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Extended Polarization Potential: Applications to Atomic Scattering*

JOSEPH CALLAWAY AND R. W. LABAHN
Department of Physics, Louisiana State University, Baton Rouge, Louisiana

AND

R. T. PU AND W. M. DUXLER
Department of Physics, University of California, Riverside, California

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In the calculation of the scattering of low-energy charged particles by atoms, corrections must be made to the usual polarization potential. The most important of these is a distortion potential, arising from the action of the kinetic-energy operator for the scattered particle on the perturbed wave function for the atom. A formal expression for this potential is obtained for any atom. It is evaluated approximately for hydrogen and helium. The combination of the distortion potential and the ordinary polarization potential is called the extended polarization potential; it is much weaker than either separately. Calculations of the scattering of low-energy positrons and electrons by hydrogen and helium atoms are performed in which the extended polarization potential is employed. Computed phase shifts and cross sections are compared with experiment and with other theoretical calculations.

I. INTRODUCTION

LET us consider the scattering of a low-energy charged particle by an isolated atom. Initially, the particle is at a large distance R from the atom. The atom distorts slightly in the electric field of the particle. The field produced by the induced multipoles alters the potential energy of the incident particle. This change is called the polarization potential. It is easy to see that the polarization potential must be proportional to $-\alpha/R^4$ when R is sufficiently large, where α is the atomic dipole polarizability. When R is small, that is, when the incident particle penetrates the atom, a more complicated expression can be obtained for the polarization potential which is not singular at the origin.[1–7]

There are other related effects which also must be considered. The wave function of the atom comes to depend on the coordinates of the incident particle. This means there will be a contribution to the kinetic energy of the system from the action of the kinetic-energy operator of the external particle on the atomic wave function. Since this contribution depends on R, it contributes to the effective potential experienced by the external particle. This effect is repulsive: that is, it tends to counterbalance the attractive polarization potential. At large R, it falls off asymptotically as R^{-6}, and thus is less important than the polarization potential; however, for small R it is of the same order as the polarization potential. Since the corrections to the particle-atom interaction from third-order effects usually neglected in polarization potential calculations are of order R^{-7} at large R,[8] the term we are discussing is the leading correction to the polarization. We shall refer to this term as the distortion potential; the combination of it and the ordinary polarization potential will be called the *extended polarization potential.*

A reasonable approximation to the extended polarization potential may be readily computed. We have used this potential in calculations of the scattering of low-energy electrons and positrons by hydrogen and helium atoms. Use of the extended polarization potential corrects much of the error resulting from too large polarization effects found in the adiabatic exchange approximation, particularly when monopole components of the polarization potential are included. In this respect, the results are similar to those of the so-called dynamic exchange approximation,[9] which this work supersedes.

The plan of this paper is as follows. In Sec. II, the distortion potential is defined and a formal expression given which is applicable to any atom. Section III contains a brief discussion of the relation between the present work and some other treatments of low-energy scattering. In Sec. IV, the distortion potential and extended polarization potential are constructed approximately for hydrogen and helium. The calculation of the cross section for the scattering of low-energy electrons and positrons by hydrogen and helium atoms using the extended polarization potential is described in Sec. V. The results are compared with experiments and other calculations. Our conclusions are summarized in Sec. VI.

II. THEORY

We wish to investigate the scattering of a charged particle by an atom using a form of the polarized orbital

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

[2] A. Dalgarno and N. Lynn, Proc. Phys. Soc. (London) **70A**, 223 (1957).

[3] J. Callaway, Phys. Rev. **106**, 868 (1957).

[4] A. Temkin, Phys. Rev. **107**, 1004 (1957); **116**, 358 (1959); A. Temkin and J. C. Lamkin, *ibid.* **121**, 788 (1961).

[5] H. Reeh, Z. Naturforsch. **15a**, 377 (1960).

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

[7] P. M. Stone, Phys. Rev. **141**, 137 (1966).

[8] A. Dalgarno and J. T. Lewis, Proc. Phys. Soc. (London) **A69**, 67 (1956).

[9] R. W. LaBahn and J. Callaway, Phys. Rev. **147**, 28 (1966).

method.[3] Because severe problems arise in connection with the proper selection of a certain projection operator in the case that the incident particle is identical with those in the atom, we will have to restrict our considerations formally to that in which the incident particle is distinguishable from those in the atom. However, if the corrections to the exchange interaction due to polarization and distortion effects may be neglected, the extension to include identical scattering and target particles appear to be straightforward.

