where $\theta_i' = k_i r - \eta_i \ln 2k_i r$. From Eq. (2a)

$$F_{ij}(r) \sim k_i^{-1/2}[(\sin\theta_i' \cos\phi_i - \cos\theta_i' \sin\phi_i)\delta_{ij} + (\cos\theta_i' \cos\phi_i + \sin\theta_i' \sin\phi_i)\mathcal{R}_{ij}],$$

where $\phi_i = l_i \pi/2 - \sigma_{l_i}$. Combining this result with (40) gives the required N_A equations

$$\cos\phi_i\, \omega_i^j - \sin\phi_i\, \omega_{N_A+i}^j = k_i^{-1/2}\delta_{ij}, \tag{41}$$

where the superscript j denotes that the linear equations at the matching point for the parameters $\nu_1 \cdots \mu$ must be solved N_A times, with j characterizing these matched solutions. The elements of the real symmetric reactance matrix are then given by

$$\mathcal{R}_{ij} = k_i^{1/2}[\sin\phi_i\, \omega_i^j + \cos\phi_i\, \omega_{N_A+i}^j]. \tag{42}$$

Having obtained the $\mathcal{R}$ matrix it is a simple matter of matrix manipulation to obtain the T matrix and cross section using Eqs. (35) and (36).

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Elastic Scattering of Low-Energy Electrons from Atomic Helium*

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Scattering phase shifts have been computed for elastic electron scattering from neutral helium for an energy range from 0 to 50 eV. These computations were based upon an extension of Hartree-Fock theory in which the distortion induced in the atom by the incident electron is considered in the adiabatic approximation and developed in a perturbation expansion in the interaction between incident and atomic electrons. This expansion contains terms describing both the adiabatic polarization interaction and velocity-dependent corrections to it. The effects of these two interactions are examined by calculating the scattering in two approximations: first, a pure adiabatic-exchange calculation using the total polarization potential consistent with second-order perturbation theory; and second, a "dynamic-exchange" calculation in which all the dynamic terms consistent with second-order perturbation theory are included along with the polarization potential. An additional dynamic-exchange calculation in which only the dipole components of all the distortion terms are included is also considered. The computed phase shifts were used to determine the scattering cross sections and these are compared with other calculations and experimental data. Scattering lengths were also calculated by iteration of the pertinent equations at zero energy, and resulted in the values $1.097a_0$ for the adiabatic-exchange approximation and $1.186a_0$ and $1.181a_0$ for the dynamic-exchange approximations using, respectively, the total-distortion terms and the dipole components of these terms only. The dynamic-exchange values for the scattering length compare very favorably with the experimental value $1.18a_0$ determined independently from experimental data by Frost and Phelps and by Crompton and Jory. The dynamic-exchange approximation for the total scattering cross section agrees quite closely with the experimental data of Ramsauer and Kollath, while the corresponding diffusion cross section agrees quite well with the data of Crompton and Jory. These calculations show that best agreement with experiment is obtained when only the dipole components of *all* of the distortion terms are included in the formalism.

I. INTRODUCTION

In a previous paper,[1] the scattering of electrons by helium atoms was considered in an approximation in which the distortion of the target atom by the incident electron gave rise to an effective polarization potential which was added to the usual Hartree-Fock equations. The results of these calculations gave a cross section which was in good agreement with experiment at very low energies but was larger than the experimental values at higher energies. This discrepancy arises in part from oversimplification of the dynamics of the scattering electron in describing the distortion interaction. The main purpose of this paper is to report on some extended calculations for helium in which a velocity-dependent correction to the adiabatic theory is incorporated into the scattering equation.

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† Based in part on a dissertation submitted to the University of California, Riverside, in partial fulfillment of the requirements for the Doctor of Philosophy degree.

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The importance of the long-range $-\alpha/R^4$ polarization interaction for the energy dependence of the very-low-energy electron-atom cross section has been amply demonstrated in numerous calculations.[1–12] All of these, however, were based upon the adiabatic approximation in which the mutual distortion interaction is calculated by assuming the atom to be perturbed by the electric field of a stationary external charge. This approximation thereby assumes that the atomic electron distribution can readjust instantaneously for each position of the incident electron. Good results are obtained as long as the average velocity of the atomic electrons greatly exceeds that of the scattering electron. The latter condition is only satisfied in general for very low velocities (or energies) of the incident electron, since, even though this electron may have started at infinity with negligible velocity, it is accelerated by the attractive polarization interaction. This effect leads to velocity-dependent interactions which must be incorporated in the formalism to give an adequate treatment of the problem.

To date, specifically velocity-dependent interactions have generally been neglected in atomic-scattering calculations. The eigenfunction expansion (or close-coupling) methods do contain implicitly some account of this interaction according to the number of atomic states retained in the expansion.[13] Our approach is rather different, being based upon perturbed Hartree-Fock theory. In second order we obtain a velocity-dependent term in the final scattering equation. This interaction is repulsive and acts as a correction for the fact that when the velocity of the incident electron is not negligible the atomic-electron distribution cannot completely follow its motion. We moreover find that the velocity-dependent interaction determined in this approximation has the correct long-range behavior rather than being a truncated form like obtained in a limited-eigenfunction-expansion calculation.[13]

The extended Hartree-Fock (HF) formalism of our work is discussed in Sec. II. The resulting scattering equation is found to be very similar to the adiabatic-exchange equation of our previous paper,[1] differing mainly by the presence of a first-derivative term from the velocity-dependent interaction. This velocity-dependent term is discussed in Sec. III along with some additional distortion interaction terms which arise out of the formalism. A more complete expression for the polarization potential is also included. In Sec. IV we discuss the numerical procedures used to solve the scattering equation. The results of our calculations are given in Sec. V and discussed in relation to other recent theoretical predictions and experimental data.

II. DERIVATION OF THE SCATTERING EQUATION

The HF scattering equation is obtained by requiring that the variation of the integral

$$I=\int \Psi^*(H-E)\Psi d\tau \tag{1}$$

be zero, where Ψ is the total wave function for the three-electron system consisting of two bound electrons and the scattering electron. H is the total Hamiltonian,[14]

$$H=-\nabla_1{}^2-\nabla_2{}^2-\nabla_3{}^2-4/r_1-4/r_2-4/r_3 \\ +2/r_{12}+2/r_{23}+2/r_{13}, \tag{2}$$

$$r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|,$$

and E is the total energy,

$$E=E_A+k^2, \tag{3}$$

where E_A is the total electronic binding energy of the atom and k^2 is the energy of the scattering electron at infinite separation.

The importance of the electron-electron exchange interaction in low-energy atomic scattering theory is well established.[15] We thus require that the total wave function Ψ be completely antisymmetric in the interchange of any two electrons to satisfy the Pauli principle. To include both this and the distortion of the atom produced by the external electron, the total wave function is approximated as follows:

$$\Psi(1,2,3)=(3)^{-1/2}[\psi^{(3)}(1,2)\mathbf{S}(1,2)\varphi(3)\boldsymbol{\alpha}(3) \\ +\psi^{(1)}(2,3)\mathbf{S}(2,3)\varphi(1)\boldsymbol{\alpha}(1) \\ +\psi^{(2)}(3,1)\mathbf{S}(3,1)\varphi(2)\boldsymbol{\alpha}(2)], \tag{4}$$

in which $\varphi(n)$ represents the wave function for the scattering electron, $\psi^{(n)}(i,j)$ is the wave function of the two bound electrons i and j, perturbed by the field of a separated electron n, and $\mathbf{S}$ is the singlet spin function for the bound electrons,

$$\mathbf{S}(i,j)=(2!)^{-1/2}[\boldsymbol{\alpha}(i)\boldsymbol{\beta}(j)-\boldsymbol{\alpha}(j)\boldsymbol{\beta}(i)], \tag{5}$$

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[13] Cf. R. Pu, Lawrence Radiation Laboratory Report UCRL 10878, 1963 (unpublished), where it is shown that a $1s$-$2s$-$2p$ close-coupling configuration for hydrogen implicitly includes 73.5% of the long-range dipole component of the velocity-dependent interaction.

[14] Atomic units of length in Bohr radii and energy in rydbergs (13.6 eV) are used throughout this paper.

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

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are single-electron spinors with projections $m_s=+\frac{1}{2}$ and $-\frac{1}{2}$, respectively.

