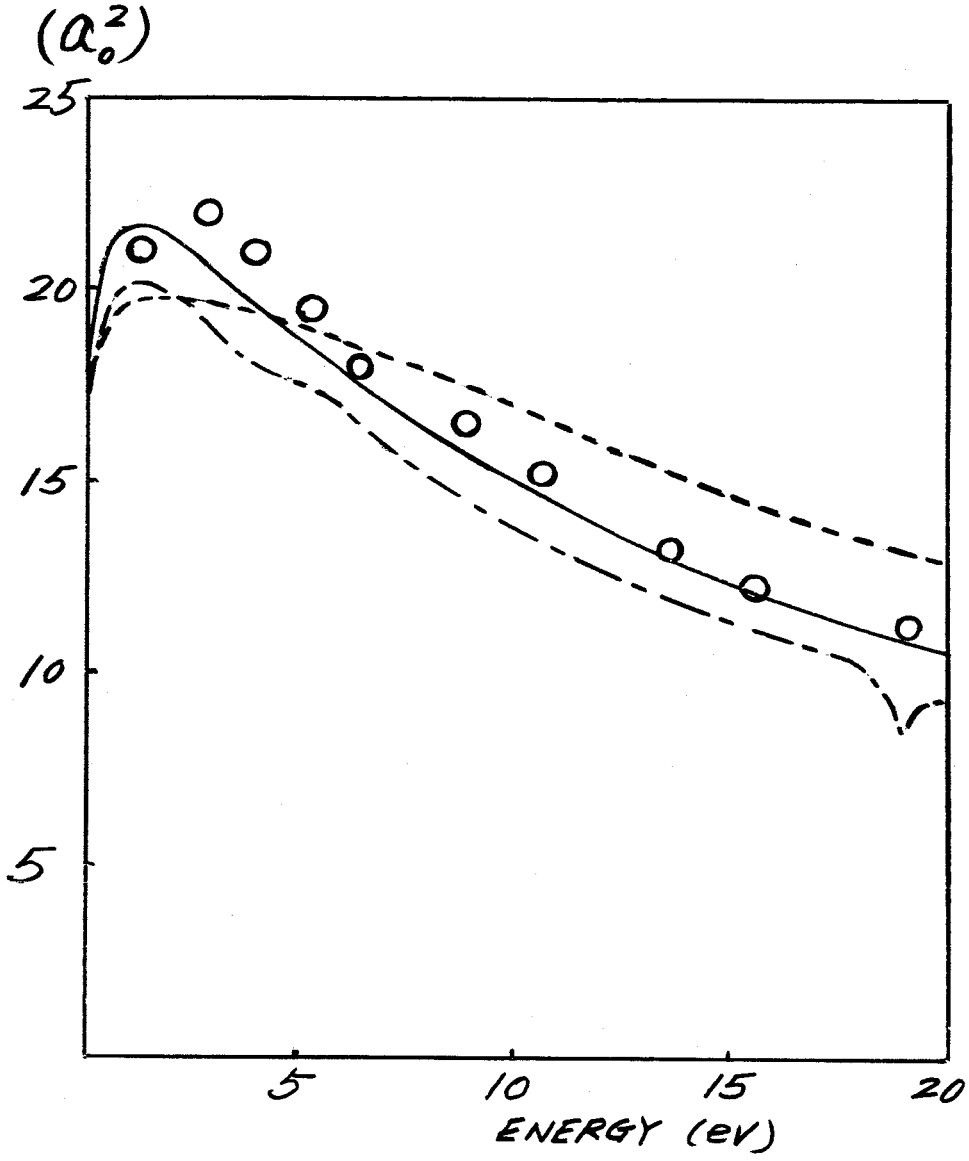


FIG. 7

TOTAL CROSS SECTION $\sigma\ (a_0^2)$

- - - - - - - - LA BAHN & CALLAWAY[17]

———————— PRESENT CALCULATION

O RAMSAUER & KOLLATH[18] } EXP.

— — — — — GOLDEN & BANDEL[19] } EXP.