Our approach is an extension of the optical potential method of Feshbach.[10] Central to this work is the introduction of a projection operator P which has the property that, operating on an arbitrary wave function for the system, it produces a function which, when the coordinates of the scattering particle become arbitrarily large, approaches the product of the wave function for the undisturbed atom in its ground state and a function of the scattering particle coordinates only. Let us suppose that the target atom contains N electrons. We will denote their coordinates (and spins where necessary) by x_a. The coordinates of the scattering particle are labeled x_s. Then P has the property that

$$\lim_{x_s\to\infty} P\Psi(x_a,x_s)=\phi(x_s)\psi_0(x_a)\,. \tag{1}$$

ψ_0 is the ground-state wave function for the atom. P must also be Hermitian and satisfy

$$P^2=P\,. \tag{2}$$

Now let Q be the complement of P

$$Q=1-P\,. \tag{3}$$

Feshbach shows that an exact equation which gives rise to the correct elastic scattering is

$$H_{\text{opt}}(P\psi)=E(P\psi)\,, \tag{4}$$

where the "optical" Hamiltonian H_{opt} is given by

$$H_{\text{opt}}=PHP-PHQ[1/(E-QHQ)]QHP\,. \tag{5}$$

When the wave function of the undistorted atom is known, the conventional choice of projection operator is

$$P=\psi_0(x_a)\psi_0^*(x_a')\,. \tag{6}$$

Then the second term in Eq. (5) contains the effects of virtual excitation of the core levels, and in particular contains the core polarization effects. There is, however, no compelling reason for the particular choice of P specified by Eq. (6). Any operator P which satisfies Eqs. (1) and (2) will do. The polarized orbital method results if the projection operator P is constructed from the wave function of the atom as distorted by the external particle.

Let $\psi^{(d)}(x_a,x_s)$ be the wave function for the atom as distorted by an external particle at x_s. We will choose

$$P=\psi^{(d)}(x_a,x_s)\psi^{(d)*}(x_a',x_s)\,. \tag{7}$$

In order that P satisfy Eq. (2), it is necessary that $\psi^{(d)}(x_a,x_s)$ be normalized to unity for all values of x_s.

$$\int|\psi^{(d)}(x_a,x_s)|^2dx_a=1\,. \tag{8}$$

If $\psi^{(d)}(x_a,x_s)$ is obtained by Hartree-Fock perturbation theory,[10–12] the normalization requirement will be satisfied. It is also apparent that, since

$$\lim_{x_s\to\infty}\psi^{(d)}(x_a,x_s)=\psi_0(x_a)\,, \tag{9}$$

our projection operator satisfies Eq. (1).

We next make the approximation of neglecting the second term in Eq. (5) altogether. The Hamiltonian H may be expressed as

$$H=H(x_a)+H(x_s)+V(x_a,x_s) \tag{10}$$

in which $H(x_a)$ contains the kinetic energy, the potential energy in the field of the nucleus, and the electron interaction terms pertaining to the bound electrons; $H(x_s)$ contains the kinetic energy and interaction with the atomic nucleus of the incident particle, and $V(x_a,x_s)$ contains the interaction between the bound electrons the the external particle. We define

$$\phi(x_s)=\int\chi^{(d)*}(x_a,x_s)\Psi(x_a,x_s)dx_a\,, \tag{11}$$

where $\Psi(x_a,x_s)$ is the complete wave function for the entire system. A short calculation shows that the reduced form of Eq. (5)

$$[E-PH]P\Psi=0$$

now becomes

$$[E-H_D(x_s)]\phi(x_s)=0 \tag{12}$$

in which

$$H_D(x_s)=\int\psi^{(d)*}(x_a,x_s)[H(x_a)+H(x_s)+V(x_a,x_s)]\times\psi^{(d)}(x_a,x_s)dx_a\,. \tag{13}$$

Now we express $\psi^{(d)}(x_a,x_s)$ in the form

$$\psi^{(d)}(x_a,x_s)=\psi_0(x_a)+\chi(x_a,x_s)\,. \tag{14}$$

The unperturbed atomic wave function $\psi_0(x_a)$ is normalized. Then Eq. (8) implies that $\chi(x_a,x_s)$ satisfies

$$\int[\psi_0^*(x_a)\chi(x_a,x_s)+\chi^*(x_a,x_s)\psi_0(x_a)]dx_a=-\int|\chi(x_a,x_s)|^2dx_a\,. \tag{15}$$

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[10] H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958); **19**, 287 (1962).