The bound-state wave functions $\psi^{(n)}(i,j)$ are determined to first order in the interaction with the scattering electron. They are thus of the form[3]

$$\psi^{(n)}(i,j)=\psi_{100}(i)\psi_{100}(j)+\psi_{100}(i)\chi(j;n)+\psi_{100}(j)\chi(i;n)\,,\quad(6)$$

where ψ_{100} denotes the unperturbed HF wave function for the helium ground state and $\chi(j;n)$ is the first-order perturbation correction describing the changes in the wave of atomic electron j under the influence of the electric field of a separated electron n. This perturbed wave function χ is determined in the adiabatic approximation and thus the total atomic wave function $\psi^{(n)}(i,j)$ is known beforehand and not subjected to variation.

Now, since the total energy of the system is known [given by Eq. (3)] and we are using known wave functions to represent the motion of the atomic electrons, the application of the variational principle to Eq. (1) is restricted to a variation of the unknown scattering electron wave function φ^*. When this is done and the results integrated over the atomic electron spin coordinates and rearranged slightly, we obtain the basic scattering equation

$$\int\psi^{*(3)}(1,2)[H-E][\psi^{(3)}(1,2)\varphi(3)-\psi^{(2)}(3,1)\varphi(2)]d\mathbf{r}_1d\mathbf{r}_2=0\quad(7)$$

for the scattering electron wave function φ. This equation is very complex as it stands and we thus resort to further approximations to obtain equations which can be reasonably adapted to numerical solution.

The first approximation to Eq. (7) that we considered was the subject of our previous paper[1] and referred to as the adiabatic-exchange approximation. This approximation may[16] be obtained by neglecting the perturbed orbital components in all the functions $\psi^{(n)}(i,j)$, except in one term of the direct-interaction part. The resulting adiabatic-exchange scattering equation may then be written in the form

$$\int\psi_{100}^*(1)\psi_{100}^*(2)[H-E][\psi^{(3)}(1,2)\varphi(3)-\psi_{100}(1)\psi_{100}(3)\varphi(2)]d\mathbf{r}_1d\mathbf{r}_2=0\,.\quad(8)$$

A second approximation to Eq. (7) which is somewhat more inclusive is the subject of this paper. In this approximation, we will retain the perturbed orbital components of both of the functions $\psi^{(3)}(1,2)$ in the direct interaction part, while all perturbed orbital components are neglected in the exchange interaction part. This approximation, which we will call the "dynamic-exchange" approximation, replaces Eq. (7) by

$$\int\psi^{*(3)}(1,2)[H-E]\psi^{(3)}(1,2)d\mathbf{r}_1d\mathbf{r}_2\varphi(3)-\int\psi_{100}^*(1)\psi_{100}^*(2)[H-E]\times\psi_{100}(1)\varphi(2)d\mathbf{r}_1d\mathbf{r}_2\psi_{100}(3)=0\,.\quad(9)$$

We now use the equations for the unperturbed and perturbed atomic orbital components to reduce the dynamic-exchange equation to a more explicit form. Our functions satisfy the equations:

$$[-\nabla_1^2-4/r_1+V_c(r_1)-\epsilon]\psi_{100}(\mathbf{r}_1)=0\,,\quad(10)$$

in the case of the unperturbed function ψ_{100}, and [17]

$$[-\nabla_1^2-4/r_1+V_c(r_1)-\epsilon]\chi(\mathbf{r}_1;\mathbf{r}_3)=[V_c(r_3)-2/r_{13}]\psi_{100}(\mathbf{r}_1)\,,\quad(11)$$

for the first-order perturbation function χ. In these equations

$$V_c(r_i)=\int|\psi_{100}(\mathbf{r}_j)|^2\frac{2}{r_{ij}}d\mathbf{r}_j\,,\quad(12)$$

and ϵ is the HF single-electron eigenenergy for the helium ground state. The atomic orbital components also satisfy the orthogonality relation

$$\int\psi_{100}(\mathbf{r}_i)\chi(\mathbf{r}_i;\mathbf{r}_j)d\mathbf{r}_i=0\quad(13)$$

for all values of $\mathbf{r}_j$.

The reduced form of the dynamic-exchange equation obtained by using Eqs. (10)–(13) to integrate Eq. (9) over the atomic coordinates (1 and 2) is

$$[-\nabla_3^2-4/r_3+2V_c(r_3)+2V_p(r_3)-2D(\mathbf{r}_3)-k^2]\varphi(\mathbf{r}_3)=\left[(\epsilon-k^2)\int\psi_{100}^*(\mathbf{r}_2)\varphi(\mathbf{r}_2)d\mathbf{r}_2+\int\psi_{100}^*(\mathbf{r}_2)\frac{2}{r_{23}}\varphi(\mathbf{r}_2)d\mathbf{r}_2\right]\psi_{100}(\mathbf{r}_3)\,.\quad(14)$$

In this equation, V_p is the adiabatic polarization potential,

$$V_p(r_3)=\int\psi_{100}^*(\mathbf{r}_3)\frac{2}{r_{23}}\chi(\mathbf{r}_2;\mathbf{r}_3)d\mathbf{r}_2\,,\quad(15)$$

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[16] In our previous paper, we began with a slightly more general approximation to the basic scattering equation and then reduced this to the adiabatic-exchange form by neglecting all dynamic terms.

[17] We are also using here the same truncated form of the perturbed orbital component equation as was considered in our previous paper (Ref. 1). The validity of this approximation has been considered to some extent in Appendix A of Ref. 18.

and D is the dynamical operator,

$$D(\mathbf{r}_3)\varphi(\mathbf{r}_3)=\int\chi^*(\mathbf{r}_2;\mathbf{r}_3)[\{\nabla_3^2\chi(\mathbf{r}_2;\mathbf{r}_3)\}+2\nabla_3\chi(\mathbf{r}_2;\mathbf{r}_3)\cdot\nabla_3]d\mathbf{r}_2\varphi(\mathbf{r}_3)\,. \quad (16)$$

This last term constitutes the only formal difference between the adiabatic-exchange approximation of our previous work[1] and the dynamic-exchange approximation of this paper. However, this term gives rise to a long-range velocity-dependent interaction which we have found to have a significant effect upon the scattering even at very low energies. We shall discuss this term at some length in the following section. In a subsequent calculation, we intend to consider a more complete approximation to the basic scattering equation (7) in which the first-order perturbed orbital components are retained in the exchange-interaction part. The resulting approximation has a form similar to the polarized-orbital equation of Temkin and Lamkin[6] for atomic hydrogen.

III. THE DISTORTION-INTERACTION TERMS

The polarization and dynamic terms V_p and D, defined in Eqs. (15) and (16), respectively, are seen to depend upon the atomic orbital components ψ_{100} and χ. We thus begin this section with a brief discussion of these functions. (A more detailed derivation and discussion of the perturbed orbital component χ is given in Ref. 18).

The exact solution of the HF self-consistent-field (SCF) equation (10) for the unperturbed atomic orbital ψ_{100} must be obtained numerically. However, in our previous paper,[1] we found that the 12-parameter analytical approximation to ψ_{100} given by Roothaan, Sachs, and Weiss[19] is sufficiently accurate to represent the unperturbed motion of the atomic electrons for this scattering problem. We thus have used this analytical approximation for ψ_{100} in all places in this paper except where an exception is specifically noted. (The HF eigenenergy corresponding to the Roothaan, Sachs, and Weiss functions is $\epsilon=1.835912$ Ry.)

The solution of the truncated perturbation equation (11) for the perturbed orbital component χ is only known for the case of atomic hydrogen [in which case Eq. (11) is the exact equation] and the uperturbed function ψ_{100} has the simple form $\exp(-zr)$. The desire to have a tractable analytical approximation for the perturbed orbital component χ was dictated by the complexity of the expression (16) for the operator D and the form of the exchange terms in the polarized-orbital equation mentioned at the end of the previous section. We thus have drawn upon the known solutions of Eq. (11) for the case of atomic hydrogen to obtain an approximate analytical solution for helium.

The approximate analytical solution of Eq. (11) for helium was obtained as follows. We begin with a transformation given by Schwartz[20] to write

$$\chi(\mathbf{r}_2;\mathbf{r}_3)=[F(\mathbf{r}_2;\mathbf{r}_3)-\langle F\rangle]\psi_{100}(\mathbf{r}_2)\,, \quad (17)$$

where

$$\langle F\rangle=\int|\psi_{100}(\mathbf{r}_2)|^2F(\mathbf{r}_2;\mathbf{r}_3)d\mathbf{r}_2\,. \quad (18)$$

The function F is then analyzed in partial waves through the relation

$$F(\mathbf{r}_2;\mathbf{r}_3)=\sum_l F_l(r_2;r_3)P_l(\cos\theta_{23})\,. \quad (19)$$

Since ψ_{100} is spherically symmetric, we see from Eq. (18) that $\langle F\rangle$ vanishes for all $l\neq0$. [A nonzero value of $\langle F_0\rangle$ insures that χ as given by Eq. (17) satisfies the orthogonality relation (13).]