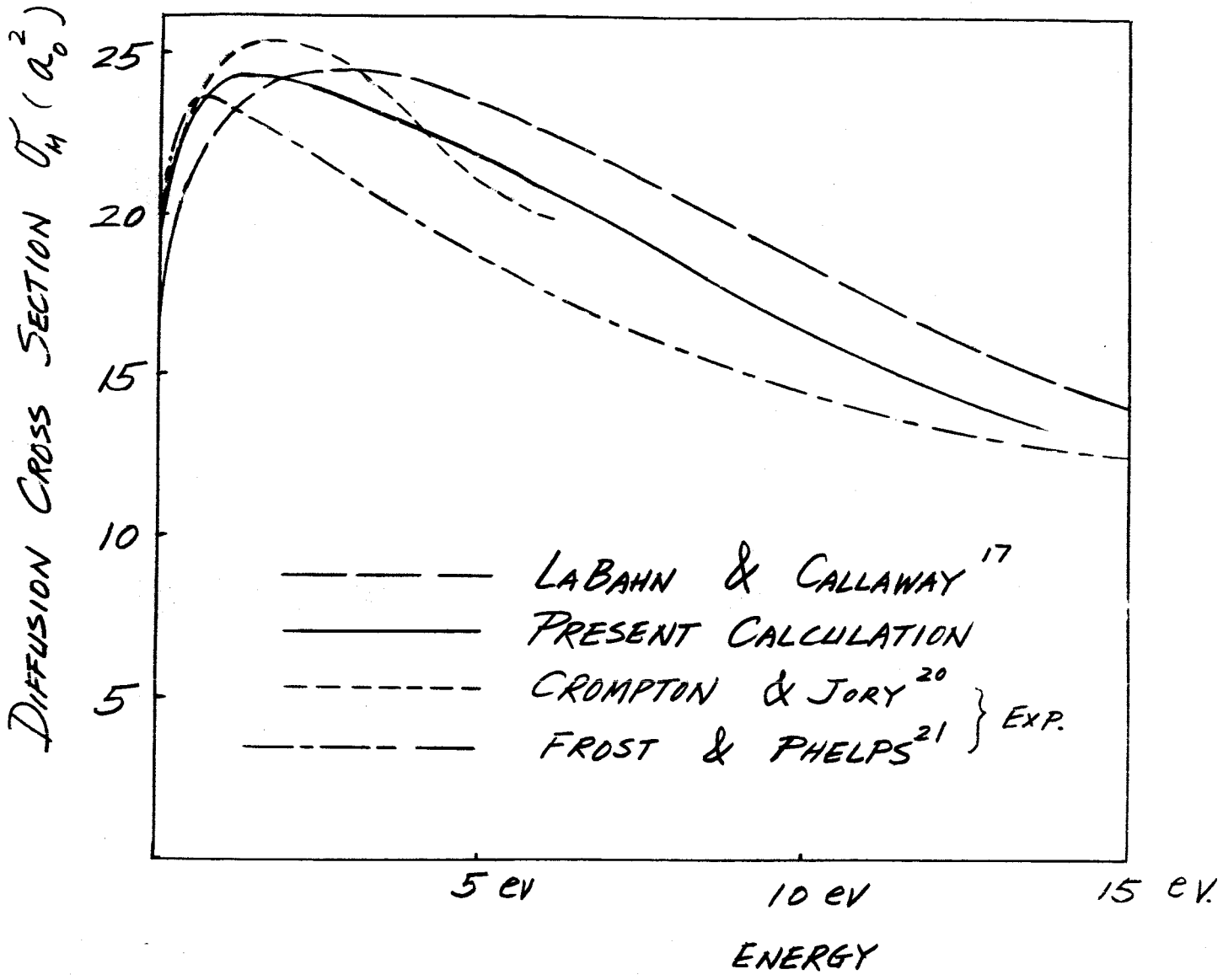

DIFFUSION CROSS SECTION σ_M (a_0^2)
25
20
15
10
5
LABAHN & CALLAWAY 17
PRESENT CALCULATION
CROMPTON & JORY 20
FROST & PHELPS 21
EXP.
5 eV
10 eV
15 eV.
ENERGY