[11] A. Dalgarno, Proc. Roy. Soc. (London) **251A**, 282 (1959).

[12] L. C. Allen, Phys. Rev. **118**, 167 (1960).

Let us now consider the terms in Eq. (12) which result from the action of $H(x_s)$. Using the normalization condition, Eq. (15), we obtain

$$\left[H(x_s)+H(x_s)\int\psi_0{}^*(x_a)\chi(x_a,x_s)dx_a+\int\chi^*(x_a,x_s)\psi_0(x_a)dx_aH(x_s)+\int\chi^*(x_a,x_s)H(x_s)\chi(x_a,x_s)dx_a\right]\phi(x_s)$$

$$=\left[H(x_s)-\tfrac{1}{2}H(x_s)\int\chi^2(x_a,x_s)dx_a-\frac{1}{2}\int\chi^2(x_a,x_s)dx_aH(x_s)+\int\chi^*(x_a,x_s)H(x_s)\chi(x_a,x_s)dx_a\right]\phi(x_s).\quad(16)$$

In the last step of Eq. (16) we have used the fact that both ψ_0 and χ may be chosen to be real. Evidently, only the kinetic-energy part of $H(x_s)$ will contribute in the evaluation of the last three terms of (16), and a straightforward calculation shows that Eq. (16) may be written as

$$[H(x_s)+V_d(x_s)]\phi(x_s),\quad(17)$$

where

$$V_d(x_s)=\int|\nabla_s\chi(x_a,x_s)|^2dx_a.\quad(18)$$

The function $V_d(x_s)$ is the distortion potential.

The remaining terms in Eq. (13) may conveniently be separated into three parts:

$$E_a+V_c(x_s)+V_p(x_s)\quad(19)$$

in which E_a is the energy of the undistorted atom

$$E_a=\int\psi_0{}^*(x_a)H(x_a)\psi_0(x_a)dx_a,\quad(20)$$

$V_c(x_s)$ is the average potential

$$V_c(x_s)=\int\psi_0{}^*(x_a)V(x_a,x_s)\psi_0(x_a)dx_a,\quad(21)$$

and V_p is the polarization potential, containing all the terms not included above.

For further analysis, we will asuppose that $\chi(x_a,x_s)$ is computed using Hartree-Fock perturbation theory.[11–13] In this approach, we regard $\psi^{(d)}$ as a determinant of perturbed one-electron wave functions which are conveniently expressed as

$$u_i(x_j)+w_i(x_j,x_s)\quad(22)$$

in which i designates one of the occupied states, x_j represents the coordinates of one of the atomic electrons, x_s is as before the coordinate of the external particle, and u_i is a one-electron wave function satisfying the Hartree-Fock equations for the undistorted atom. The interaction term in Eq. (10) is

$$V(x_a,x_s)=\sum_j V(x_j,x_s)=eq\sum_j|x_j-x_s|^{-1}.\quad(23)$$

The quantity q is the charge of the incident particle. This interaction is treated as a perturbation. The functions $w_i(x_j,x_s)$ then satisfy the perturbed Hartree-Fock equations which are given in Refs. 10–12. The individual one-electron wave functions of Eq. (23) must remain orthogonal and normalized for all values of x_s. Then we can express Eq. (13) as

$$V_d(x_s)=\sum_i\int|\nabla_sw_i(x_1,x_s)|^2dx_1\quad(24)$$

in which the sum includes all atomic states (including spin). A fourth-order term has been neglected.

Now let us suppose that the external particle is at large distances from the atom so that the interaction term is small. We may then use first-order perturbation theory to determine the perturbed wave functions w_i. The leading term in the polarization potential $V_p(x_s)$ which was defined implicitly in Eq. (19) then has the well-known form:

$$V_p(x_s)=\sum_i\int u_i(x_1)V(x_1,x_s)w_i(x_1,x_s)dx_1.\quad(25)$$

From the form of the perturbed Hartree-Fock equations, it is easy to see that the dipole component of the interaction dominates at large distances. The $l=0$ component of w_i gives rise to potentials which decay exponentially at large distances. If $R=|x_s|$, then we find that

$$w_i(x_1,x_s)\propto\frac{\cos\theta}{R^2}f(x_1),\quad(26)$$

where θ is the angle between x_s and x_1. From this we conclude immediately that $V_d(R)\propto R^{-6}$ for sufficiently large R, as was stated in the Introduction. A similar analysis applied to Eq. (25) leads to the usual R^{-4} dependence of V_p for large R.