When Eqs. (17) and (19) are substituted into Eq. (11) and the result reduced with the aid of Eq. (10),[21] we obtain the partial-wave equation for F_l,[18]

$$\left[-\frac{d^2}{dr_2^2}-2\frac{u_{1s}'(r_2)}{u_{1s}(r_2)}\frac{d}{dr_2}+\frac{l(l+1)}{r_2^2}\right]F_l(r_2;r_3)=\delta_{l,0}V_c(r_3)-2r_<^l/r_>^{l+1}\,, \quad (20)$$

where

$$u_{1s}'(r)/u_{1s}(r)=d[\ln u_{1s}(r)]/dr\,, \quad (21)$$

$u_{1s}(r)$ is the reduced radial part of the unperturbed orbital, $\psi_{100}(\mathbf{r})=[4\pi]^{-1/2}u_{1s}(r)/r$, and $r_<$ is the smaller and $r_>$ is the larger of r_2 and r_3.

The transformation of the perturbed orbital equation (11) into the form (20) is exact. However, to obtain analytical expressions for the components F_l, we must make an approximation. We do this by observing that the logarithmic derivative (21) for a hydrogenic orbital, $u_{1s}(r)=N\exp(-zr)$, has the form

$$d[\ln Ne^{-zr}]/dr=1/r-z\,. \quad (22)$$

The logarithmic derivative for the analytical approximation to $u_{1s}(r)$ that we are using here, on the other hand, has the form

$$d[\ln u_{1s}(r)]/dr=1/r-z'+ar+br^2+\cdots\,, \quad (23)$$

where z', a, b, $\cdots$, are constants depending upon the 12 parameters in the Roothaan, Sachs, and Weiss function.[19] We now approximate the logarithmic derivative in Eq. (20) by Eq. (22) and thus neglect the terms $ar+br^2+\cdots$ on the right-hand side of Eq. (23). When this is done, analytical solutions of Eq. (20) are known

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[18] R. W. LaBahn, Ph.D. thesis, University of California, 1965 (unpublished).

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[20] C. Schwartz, Ann. Phys. (N.Y.) **6**, 156 (1959).

[21] The use of Eq. (10) in the reduction here entails the so-called "Sternheimer approximation" which, however, is rigorously exact for the helium self-consistent-field equation [see R. M. Sternheimer, Phys. Rev. **96**, 951 (1954)].

and have been given (implicitly) by Reeh[22] and Bethe[23] ($l=1$ component only).

The analytical solutions to Eq. (20) given by Reeh and Bethe are complete solutions, that is, they are defined for all values of r_2 and r_3.[24] In a similar analysis for atomic hydrogen, Temkin and Lamkin[6] considered the perturbation to exist only when the scattering electron was "outside of" the atomic electron ($r_3>r_2$). Their perturbed orbital component then contained a unit step function, $\epsilon(r_2,r_3)$, to enforce this restriction. However, in derivation of their final scattering equation, they neglected all terms containing any derivative operators operating on the unit step function.

The neglect of terms coming from operating with the Laplacian on the unit step function was an unwarranted omission in the calculation of Temkin and Lamkin and the method of polarized orbitals should be understood to include these terms.[25] These terms, which were correctly included by Sloan,[26] appear in the polarization exchange portion of the scattering equation (which is neglected in our present formalism) and give rise to a velocity-dependent interaction with an exponentially decaying coefficient. The resulting terms would not be present if a perturbed orbital properly defined for all values of r_2 and r_3 had been used.

The dynamic term D defined in Eq. (16), consists of terms involving various derivatives of the perturbed orbital χ. To avoid the introduction of questionable terms, we have used the complete solutions of Eq. (20) discussed above to approximate χ. For future reference, we shall denote the equivalent components of F by the following notation:

$$\begin{aligned} F_l(r_2;r_3) &= F_l(r_2<r_3) \text{ for the region where } r_2<r_3, \\ &= F_l(r_2>r_3) \text{ for the region where } r_2>r_3. \end{aligned} \tag{24}$$

The expansion of the perturbed wave function, Eq. (19), can be used to generate a multipole expansion of the polarization potential, Eq. (15). This becomes, after substitution of Eqs. (12) and (17)-(19):

$$V_p(r_3)=\sum_l \left[\int_0^\infty |\psi_{100}(\mathbf{r}_2)|^2 F_l(r_2;r_3)\frac{2}{r_{23}}P_l(\cos\theta_{23})d\mathbf{r}_2 - \delta_{l,0}\langle F_l(r_3)\rangle V_c(r_3)\right]. \tag{25}$$

We shall denote the multipole components of V_p by $V_p^{(l)}$. They arise upon expansion of the term $2/r_{23}$ in Eq. (25). After performing the integration over the angular coordinates of r_2, these components have the form

$$V_p^{(l)}(r_3)=\frac{2}{2l+1}\left[\frac{1}{r_3^{l+1}}\int_0^{r_3} u_{1s}^2(r_2)F_l(r_2<r_3)r_2^l dr_2 + r_3^l\int_{r_3}^\infty u_{1s}^2(r_2)F_l(r_2>r_3)r_2^{-(l+1)}dr_2 - \delta_{l,0}\langle F_l(r_3)\rangle V_c(r_3)\right], \tag{26}$$

where we have used the definitions of Eq. (24).

Inspection of Eq. (20) shows that for large values of the separation r_3, $F_l(r_2<r_3)$ behaves like $r_3^{-(l+1)}$ for $l\neq 0$ [for $l=0$, $F_0(r_2<r_3)$ decays exponentially with increasing r_3]. Thus, from Eq. (26), we see that

$$V_p^{(l)}(r_3)\xrightarrow[r_3\to\infty]{}\frac{\text{const}}{r_3^{2l+2}}, \quad \text{for } l\neq 0. \tag{26'}$$

The perturbation analysis we are using here uses a first-order perturbed orbital χ, to determine a second-order polarization potential or energy correction V_p. If we were to consider a second-order perturbed orbital in addition to χ, we would introduce third-order interaction terms. The long-range nature of these third-order interactions has been shown[27] to exhibit a behavior beginning with terms proportional to r_3^{-7}. Thus, to be consistent with the inclusion of distortion effects up through second order, we may only retain terms which are larger than those given by third or higher order perturbation theory. From this analysis, it follows that only the first three, or $l=0, 1, 2$, components of V_p can be included under this criteria. Moreover, by a similar analysis, it is seen that only the first two components of the dynamic terms D can be retained under this criteria.

An additional comment in regard to the $l=0$ components of the distortion terms is in order. We have noted above that $F_0(r_2<r_3)$ decays exponentially with increasing r_3 and thus the $l=0$ components of the distortion terms will vanish exponentially. Under the above restrictions, then, it would appear that the $l=0$ components should also be neglected here. However, the $l=0$ components of all the distortion terms are significantly larger for small r_3 than any other components. We thus feel that they should be included to be consistent with our perturbation formalism. Moreover, in all previous electron-helium scattering calculations, excepting the recent work of Kestner, Jortner, Cohen, and Rice,[10] the $l=0$ component of the

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[22] H. Reeh, Z. Naturforsch., **15A**, 377 (1960).

[23] H. A. Bethe, *Handbuch der Physik* (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943), Vol. 24, pt. 1, p. 339 ff.

[24] The $r_<^l/r_>^{l+1}$ factor on the right-hand side of Eq. (20) results in a discontinuity in the equation for F_l as r_2 goes from values smaller than r_3 to values larger than r_3 (or vice versa). The usual procedure in solving equations of this form is to find separate solutions of the complete inhomogeneous equation valid in the regions $r_2<r_3$a nd $r_2>r_3$. Arbitrary multiples of the equivalent homogeneous equation solutions are then added to these inhomogeneous equation solutions and the multiplicative constants determined by matching the functions in magnitude and slope at the boundary $r_2=r_3$. See Ref. 22 for more specific details.

[25] A. Temkin (private communication).

[26] I. H. Sloan, Proc. Roy. Soc. (London) **A281**, 151 (1964).

[27] A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) **A233**, 70 (1955); Proc. Phys. Soc. (London) **A69**, 57 (1956).

polarization potential has been neglected. Thus, by including it here, we may examine the consequences of this omission in other works.