FIG. 8

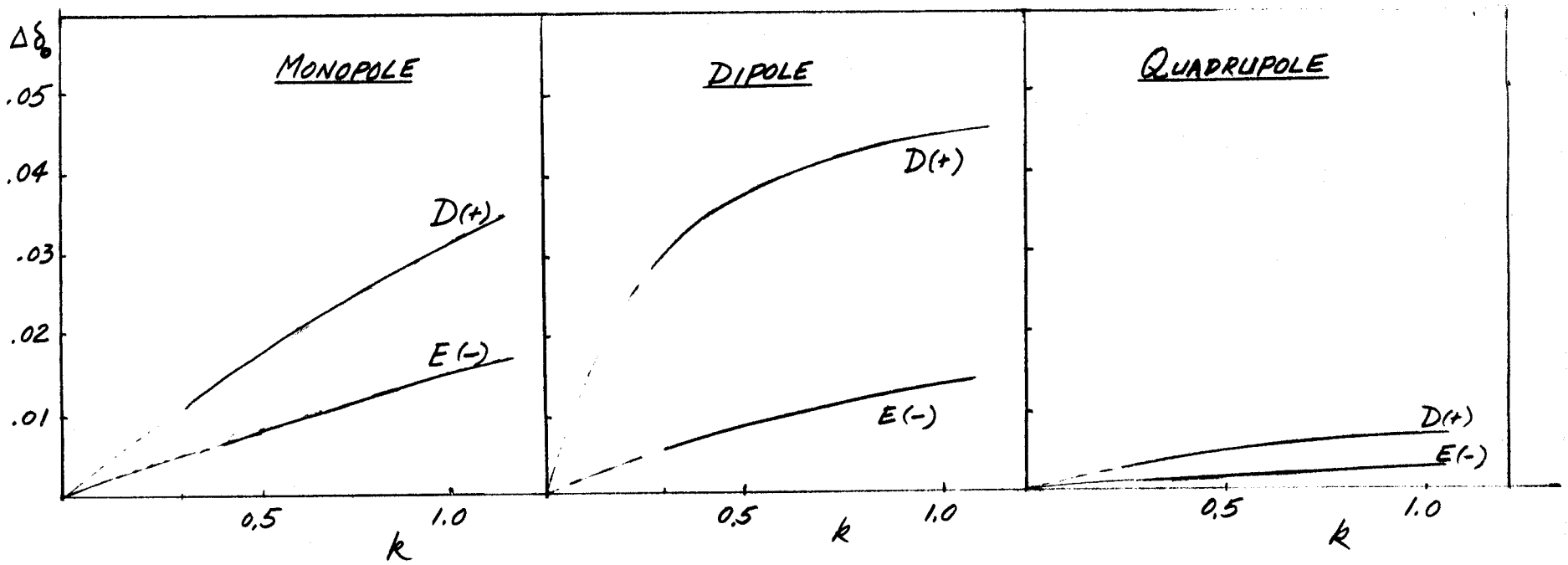


FIGURE 9.

CONTRIBUTIONS TO THE S-WAVE PHASE SHIFTS FROM MULTIPOLE COMPONENTS. D : DIRECT PART E : EXCHANGE PART. (±) DENOTES THE SIGN OF CONTRIBUTION

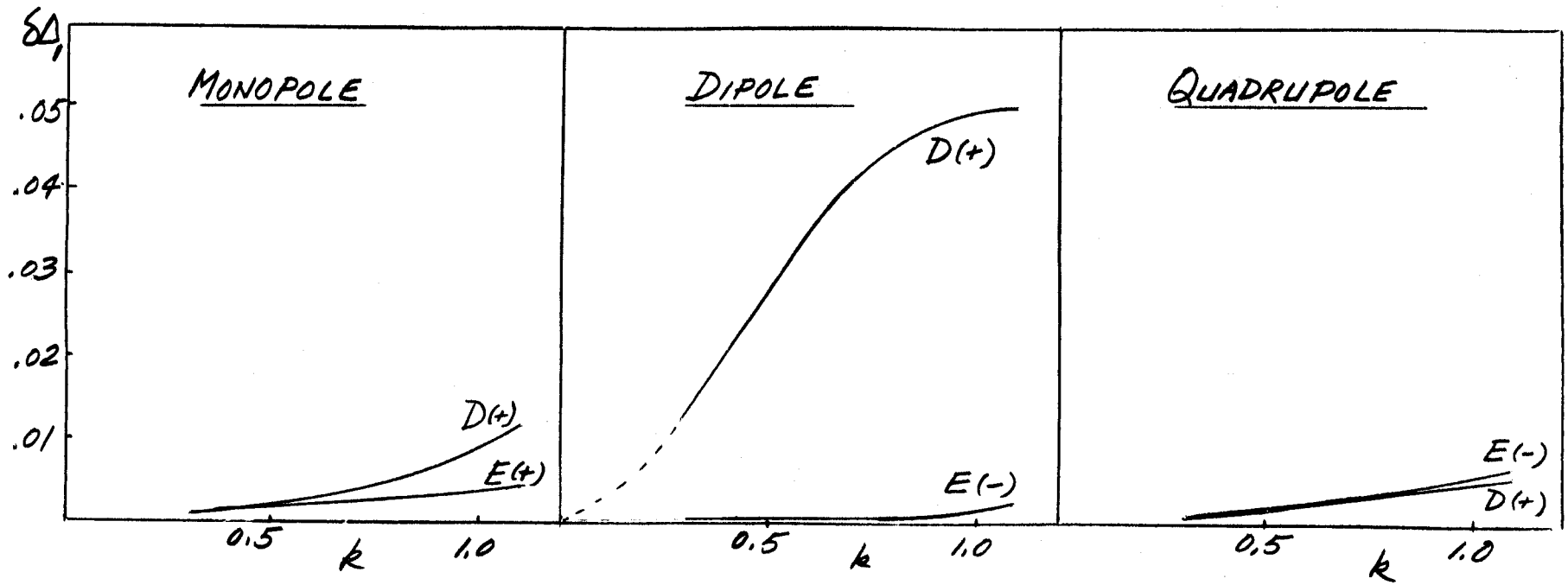


FIGURE 10

CONTRIBUTIONS TO THE P-WAVE PHASE SHIFTS FROM MULTIPOLE COMPONENTS. D = DIRECT PART E = EXCHANGE PART. (±) DENOTES THE SIGN OF CONTRIBUTION.

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