If the incident particle is an electron, it is necessary to antisymmetrize the total wave function of the system with respect to exchange between the incident electron and electrons in the target atom. This poses severe problems, and it has not been possible to obtain a satisfactory generalization of our projection operator P, Eq. (7), which satisfies all the requirements. In lowest order, however, the result is clear from a physical argument. If the distortion of the atom by the external electron is neglected, and the Hartree-Fock approxima-

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[13] S. Kaneko, J. Phys. Soc. Japan 14, 1600 (1959).

tion is used for the atomic wave function, the projection operator given by Feshbach must result. This is

$$P' = (N+1)^{-1/2} A \psi_0(x_a) \psi_0^*(x_a') A (N+1)^{-1/2} \qquad (27)$$

in which A antisymmetrizes with respect to coordinates x_s and x_a:

$$A = 1 - \sum_{j=1}^{N} P_{sj} \qquad (28)$$

and P_{sj} permutes x_s and x_j.

The usual exchange interaction between an electron and an atom decays exponentially with distance and becomes negligible in comparison with the direct terms at large distances. For this reason, it should be a reasonable approximation to neglect the distortion of the atom insofar as the exchange terms are concerned; that is, we use for this purpose P' as given in Eq. (27), combining the result with H_D of Eq. (13). The resulting approximate wave equation is (with $k^2 = E - E_a$ and ϵ_j the energy of atomic state j)

$$\begin{aligned}[H(x_s) + V_c(x_s) + V_p(x_s) + V_d(x_s) - k^2]\phi(x_s) \\ = \sum_j \biggl\{ \int u_j^*(x_1)[\epsilon_j - k^2 + V(x_1,x_s)] \\ \times \phi(x_1) dx_1 \, u_j(x_s) \biggr\} . \qquad (29)\end{aligned}$$

We will call this the extended polarization approximation.

III. COMPARISON WITH PREVIOUS WORK

The distortion potential V_d of Eq. (18) has not appeared in previous applications of the polarized orbital method. Temkin[4] has employed instead of our H_D, Eq. (13), the expression

$$\begin{aligned}H_D(x_s) = \int \psi_0^*(x_a)[H(x_a) + H(x_s) \\ + V(x_a,x_s)]\psi^{(d)}(x_a,x_s) dx_a \qquad (30)\end{aligned}$$

in which the undistorted atomic wave function ψ_0 appears on the left of the bracket in the integrand. Although this approach yields the usual polarization potential of Eq. (25), it will not contain V_d. Temkin's approach is apparently inconsistent with the projection operator formalism we have employed.

In our previous calculations of the scattering of electrons by helium atoms, the distortion potential derived here was absent, and in its place two other terms appeared.[9] These calculations employed the equation

$$\begin{aligned}[-\nabla_s^2 + V_c(x_s) - 4/R + V_p(x_s) - D_v(x_s) \cdot \nabla_s - V_L(x_s) \\ - k^2]\phi(x_s) = \int u_{1s}^*(x_1)[\epsilon_{1s} - k^2 + V(x_1,x_s)] \\ \times \phi(x_1) dx_1 \, u_{1s}(x_s) \qquad (31)\end{aligned}$$

in which

$$D_v(x_s) = 4 \int w(x_1,x_s) \nabla_s w(x_1,x_s) dx_1 \qquad (32)$$

and

$$V_L(x_s) = 2 \int w(x_1,x_s) \nabla_s^2 w(x_1,x_s) dx_1 . \qquad (33)$$

These equations were obtained by reducing H_D, neglecting the normalization condition, and retaining only the first-order perturbed atomic wave functions. Although the approach used in Ref. 9 is inadequate in a formal sense, it turns out, as will be placed in evidence below, that the difference in phase shifts for electron-helium scattering between those obtained from Eq. (29) and from Eq. (31) are reasonably small. The reason for this is the following: We define a new function ϕ' by

$$\phi(x_s) = \phi'(x_s) \exp\left[- \int w^2(x_1,x_s) dx_1 \right] . \qquad (34)$$