The analytical solutions to Eq. (20) obtained by using the first two terms of Eq. (23) to approximate the logarithmic derivative depend upon the constant z'. The value chosen for this constant was not taken as that deduced from the 12 parameters in ψ_{100} but rather chosen to best approximate the exact solution of Eq. (20) in the region where the perturbed orbital has the greatest significance. These criterions lead to a different choice of z' for each partial wave component F_l and also for $l\neq 0$, a different choice for a particular component depending upon whether it was used in the polarization potential or the dynamic terms.

The $l=0$ component of the polarization potential was obtained by numerical integration of the analytic approximation for $F_0(r_2;r_3)$ and 12-parameter SCF orbital ψ_{100} in Eq. (26). The constant z' in $F_0(r_2;r_3)$ was chosen to make the analytic approximation to F_0 equal to the exact function at $r_3=0$ since this is where the $l=0$ component of χ has the greatest significance. This selection determined z' for $F_0(r_2;r_3)$ through the relation

$$z_0'=\tfrac{1}{2}V_c(0)=1.6872761. \qquad (27)$$

The $l=0$ component of the polarization potential was also obtained by numerical integration of Eq. (26) with the analytic approximation for $F_1(r_2;r_3)$ and the 12-parameter SCF orbital ψ_{100}. The constant z' in F_1 was chosen here to make the asymptotic form $2V_p^{(1)}(r_3)\rightarrow -\alpha/r_3^{-4}$ as $r_3\rightarrow\infty$, exhibit the correct polarizability, α, for helium. We have used the recent value, $\alpha=1.395a_0^3$, determined from the experimental data of Johnston, Oudemans, and Cole[28] for the polarizability and this selection resulted in the value $z_1'=1.6245458$ for the constant in $F_1(r_2;r_3)$. The resulting single-electron polarization potential is shown by the solid curve in Fig. 1.

In our previous paper,[1] we used an earlier value of $\alpha=1.376a_0^3$ for the polarizability of helium and the analytic form for $V_p^{(1)}$ obtained by Bethe[23] upon using the hydrogenic form, $\psi_{100}(\mathbf{r})=(z^3/\pi)^{1/2}\exp(-zr)$, for the unperturbed atomic orbital. This form of $V_p^{(1)}$ is shown by the dashed curve in Fig. 1. Because of the importance of this component of the polarization potential, we have examined it in still greater detail. This examination entailed an exact numerical solution of the perturbed orbital equation (20) with the proper logarithmic derivative term Eq. (23). The resulting solution was properly continued[24] through the boundary $r_2=r_3$ and then integrated numerically, along with the 12-parameter SCF orbital, in Eq. (26). Only selected values of the separation r_3 were considered [because of the complexity of the numerical processing required to determine the function $F_1(r_2;r_3)$] and the resulting values of this "exact" form of $V_p^{(1)}$ are shown by the crosses in Fig. 1. Comparison of the three forms of $V_p^{(1)}$ in Fig. 1 shows only negligible differences for all values of r_3 and thus one could use any one of these in scattering calculations. We have used the approximate form first discussed above (solid curve in Fig. 1) in all of the new calculations reported in this paper.

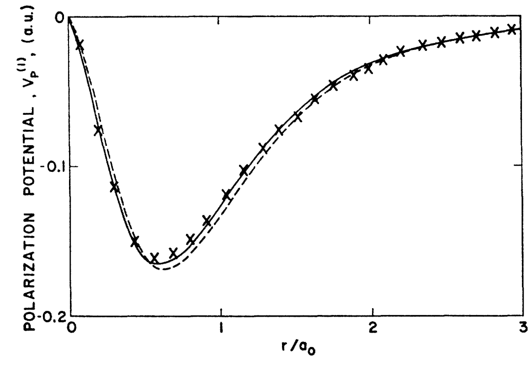

FIG. 1. Comparison of various forms of the $l=1$ component of the single-electron polarization potential. The dashed curve is Bethe's analytic form, the solid curve is the approximate form discussed in the text, and the crosses are from the exact numerical solution of Eq. (20). (a.u. ≡ atomic units.)

Because of the similarity of the analytical and approximate forms of $V_p^{(1)}$ and the fact that $V_p^{(2)}$ is small for all values of r_3, we have used the analytical form of $V_p^{(2)}$ instead of performing the numerical integration as done for $V_p^{(0)}$ and $V_p^{(1)}$. The analytic form of $V_p^{(2)}$ was obtained by Reeh[22] by using the hydrogenic form of ψ_{100} in Eq. (26) and is given by

$$\begin{aligned}V_p^{(2)}(r_3)=\frac{-15}{x^6}\Big\{1-e^{-2x}\Big[&1+2x+\tfrac{4}{3}x^2+\tfrac{1}{3}x^3+\frac{2}{9}x^4\\&+\frac{2}{9}x^5+\frac{1}{18}x^6-\frac{1}{135}x^7+\frac{1}{135}x^8-\frac{2}{135}x^9\Big]\\&+e^{-4x}\Big[1+4x+\frac{20}{3}x^2+6x^3+\frac{28}{9}x^4+\frac{8}{9}x^5+\tfrac{1}{9}x^6\Big]\\&+\frac{8}{135}x^{10}\,\mathrm{Ei}(-2x)\Big\}, \qquad (28)\end{aligned}$$

where $x=zr_3$ and $\mathrm{Ei}(-2x)$ is the negative exponential integral.[29] The constant z in Eq. (28) was chosen to make the asymptotic form, $2V_p^{(2)}(r_3)\rightarrow -q/r_3^6$ for $r_3\rightarrow\infty$, exhibit the correct quadrupole polarizability q for helium. There is no experimental value for q and thus we have used the value $q=2.3265a_0^5$ calculated by Dalgarno and McNamee[30] through a variational

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[28] D. R. Johnston, G. J. Oudemans, and R. H. Cole, J. Chem. Phys. 33, 1310 (1960).

[29] E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, Inc., New York, 1945), p. 1.

[30] A. Dalgarno and J. M. McNamee, Proc. Phys. Soc. (London) 77, 673 (1961).

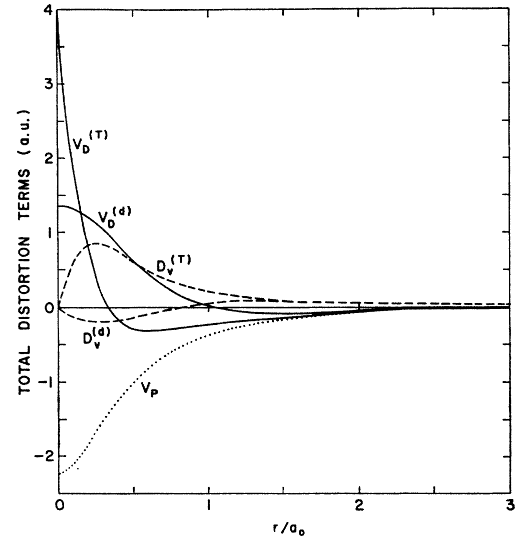

FIG. 2. Total distortion terms in the electron-helium interaction. The dotted and solid curves display interaction potentials while dashed curves represent coefficients for the velocity-dependent interaction.

method using the same 12-parameter SCF orbital we are using here. A value of $z=1.5313332$ was obtained from this analysis.

The total polarization potential is composed of twice the sum of the first three partial-wave components,

$$2V_p(r)=2\sum_{l=0}^{2} V_p^{(l)}(r) \tag{29}$$

and is displayed by the dotted curve in Fig. 2. This potential was used to represent the adiabatic polarization interaction in two of the calculations reported in Sec. V, while in a third calculation we used only the $l=1$ component of this potential.

The dynamic terms D defined in Eq. (16) are also subjected to a multipole analysis and, as mentioned above, only the first two or $l=0$ and 1, components are retained. Before discussing these though, we must consider briefly the method used to solve the scattering equation which will be discussed in more detail in Sec. IV. This preview is required to provide proper treatment of the term $\nabla_3\varphi(\mathbf{r}_3)$ in Eq. (16).

The scattering equation (14) is actually sloved for the reduced radial components of a partial-wave expansion of the scattering electron wave function $\varphi(\mathbf{r}_3)$. For this, the scattering equation is first reduced to the corresponding radial equation by substituting the expansion

$$\varphi(\mathbf{r}_3)=\sum_{l=0}^{\infty}\frac{u_l(r_3)}{r_3}Y_l^0(\Omega_3) \tag{30}$$

for the scattering electron wave function. The resulting equation is then multiplied on the left by $r_3Y_l^{0*}(\Omega_3)$ and integrated over the solid angle $d\Omega_3$, to obtain equations for the various reduced radial components $u_l(r_3)$. This transformation has no effect upon the various potential terms in the scattering equation excepting that they now multiply the reduced radial components $u_l(r_3)$, instead of the total wave function $\varphi(\mathbf{r}_3)$. However, the velocity-dependent interaction must now be redefined in terms of the corresponding operator for the reduced radial components of the scattering electron wave function.