Since for large $|x_s| = R$

$$w^2(x_1,x_s) \propto R^{-4} ,$$

the same phase shifts will be obtained from ϕ' as from ϕ. We substitute Eq. (34) into Eq. (31). A straightforward calculation shows that ϕ' satisfies the equation

$$\begin{aligned}\biggl[-\nabla_s^2 - 4/R + V_c(x_s) + V_p(x_s) + 2\int |\nabla_s w(x_1,x_s)|^2 dx_1 \\ - k^2 + 4 \left| \int w(x_1,x_s) \nabla_s w(x_1,x_s) dx_1 \right|^2 \biggr] \phi'(x_s) \\ = \int u_{1s}(x_1)\{\epsilon_{1s} - k^2 + V(x_1,x_s)\} \exp\left[- \int w^2(x_2,x_1) dx_2 \right] \\ \times \phi'(x_1) dx_1 \left[\exp \int w^2(x_1,x_s) dx_1 \right] u_{1s}(x_s) . \qquad (35)\end{aligned}$$

This differs from Eq. (29) in two respects: A fourth-order direct term

$$4 \left| \int w(x_1,x_s) \nabla_s w(x_1,x_s) dx_1 \right|^2$$

is present, and the exchange terms are modified slightly. Both these effects would be expected to be reasonably small and this is confirmed by explicit calculations for helium.

IV. CONSTRUCTION OF THE DISTORTION POTENTIAL

We will consider the construction of the distortion potential for hydrogen and helium. In these atoms, there is a single one-electron wave function and, following Schwartz,[14] it is convenient to introduce a function

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

$F(x_1,x_s)$ by

$$w(x_1,x_s)=[F(x_1,x_s)-\langle F\rangle]u_0(x_1) \tag{36}$$

in which $u_0(x_1)$ is the unperturbed one-electron wave function for the atom, and

$$\langle F\rangle=\int u_0^2(x_1)F(x_1,x_s)dx_1. \tag{37}$$

The inclusion of $\langle F\rangle$ is a device to ensure that the perturbed wave function is orthogonal to u_0. It is then easy to show that $F(x_1,x_s)$ satisfies the equation

$$\begin{aligned}[\nabla_1^2+[2/u_0(x_1)]\nabla_1 u_0(x_1)\cdot\nabla_1]F(x_1,x_s)&=2/|x_1-x_s|-V_c(x_s),\\ V_c(x_s)&=2\int u_0^2(x_1)|x_1-x_s|^{-1}dx_1.\end{aligned} \tag{38}$$

For a hydrogenic atom we have, with $r=|x_1|$, $u_0=(Z^3/\pi)^{1/2}e^{-Zr}$. This is, of course, exact for hydrogen with $Z=1$, and we shall use this form for u_0 also in the case of helium as an approximation. In that case Z is a parameter which can be determined by fitting the observed atomic polarizability ($Z=1.594$), or from a variational calculation for the ground state ($Z=1.6875$).

Dalgarno and Lynn have solved Eq. (38) with the hydrogenic u_0, and have used this solution to determine the polarization potential V_p. We will use this polarization potential (referred to as the "complete" polarization potential) occasionally in the following. However, a distortion potential V_d has not yet been constructed from their solution. Instead, we will use the simpler approach in which a partial-wave expansion of F is made, and Eq. (38) is replaced by a set of ordinary differential equations for the components of F. Let $R=|x_s|$, and let θ be the angle between x_1 and x_s. We write

$$F(x_1,x_s)=\sum_l F_l(r,R)P_l(\cos\theta). \tag{39}$$

We then have

$$\frac{d^2F_l}{dr^2}+2\left(\frac{1}{r}-Z\right)\frac{dF_l}{dr}-\frac{l(l+1)}{r^2}F_l=\frac{2r_<^l}{r_>^{l+1}}-V_c(R)\delta_{l,0} \tag{40}$$

in which $r_<$ ($r_>$) is the lesser (greater) of r and R. The polarization and distortion potentials in the case of a single bound electron may then be expressed as

$$V_p(R)=\sum_l V_p^{(l)}(R);\quad V_d(R)=\sum_l V_d^{(l)}(R), \tag{41a}$$

with

$$V_p^{(l)}(R)=\frac{8\pi}{2l+1}\int u_0^2(r)\left(\frac{r_<^l}{r_>^{l+1}}\right)F_l(r,R)r^2dr, \tag{41b}$$

$$V_d^{(l)}(R)=\frac{4\pi}{2l+1}\int u_0^2(r)\left[\left(\frac{dF_l}{dr}\right)^2+\frac{l(l+1)}{R^2}F_l^2\right]r^2dr. \tag{41c}$$

In the case of helium, these results are to be multiplied by a factor of 2.

The $l=1$ component of the perturbed wave function was first obtained by Bethe,[1] who constructed from it the now well-known dipole polarization potential. Solutions for $l=0$ and 2 were obtained by Reeh,[5] who also obtained their contributions to the polarization potential. The $l=0$, 1, and 2 components of the polarization potential are also given by Kestner *et al.*[15] Components of the distortion potential have not been published previously, and we believe that it is of interest to give the largest one, the dipole ($l=1$) distortion potential:

$$\begin{aligned}V_d^{(1)}(R)=y^{-6}\{&129/4+3(y+1)^2(2y^4+4y^3+7y^2+6y+3)\\ &\times e^{-4y}[\mathrm{Ei}(2y)-2\ln 2y-2\gamma]+\mathrm{Ei}(-2y)\\ &\times[2e^{-2y}(9+18y+12y^2-3y^4-2y^5-2y^6)\\ &-2y^6+4y^5-3y^4+6y^2-9]+e^{-2y}[57/4-(15/2)y\\ &-(127/2)y^2-77y^3-45y^4-(46/3)y^5-(4/3)y^6]\\ &-e^{-4y}[93/2+150y+226y^2+216y^3+(305/2)y^4\\ &+86y^5+39y^6+12y^7]\}\end{aligned} \tag{42}$$

in which $y=ZR$, and γ is Euler's constant.

It is also possible to obtain limiting forms of these potentials for all l both when R is very large, and when it is close to zero. The large R result for $l>0$ is given in Ref. 2 for V_p:

$$V_p^{(l)}(R)=\frac{-4(2l+1)!}{(2ZR)^{2l+2}}\left(\frac{l+2}{l}\right) \tag{43}$$

while we find in the case of V_d:

$$V_d^{(l)}(R)=\frac{8(2l+2)!}{l^2(2ZR)^{2l+4}}\times\left[2l^2+4l+1+\frac{l^2(l+2)(2l+3)}{2(l+1)}\right]. \tag{44}$$

Thus, the lth component of V_d in the asymptotic region depends on the same power of R as the $l+1$ component of V_p. The $l=0$ forms decrease exponentially to zero in both cases.

For small R, it can be shown by expansion of Eq. (42), or directly, that $V_d^{(1)}(0)=1$ Ry. This is equal in magnitude but opposite in sign to the value of $V_p^{(0)}(0)$. Further it can be shown that all other contributions to V_p and V_d vanish for $R=0$. Thus we have an interesting result: For a hydrogenic bound-electron wave function,

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[15] N. R. Kestner, J. Jortner, M. H. Cohen, and S. A. Rice, Phys. Rev. **140**, A56 (1965).

the sum of the polarization and distortion potentials vanishes for $R=0$.

In Fig. 1 we show the distortion and polarization potentials and their sum for a single bound hydrogenic electron. The $l=0$, 1, and 2 components of the polarization potential and the $l=0$, 1 components of the distortion potential have been included. The sum is correct to order R^{-6} at large R and also has the appropriate behavior at small R. If we had included the "complete" polarization potential of Dalgarno and Lynn, the result would have shown a slight decrease in the effective repulsion for small R and a small increase in the attractive at intermediate R. The result would not, however, be noticeably different on the scale of Fig. 1. Inclusion of the neglected components of V_d would give an effect in the opposite direction.

V. APPLICATIONS TO HYDROGEN AND HELIUM

The elastic scattering of low-energy electrons and positrons by hydrogen and helium atoms has been calculated to illustrate the effectiveness of the new distortion potential. The calculations for helium parallel closely our previous work[9] and we shall consider these first.

Helium

The scattering equation (29) is first reduced for solutions by expanding the scattering function in partial waves

$$\phi(x_s)=\sum_l R^{-1}u_l(R)Y_l^0(\Omega). \qquad (45)$$

Substituting this into Eq. (29) and integrating out the angular dependence yields the radial equation

$$\left[-\frac{d^2}{dR^2}+\frac{l(l+1)}{R^2}-\frac{2Z}{R}+V_c(R)+V_p(R)+V_d(R)-k^2\right]u_l(R)=\frac{2}{2l+1}\left[\tfrac{1}{2}\delta_{l,0}(\epsilon_{1s}-k^2)\int_0^\infty u_{1s}(r)u_0(r)dr+\int_0^\infty u_{1s}(r)\frac{r_<^{\,l}}{r_>^{\,l+1}}u_l(r)dr\right]u_{1s}(R), \qquad (46)$$

where Ze is the charge of the nucleus.[16] The coordinates R and r are as defined in Sec. IV. For positron scattering, all terms on the right-hand side of Eq. (46) are set to zero.