The transformation of the dynamic terms defined in Eq. (16) is accomplished as follows: we first substitute expression (19) into Eq. (17) and substitute the result along with Eq. (30) into Eq. (16). Since the Laplacian ∇_3^2 and gradient ∇_3 are independent of the atomic electron coordinate $\mathbf{r}_2$, we can perform the integration over $d\mathbf{r}_2$; we multiply then on the left by $r_3Y^{0*}(\Omega_3)$ and integrate over $d\Omega_3$. The transformed dynamic interaction may then be written as

$$D(r_3)u_l(r_3)=-\sum_{l'=0}^{\infty}\left[D_L^{(l')}(r_3)+D_v^{(l')}(r_3)\frac{d}{dr_3}\right]u_l(r_3), \tag{31}$$

where we have introduced the notation

$$D_L^{(l)}(r_3)=-\left[\int_0^\infty F_l(r_2;r_3)\left(\frac{\partial^2}{\partial r_3^2}-\frac{l(l+1)}{r_3^2}\right)F_l(r_2;r_3)\times u_{1s}^2(r_2)dr_2-\delta_{l,0}\langle F_0(r_3)\rangle\frac{d^2}{dr_3^2}\langle F_0(r_3)\rangle\right], \tag{32}$$

and

$$D_v^{(l)}(r_3)=-2\left[\int_0^\infty F_l(r_2;r_3)\frac{\partial}{\partial r_3}F_l(r_2;r_3)u_{1s}^2(r_2)dr_2-\delta_{l,0}\langle F_0(r_3)\rangle\frac{d}{dr_3}\langle F_0(r_3)\rangle\right], \tag{33}$$

for the multipole components of the respective terms.

The first term $D_L^{(l)}$, defined in Eq. (32), gives the components of the Laplacian part of the dynamic terms; that is, it corresponds to the

$$\int \chi^*(\mathbf{r}_2;\mathbf{r}_3)\nabla_3^2\chi(\mathbf{r}_2;\mathbf{r}_3)d\mathbf{r}_2$$

part of Eq. (16). This term acts as an additional distortion interaction potential to be added to the polarization potential, Eq. (29).

The second term $D_v^{(l)}(r_3)$, defined in Eq. (33), gives the coefficient of the gradient operator in the equation for the reduced radial components of the scattering electron wave function. This term can be interpreted pictorially as a correction to the adiabatic theory to account for the fact that the atomic electron distribution cannot instantaneously follow the motion of the scattering electron if this possesses a finite velocity.

The $l=0$ components of Eqs. (32) and (33) were obtained by numerical integration using the approximate perturbed orbitals discussed above and the same constant z_0', defined by Eq. (27) for the polarization potential.

The $l=1$ components of Eqs. (32) and (33) were obtained in more approximate form. Since the numerical polarization potential agrees quite well with Bethe's analytic expression, we have omitted the numerical integration procedure here and used the hydrogenic form of ψ_{100} to determine analytic forms for $D_v^{(1)}$ and $D_L^{(1)}$. These are given by

$$\begin{aligned}D_L^{(1)}(r_3)=&-(1/x^6)\{43/2+\mathrm{Ei}(-2x)[\tfrac{4}{3}x^6-4x^5+3x^4-2x^3+3x^2-6+e^{-2x}(4x^7+2x^6-4x^5-2x^4+8x^3+18x^2+24x\\&+12)]+e^{-2x}[19/2-5x-39x^2-45x^3-(69/2)x^4-(47/2)x^5-(13/3)x^6-\tfrac{2}{3}x^7]-e^{-4x}\{31+100x+154x^2\\&+157x^3+(237/2)x^4+72x^5+37x^6+12x^7+12(x+1)^2(1+2x+\tfrac{5}{2}x^2+2x^3+x^4)[\gamma-\tfrac{1}{2}\,\mathrm{Ei}(2x)+\ln 2x]\}\}\,, \qquad (34)\end{aligned}$$

and

$$\begin{aligned}D_v^{(1)}(r_3)=&(1/zx^5)\{43/2+\mathrm{Ei}(-2x)[\tfrac{4}{3}x^6-2x^5-2x^3+6x^2-6+4e^{-2x}(x^6-2x^4-x^3+3x^2+6x+3)]+e^{-2x}[19/2-5x\\&-49x^2-53x^3-29x^4-(16/3)x^5-\tfrac{2}{3}x^6]-e^{-4x}\{31+100x+144x^2+129x^3+82x^4+40x^5\\&+12x^6+12(x+1)^3[(x+1)^2-x][\gamma-\tfrac{1}{2}\,\mathrm{Ei}(2x)+\ln 2x]\}\}\,, \qquad (35)\end{aligned}$$

where $x=zr_3$, γ is Euler's constant, and $\mathrm{Ei}(2x)$ is the positive exponential integral.[29]

The constant z used in Eqs. (34) and (35) was chosen as the value which gives the proper polarizability for the corresponding analytical (Bethe's) form of $V_p^{(1)}$. This was shown in our previous paper[1] to be given by

$$z=(9/\alpha)^{1/4} \qquad (36)$$

which, for $\alpha=1.395a_0^3$, gives $z=1.5937387$.

Specific forms for the dynamic terms are shown in Fig. 2 as summed together with the corresponding polarization potentials. The dashed curve marked $D_v^{(T)}$ corresponds to twice the sum of the $l=0$ and 1 forms of Eq. (33) $[2(D_v^{(0)}+D_v^{(1)})]$ which constitutes the total coefficient of the velocity-dependent interaction consistent with second-order perturbation theory. The dashed curve marked $D_v^{(d)}$ corresponds to $2D_v^{(1)}$ which is required in the calculation using only the $l=1$, or dipole, components of the distortion terms. The long-range behavior of both $D_v^{(T)}$ and $D_v^{(d)}$ are dictated by the form of $D_v^{(1)}$ since $D_v^{(0)}$ vanishes exponentially. Observation of Eq. (35) shows that

$$D_v^{(T)}(r_3)\rightarrow D_v^{(d)}(r_3)\rightarrow v/r_3^5, \quad \text{as} \quad r_3\rightarrow\infty\,, \qquad (37)$$

where

$$v=43/z^6=2.624a_0^5\,. \qquad (38)$$

The total potential part of the distortion terms is shown in Fig. 2 by the solid curve marked $V_D^{(T)}$. This curve represents twice the sum of the total polarization potential V_p defined in Eq. (29), and the $l=0$ and 1 forms of Eq. (32). Specifically

$$D_D^{(T)}(r_3)=2\Big[\sum_{l=0}^{2} V_p^{(l)}(r_3)+\sum_{l=0}^{1} D_L^{(l)}(r_3)\Big] \qquad (39)$$

and by observation of Eqs. (26′), (34), and (38) we find that asymptotically,

$$V_D^{(T)}(r_3)\rightarrow -\alpha/r_3^4-(q+v)/r_3^6, \quad \text{as} \quad r_3\rightarrow\infty\,, \qquad (40)$$

with $\alpha=1.395a_0^3$, $q=2.3265a_0^5$, and $v=2.624a_0^5$.

The solid curve marked $V_D^{(d)}$ in Fig. 2 represents the sum of the dipole components of the potential part of the distortion terms $[2V_p^{(1)}(r_3)+2D_L^{(1)}(r_3)]$. This term is used in conjunction with $D_v^{(d)}$ to examine the effects of using only the dipole components of the distortion terms and has the asymptotic form as given by Eq. (40) with $q=0$. The results of using these various approximations for the distortion interaction are considered in Sec. V following a discussion in the next section of the methods used to solve the scattering equation.