We have performed one new calculation for electron-helium scattering and four for positron-helium scattering. The electron-helium calculations will be discussed first.

The distortion interaction used for the electron-helium calculation consisted of the sum of the first three multipole components ($l=0$, 1, 2) of the polarization potential (dashed curve labeled V_p in Fig. 1)[17] plus the first two components ($l=0$, 1) of the distortion potential (dashed curve labeled V_d in Fig. 1) as displayed by the solid curve in Fig. 1. Using this distortion interaction, the scattering equation (46) was solved numerically using a noniterative method and the resulting phase shifts corrected for the long-range interactions as discussed in Ref. 9. The resulting phase shifts are tabulated in Table I. These phase shifts were then used to calculate the total scattering cross section which is displayed by the heavy solid curve in Fig. 2 in comparison with some of our earlier calculations and experiments. The adiabatic-exchange-dipole (AED) curve employs only the dipole ($l=1$) component of the polarization potential.[6] The adiabatic-exchange-total (AET) curve represents using the sum of the first 3 multipole components of the polarization potential.[9] The crosses represent the most recent experimental data of Golden and Bandel.[18]

The scattering lengths resulting from these calcula-

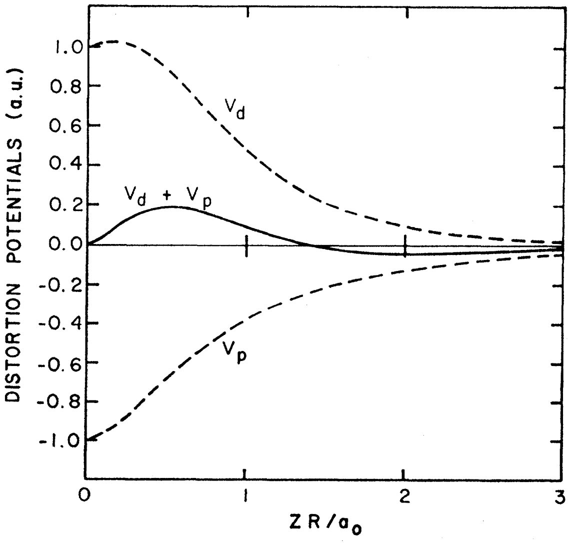

FIG. 1. Single-electron distortion potential, partial polarization potential, and their sum.

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[16] In the helium calculations, we have used the Hartree-Fock SCF functions of C. C. J. Roothaan, L. M. Sachs, and A. W. Weiss [Rev. Mod. Phys. 32, 186 (1960)], for both the u_{1s} in the exchange terms and in determining the screening potential $V_c(R)$. The value of ϵ_{1s} appropriate to these functions is -1.835912 a.u. In Eq. (46), $u_{1s}(r)$ is r times the function called u_0 in Sec. IV, while u_0 is now the $l=0$ component of ϕ.

[17] The $l=1$ and 2 components of V_p were identical to those used in Ref. 9 but the $l=0$ component used here was the analytic form given by Reeh (Ref. 5) instead of that used in Ref. 9. The reason for this change was that at the origin, the potential used in Ref. 9 went to -2.258 a.u. while the analytic form goes to -2.0 a.u. and thus gives the exact cancellation as discussed in Sec. IV. The calculated cross sections for electron-helium scattering differed negligibly between use of these two forms of the $l=0$ potential while the positron-helium cross section differed by at most 6.5%.

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

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

k	Energy (eV)	η_0	η_1	η_2
0.01	0.00136	3.12995	0.000029	0.000004
0.05	0.034	3.0812	0.00075	0.00010
0.10	0.136	3.0170	0.00306	0.00035
0.1917	0.50	2.8945	0.0118	0.00134
0.25	0.85	2.8156	0.0204	0.00245
0.2712	1.00	2.7869	0.0242	0.0029
0.3835	2.00	2.6371	0.0497	0.0060
0.4287	2.50	2.5783	0.0625	0.0076
0.50	3.40	2.4878	0.0845	0.0104
0.6063	5.00	2.3590	0.1213	0.0154
0.75	7.65	2.1979	0.1729	0.0239
0.8575	10.00	2.0877	0.2094	0.0312
1.00	13.60	1.9550	0.2508	0.0419
1.25	21.25	1.7560	0.3014	0.0620
1.50	30.60	1.5932	0.3277	0.0813
1.75	41.65	1.4584	0.3383	0.0980
2.00	54.40	1.3450	0.3399	0.1118

tions and from experiment are: 1.132 a_0, for the adiabatic-exchange-dipole polarization potential; 1.097 a_0 for the adiabatic-exchange-total polarization potential; 1.151 a_0 for the extended polarization potential. The most recent experimental value is 1.15 a_0 as determined by Golden and Bandel.