IV. SOLUTION OF THE SCATTERING EQUATION

The radial form of the scattering equation obtained by substituting Eq. (30) into Eq. (14) and integrating out the angular dependence becomes

$$\begin{aligned}\Big[-\frac{d^2}{dR^2}+2D_v(R)\frac{d}{dR}+\frac{l(l+1)}{R^2}-\frac{4}{R}+2V_c(R)+2V_p(R)+2D_L(R)-k^2\Big]u_l(R)=\frac{2}{2l+1}\Big[\tfrac{1}{2}\delta_{l,0}(\epsilon-k^2)\int_0^\infty u_{1s}(r)u_l(r)dr\\+R^{-(l+1)}\int_0^R u_{1s}(r)u_l(r)r^l dr+R^l\int_R^\infty u_{1s}(r)u_l(r)e^{-(l+1)}dr\Big]u_{1s}(R)\,, \qquad (41)\end{aligned}$$

where, for convenience, we have introduced the new notation $R=r_3$ and $r=r_2$. This equation was solved by using the noniterative method independently introduced by Omidvar[31] and Marriott.[32]

The noniterative method as applied to Eq. (41) consists of first defining the operator

$$\mathcal{O}(R)f(R)=\left[-\frac{d^2}{dR^2}+2D_v(R)\frac{d}{dR}+\frac{l(l+1)}{R^2}-\frac{4}{R}+2V_c(R)+2V_p(R)+2D_L(R)-k^2\right]f(R)$$
$$-\frac{2}{2l+1}\left[R^{-(l+1)}\int_0^R u_{1s}(r)f(r)r^l dr-R^l\int_0^R u_{1s}(r)f(r)r^{-(l+1)}dr\right]u_{1s}(R). \quad (42)$$

We then solve the two uncoupled equations

$$\mathcal{O}(R)u_l^{(0)}(R)=0,$$
$$\mathcal{O}(R)u_l^{(1)}(R)=[R^l/(2l+1)]u_{1s}(R), \quad (43)$$

and join these to obtain the complete solution of Eq. (41). The joining relation is

$$u_l(R)=u_l^{(0)}(R)+C_l u_l^{(1)}(R), \quad (44)$$

where

$$C_l=\frac{2I_{l0}^{(0)}+\delta_{l,0}(\epsilon-k^2)I_{l1}^{(0)}}{1-2I_{l0}^{(1)}+\delta_{l,0}(\epsilon-k^2)I_{l1}^{(1)}}, \quad (45)$$

with

$$I_{ln}^{(i)}=\int_0^\infty u_{1s}(r)u_l^{(i)}(r)r^{n-l-1}dr. \quad (46)$$

The integro-differential equations (43) were solved on a digital computer using a new method introduced by Sloan[26] to iterate the differential equation and Simpson's rule for the integrals. Sloan's method requires four starting values, two of the function and the two corresponding second derivatives. The function starting values were obtained by expanding the $u_l^{(i)}(R)$ near the origin in a power series in R, substituting these into Eqs. (43), and solving for the first few coefficients.[33] The second-derivative starting values were computed from the expression obtained by taking the second derivative of the function starting-value expansion.

Having a set of starting values, the integro-differential equations (43) were iterated from the origin out to $R=25a_0$. [The integral parts of these equations were stopped at $R=22a_0$ since the integrands become vanishingly small by this point due to the exponential decay of the atomic orbital $u_{1s}(r)$.] The resulting functions $u_l^{(0)}(R)$ and $u_l^{(1)}(R)$ were then joined by relations (44), (45), and (46), to form the partial-wave components of the scattering-electron wave function. Only the first three, or $l=0$, 1, and 2, partial-wave components were determined and approximate phase shifts were extracted from these by matching them with the spherical Bessel functions in the form

$$u_l(R)\to R[Cj_l(kR)-Dn_l(kR)]. \quad (47)$$

The scattering phase shifts were then found from the relation

$$\eta_l(R)=\tan^{-1}(D/C), \quad (48)$$

where $\eta_l(R)$ indicates the phase shift induced by the interaction between the origin and the point R.

By a similar procedure, we determined a scattering length by iteration of the $l=0$ component equations with $k=0$. The corresponding scattering length was then determined from the composite solution by matching this to the form

$$u_0(R)\to G[1-R/a(R)], \quad (49)$$

where G is some constant and $a(R)$ is the scattering length appropriate to the interaction between the origin and the point R.

The actual phase shift and scattering length required to calculate the cross section are $\eta_l=\eta_l(\infty)$ and $a=a(\infty)$. These generally differ from $\eta_l(R)$ and $a(R)$ because of the long-range nature of the polarization potential and velocity-dependent interaction which are truncated when the iteration process is terminated at some finite value of R.

To correct for this truncation, we have modified the formalism developed by Levy and Keller[34] for pure potential scattering to include the velocity-dependent interaction. This modification leads to the correction formula[18]

$$\tan\eta_l=\tan\eta_l(R)-k\int_R^\infty\{[rD_v(r)+r^2V(r)]$$
$$\times[j_l(kr)-\tan\eta_l(r)n_l(kr)]$$
$$+r^2D_v(r)[j_l'(kr)-\tan\eta_l(r)n_l'(kr)]\}$$
$$\times[j_l(kr)-\tan\eta_l(r)n_l(kr)]dr \quad (50)$$

for the phase shift, where primes indicate differentiation with respect to r and $D_v(r)$ and $V(r)$ are (for $R=25a_0$) the asymptotic forms (37) and (40), respectively, for the velocity-dependent interaction and polarization potential. In using Eq. (50) to correct the iterated

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[31] K. Omidvar, New York University Research Report No. CS-37 (unpublished) quoted in the paper by Temkin and Lamkin (Ref. 6).

[32] R. Marriott, Proc. Phys. Soc. (London) 72, 121 (1958).

[33] We actually extended the starter value power series out to the point where the first $\ln R$ term appeared so as to get very accurate starting values. The $\ln R$ terms arise in our equation whenever the $l=0$ or 2 components of the polarization potential and/or any of the dynamic terms are included.

[34] B. R. Levy and J. B. Keller, J. Math. Phys. 4, 541 (1963).

phase shifts, we have also made the first-order approximation of replacing $\eta_l(r)$ inside the integral by the constant $\eta_l(R)$. This approximation is reasonably valid here since for R as large as $25a_0$, the difference between $\eta_l(R)$ and η_l is small.

The iterated scattering length $a(R)$ is also corrected by this technique. The appropriate correction formula is obtained by dividing both sides of Eq. (50) [with $l=0$] by k and then taking the limit as $k\rightarrow 0$. This limit yields the formula

$$\begin{aligned} a=a(R)-\alpha[1/R-a(R)/R^2+a^2(R)/3R^3] \\ +v[a(R)/4R^4-a^2(R)/5R^5] \\ -q[1/3R^3-a(R)/2R^4+a^2(R)/5R^5] \quad (51) \end{aligned}$$

for the scattering length, where α and q are the dipole and quadrupole polarizabilities, respectively, of helium and v is the velocity-dependent interaction coefficient defined in Eq. (38). The first terms in Eq. (51) [i.e., those multiplied by α] were originally obtained by Temkin[35] through similar considerations but using only the $l=1$ component of the polarization potential.

We have used the formulas (50) and (51) to correct the iterated phase shifts and scattering lengths and these are presented in Sec. V.

The mesh sizes used in these iterations were chosen as follows. The various distortion interaction terms which required evaluation by numerical integration were processed using Simpson's rule and a mesh size of $0.01a_0$. Thus, since Simpson's rule only gives values of the integral for alternate mesh points, the differential equations could be iterated for any multiple of $0.02a_0$.[36]

Preliminary solutions of Eqs. (43) were processed by a binary-coded-decimal machine (IBM 7074) using single-precision arithmetic. Two test calculations using the constant mesh sizes of $0.04a_0$ and $0.08a_0$ were conducted and comparison of the resulting phase shifts showed only negligible differences.[18] Following this, a subsidiary set of calculations were processed on a straight binary machine (IBM 7094), also in single precision, and with a mesh size of $0.04a_0$. Large differences were then observed between the low-energy phase shifts and scattering lengths obtained from the two machines. (These differences appeared to arise from conversion errors in the binary machine and round-off errors in both machines.)

A second set of test calculations were then processed on another binary machine (IBM 7040) using double-precision arithmetic. For these tests, the equations were iterated at several test energies for each of the mesh sizes 0.02, 0.04, 0.06, 0.08, and $0.1a_0$. Comparison of the resulting phase shifts and scattering lengths showed that accurate solutions were obtained with the mesh sizes $0.06a_0$ for energies corresponding to the wave-vector region $0\leqslant k\leqslant 0.5a_0^{-1}$ and $0.04a_0$ for $0.5<k\leqslant 2.0a_0^{-1}$. All new calculations reported in this paper were processed with double precision arithmetic (on the IBM 7040) using the above mesh sizes.[37]

V. RESULTS AND DISCUSSION

Electron-helium phase shifts and scattering lengths have been calculated using three different approximations for the distortion interaction terms: (1) an adiabatic-exchange calculation using the total polarization potential of Eq. (29) (dotted curve in Fig. 2); (2) the dynamic-exchange calculation using the total potential terms and velocity-dependent interaction coefficient ($V_D^{(T)}$ and $D_v^{(T)}$ curves in Fig. 2); (3) an additional dynamic-exchange calculation using only the $l=1$ (or dipole) components of all the distortion terms [$V_D^{(d)}$ and $D_v^{(d)}$ curves in Fig. 2]. The phase shifts from these calculations are listed in Table I and also plotted in Fig. 3 in conjunction with the static-exchange calculations of Morse and Allis[15] (where all distortion effects were neglected) and the adiabatic-exchange calculations of our previous paper.[1] The corresponding scattering lengths are listed in Table II in comparison with other calculations and experimentally determined values. We shall first discuss the scattering lengths.

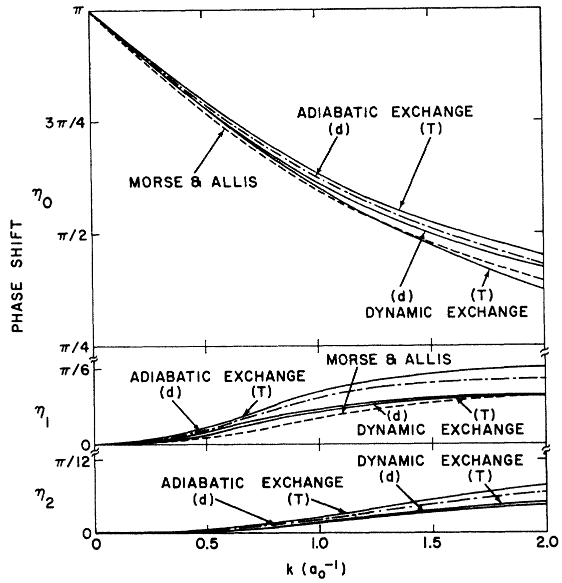

FIG. 3. Comparison of calculated electron-helium scattering phase shifts. Solid curves indicate present calculations.

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[35] A. Temkin, Phys. Rev. Letters **6**, 354 (1961).

[36] The use of Simpson's rule for the integral terms in Eqs. (43) necessitated the interlacing of two simultaneous integrals for alternate mesh points.

[37] Comparison of the double-precision calculations with the earlier binary-coded-decimal single-precision calculations showed only negligible differences in the phase shifts for $k>0.25a_0^{-1}$. Moreover, the only place where the differences seriously affected the calculated scattering cross sections where in the scattering lengths at $k=0$. Thus, the scattering lengths quoted in Ref. 18 are in error and should be replaced by the results quoted in this paper (Table I).

Table I. Electron-helium partial-wave phase shifts in radians.

k	Energy	Adiabatic exchange (Total pol. pot.)			Dynamic exchange (All components)			Dynamic exchange ($l=1$ components only)		
(a_0^{-1})	(eV)	η_0	η_1	η_2	η_0	η_1	η_2	η_0	η_1	η_2
0.01	0.00136	3.1305	0.000029	0.000005	3.1296	0.000029	0.000005	3.1296	0.000029	0.000004
0.05	0.034	3.0839	0.00078	0.00010	3.0794	0.00074	0.00010	3.0797	0.00073	0.00010
0.10	0.136	3.0222	0.0034	0.00039	3.0135	0.0030	0.00040	3.0141	0.0029	0.00038
0.1917	0.50	2.9039	0.0139	0.0015	2.8878	0.0117	0.0014	2.8893	0.0111	0.0014
0.25	0.85	2.8274	0.0251	0.0026	2.8068	0.0203	0.0026	2.8090	0.0190	0.0025
0.2712	1.00	2.7995	0.0300	0.0032	2.7774	0.0241	0.0030	2.7799	0.0225	0.0029
0.3835	2.00	2.6538	0.0647	0.0067	2.6232	0.0493	0.0061	2.6278	0.0456	0.0058
0.4287	2.50	2.5965	0.0823	0.0085	2.5624	0.0619	0.0076	2.5682	0.0574	0.0071
0.50	3.4	2.5083	0.1143	0.0119	2.4687	0.0836	0.0104	2.4765	0.0772	0.0097
0.6063	5.00	2.3830	0.1682	0.0184	2.3345	0.1198	0.0154	2.3460	0.1111	0.0141
0.75	7.65	2.2266	0.2463	0.0296	2.1648	0.1702	0.0238	2.1828	0.1590	0.0213
0.8575	10.00	2.1200	0.3021	0.0398	2.0471	0.2058	0.0310	2.0712	0.1939	0.0276
1.00	13.6	1.9923	0.3667	0.0551	1.9029	0.2460	0.0417	1.9369	0.2339	0.0369
1.25	21.25	1.8028	0.4476	0.0849	1.6799	0.2947	0.0613	1.7362	0.2849	0.0547
1.50	30.60	1.6503	0.4935	0.1149	1.4888	0.3196	0.0800	1.5732	0.3125	0.0725
1.75	41.65	1.5264	0.5175	0.1424	1.3226	0.3291	0.0962	1.4399	0.3234	0.0890
2.00	54.40	1.4243	0.5296	0.1663	1.1763	0.3300	0.1092	1.3293	0.3235	0.1033

The static-exchange value in Table II, $a=1.442a_0$, was computed by Moiseiwitsch[38] by numerical integration of the appropriate HF scattering equation without any distortion-interaction terms. This value thus closely represents the scattering length for the static atom with exchange and provides a basis for comparison with calculations including some distortion effects.

The adiabatic-exchange entries in Table II represent calculations wherein the distortion interaction was represented by some form of an adiabatic polarization potential. The first value, $a=1.132a_0$, from our previous paper, the value $a=1.21a_0$, by Bauer and Browne,[7] and the value $a=1.146a_0$ by Williamson and McDowell[9] were computed by approximating the distortion interaction with a dipole polarization potential. The resulting scattering lengths differ somewhat and this is due to differences in the scattering equations and/or forms of the polarization potentials used in these calculations.[39] The remaining two adiabatic-exchange values, $a=1.097a_0$ of the present work and $a=1.193a_0$ by Kestner, Jortner, Cohen, and Rice[10] were computed by approximating the distortion interaction with the sum of the first three ($l=0$, 1, and 2) multipole components of the total second-order adiabatic polarization potential.

Table II. Comparison of calculated and experimental electron-helium scattering lengths (in Bohr radii).

Source	Scattering length
Static exchange	
Moiseiwitsch	1.442
Adiabatic exchange	
analytic $l=1$ polarization potential[a]	1.132
total ($l=0$, 1, and 2) polarization potential	1.097
Bauer and Browne	1.21
Williamson and McDowell	1.146
Kestner, Jortner, Cohen, and Rice	1.193
Dynamic exchange	
all components of the distortion terms	1.186
$l=1$ components only	1.181
Experimental	
Ramsauer and Kollath[b]	1.19
Golden and Bandel	1.15
Frost and Phelps	1.18
Crompton and Jory	1.18

[a] Extrapolated from the very low-energy phase shifts in Ref. 1.
[b] Extrapolated from the data of Ref. 40 by O'Malley, Ref. 5.

The calculations of Kestner, Jortner, Cohen, and Rice were based upon a pseudopotential formalism in which the exchange interaction is represented by a scalar potential. They also calculated a scattering length in the static-exchange approximation (i.e., neglecting the polarization potential) and obtained a value of $a=1.502a_0$. Thus, inclusion of the total polarization potential in their formalism resulted in a decrease of 21% in the scattering length. Using Moiseiwitsch's value of $1.442a_0$, the inclusion of the total polarization potential in our formalism resulted in a decrease of 24% in the scattering length. The behavior of the scattering length upon including an adiabatic polarization potential is similar in both calculations even though the final results differ by almost 10%. The agreement between their scattering length and experiment is probably accidental, resulting from the fact that their representation of the exchange interaction gives too large a scattering length.

The dynamic-exchange values of the scattering lengths in Table II are nearly identical. This indicates

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[38] B. L. Moiseiwitsch, Proc. Phys. Soc. (London) 77, 721 (1961).

[39] Bauer and Browne solved a simplified form of HF scattering equation wherein exchange and close-range correlation were approximated by interaction potentials drawn from the quantum statistics of free electron gas. The distortion interaction was then included by replacing the close-range correlation potential for $R>4.745a_0$ by the asymptotic form, $-\alpha/R^4$, of the dipole polarization potential. Williamson and McDowell calculated the scattering in a one channel approximation using Bethe's form of the dipole polarization potential but representing the atomic electrons by a nonseparable variational wave function. Their calculation thus includes some close-range radial correlation which is completely neglected in our HF approximation.

that the $l=0$ component of the dynamic terms almost completely cancel the effects of the $l=0$ component of the polarization potential. Furthermore, these values of the scattering length are in a very good agreement with most of the experimental values listed at the end of Table II.

The Ramsauer and Kollath[40] scattering length, $a=1.19a_0$, was extrapolated from their very low-energy experimental data by O'Malley[5] using the modified effective range theory of Spruch, O'Malley, and Rosenberg.[4] The Golden and Bandel[41] scattering length, $a=1.15a_0$, was also extrapolated with the use of the modified effective range theory from their very low energy measurements. Both of these experimental data were obtained by direct measurements of the total scattering cross section using electron-beam techniques (see Fig. 4). The Frost and Phelps[42] and Crompton and Jory[43] values ($a=1.18a_0$ in both cases) on the other hand, were obtained from the diffusion cross section for helium determined by analysis of transport coefficients measured in swarm experiments (see Fig. 5). Greater accuracy can be obtained in swarm experiments as compared to electron-beam experiments at very low energies, and thus this value of $a=1.18a_0$ is the best estimate of the electron-helium scattering length presently available. Our dynamic-exchange calculations are in remarkably good agreement with this value.

The scattering phase shifts displayed in Fig. 3 show a comparison of the calculations using only the $l=1$ or dipole components of the distortion terms—the curves labeled with a (d)—and the calculations using the total distortion terms discussed in Sec. III above—the curves labeled with a (T)—along with the static-exchange phase shifts of Morse and Allis.[15] These curves show the expected differences as the various distortion terms were included in the calculations. That is, the effects of including or neglecting the $l=0$ components of the distortion terms is more pronounced in η_0 than in η_1 and η_2. This results since the centrifugal barrier prevents electrons with $l>0$ from penetrating too deeply into the atom, which is the region of greatest significance for the $l=0$ components of the distortion terms. The effects of the repulsive velocity-dependent interaction is also seen to be most pronounced in η_0 and so much so in fact that, for $k>1.5a_0^{-1}$, the dynamic-exchange calculations using the total distortion terms give values for η_0 which are lower than the (no-distortion) static-exchange calculations of Morse and Allis. The effect of the velocity-dependent interaction on η_1, on the other hand, results only in the approximate cancellation of the effects of the (attractive) adiabatic polarization potential for $k>1.5a_0^{-1}$.

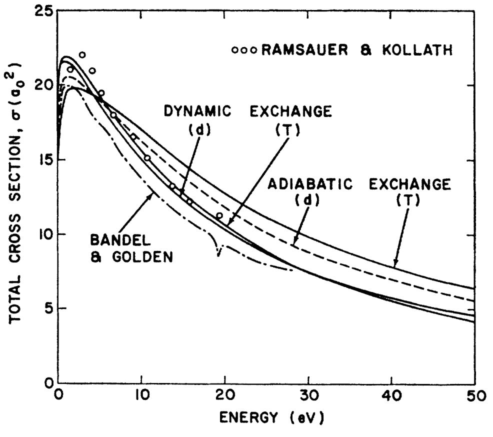

FIG. 4. Comparison of calculated electron-helium total scattering cross sections with experimental data (Ramsauer and Kollath, Golden and Bandel). Solid curves indicate present calculations.

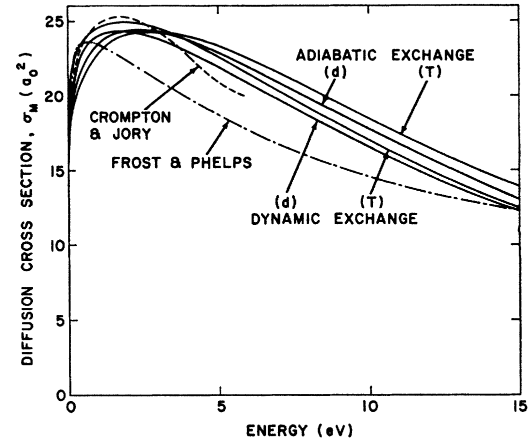

FIG. 5. Comparison of calculated electron-helium diffusion cross sections with experimental data (Frost and Phelps, Crompton and Jory).

The behavior of the dynamic-exchange $l=0$ phase shift computed using the total distortion terms is in disagreement with an informal theorem[44] on the effects that the distortion interaction has upon the scattering phase shifts.[45] This theorem states that the effect of distortion of the target is a purely attractive interaction and hence raises the phase shifts above those of the static-exchange approximation. It further states that if the distortion is divided up, either by putting in excited states one at a time as is done in the close coupling approximation, or by making a multipole decomposition of the distortion as we are doing here, then the effect of any component is purely attractive and must raise the phase shift.

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

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

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

[43] R. W. Crompton and R. L. Jory, in *IVth International Conference on the Physics of Electronic and Atomic Collisions* (Science Bookcrafters, Hastings-on-Hudson New York, 1965), p. 118–125.

[44] Y. Hahn, T. F. O'Malley, and L. Spruch, Phys. Rev. **128**, 932 (1962); I. C. Percival, *ibid.* **119**, 159 (1960).

[45] We are indebted to Dr. T. F. O'Malley for pointing out this discrepancy and informing us of the origin of the theorem.

This disagreement appears to result from neglect of the distortion effects in the exchange interaction. This hypothesis is supported by the results of some independent calculations of electron-helium scattering by Pu and Chang.[46] Their work is based upon an entirely different formalism which does not involve the adiabatic approximation. They can, however, separately determine the direct and exchange distortion effects and have found that, for the $l=0$ phase shift, these have similar magnitudes but opposite signs for higher values of k and hence tend to cancel.[47]

Some very preliminary results from solution of the polarized-orbital form of scattering equation mentioned at the end of Sec. II above also support this view by giving a value for η_0 at $k=2$ which is almost exactly equal to the Morse and Allis static-exchange value. Further work is presently in progress to obtain the polarized-orbital phase shifts and these will be reported elsewhere.

The scattering phase shifts of Table I were used in the well-known partial-wave expressions to compute the total scattering and diffusion cross sections for helium. The results of these calculations are displayed in Figs. 4 and 5 in comparison with the calculations of our previous paper and experimental data. The labeling, (*d*) and (*T*), in these is the same as in Fig. 3.

The total cross sections shown in Fig. 4 show good agreement between the adiabatic-exchange calculations and the Golden and Bandel[41] data at low energies (<3 eV) but poor agreement with these at higher energies. The adiabatic-exchange calculation of our previous paper (*d*) though, show fairly good agreement with the Ramsauer and Kollath[40] data in the high-energy region.

The dynamic-exchange calculations displayed in Fig. 4 show relatively negligible differences between the calculations using the total distortion terms (*T*) and those using only the $l=1$ components (*d*) of these terms. Moreover, both of these calculations show very good agreement with the Ramsauer-Kollath data for all energies considered and a better agreement for higher energies with the Golden and Bandel data than was obtained with the adiabatic-exchange calculations.

The diffusion cross sections in Fig. 5 show only moderately good agreement between the adiabatic-exchange calculations and experiment. The dynamic-exchange calculations, on the other hand, show very good agreement at low energies with both the Frost and Phelps[42] and Crompton and Jory[43] data. These data, though, differ quite significantly above 1 eV and the dynamic-exchange calculations follow quite closely the behavior of the Crompton and Jory data in this region.

The comparison of our calculations with each other and experimental data shows two important results. Better over-all agreement between the dynamic-exchange calculations and experiment is obtained than with the adiabatic-exchange calculations. Second, the differences between the dynamic-exchange cross sections calculated with two different approximations ($l=1$ components only or total components) to the distortion terms are generally small. These results show conclusively that the pure adiabatic approximation is only of marginal validity even at very low energies and thus some form of the velocity-dependent interaction must be included in the formalism to give adequate treatment of the scattering. Moreover, the fact that our dynamic-exchange calculations including the total distortion terms appear to produce incorrect $l=0$ phase shifts at high energies indicates that best results for this method are obtained when only the $l=1$ components of the distortion terms are included. This feature is also evident in our adiabatic-exchange cal-calculations when compared with experiment and further agrees with the results of an adiabatic analysis of positron-hydrogen scattering by Drachman.[48] This feature is also a useful one since the $l=0$ components of the distortion terms are generally quite complicated and difficult to evaluate.

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[46] R. T. Pu and E. S. Chang, Bull. Am. Phys. Soc. **11**, 40 (1966).

[47] R. T. Pu and E. S. Chang (private communication).

[48] R. J. Drachman, Phys. Rev. **138**, A1582 (1965).