The phase shifts of Table I were also used to calculate the momentum transfer cross section which is displayed by the heavy solid curve in Fig. 3. This is also compared with the corresponding results from our previous two calculations as outlined above and the recent experimental based data of Crompton, Elford, and Jory.[19] The scattering length appropriate to the Crompton, Elford, and Jory data is 1.18 a_0.

The agreement of the Crompton, Elford, and Jory results with our previous dynamic-exchange calculations[9] is superior to our present calculations. The scattering length we obtained before was 1.186 a_0. As mentioned in Sec. III, the two calculations would give very nearly the same results provided the changes in the exchange terms were negligible. It appears that these changes are of some importance here since the difference in the cross sections between using the previous explicit velocity dependence and the present distortion potential range up to a maximum of 6%.

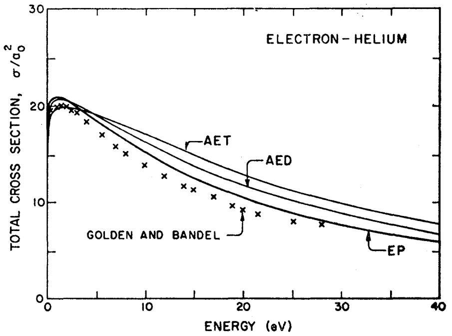

Fig. 2. Electron-helium total scattering cross sections: AED, adiabatic exchange with dipole polarization potential; AET, adiabatic exchange with three-component-sum (total) polarization potential; EP, present calculation with extended polarization potential.

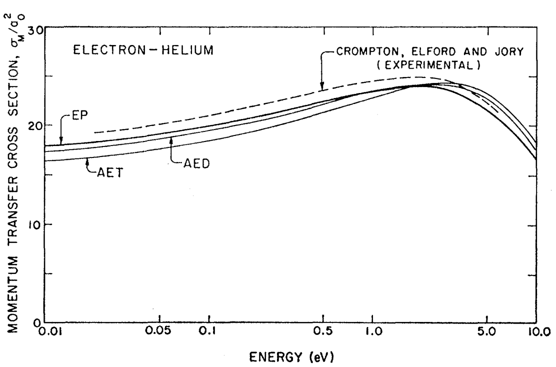

Fig. 3. Electron-helium momentum transfer cross sections. (Curve labeling identical to that of Fig. 2.)

We next discuss the positron-helium calculations.

The four calculations performed for positron-helium scattering are: (a) static atom approximation; (b) adiabatic approximation using the dipole ($l=1$) polarization potential only; (c) adiabatic approximation using the sum of the first 3 components ($l=0$, 1, 2) of the polarization; and (d) extended polarization approximation using the same potential functions applied above to electron scattering. The possibility of positronium formation was neglected in all of these calculations.

The appropriate scattering equation is Eq. (46) with all terms on the right-hand side set to zero. This was iterated numerically for the phase shifts which were then corrected as discussed in Ref. 9. The results are tabulated in Table II. These phase shifts were then used to compute the total scattering cross sections which are displayed in Fig. 4.

The static atom approximation calculation was performed to obtain a reference cross section and to check our computer program by comparing the results with the earlier calculations by Massey and Moussa.[20] A scattering length of 0.426 a_0 was obtained in this

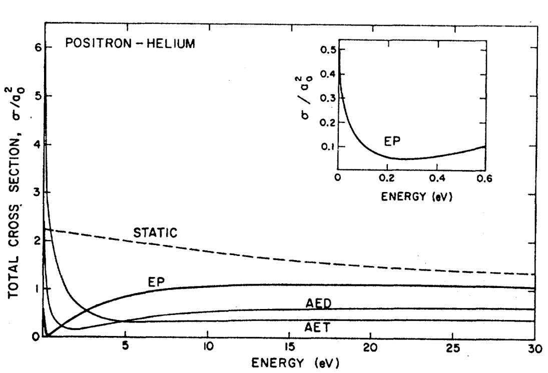

Fig. 4. Positron-helium total scattering cross sections. (Curve labeling has same meaning as those of Fig. 2.)

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[19] R. W. Crompton, M. T. Elford, and R. L. Jory, Australian J. Phys. (to be published).

[20] H. S. W. Massey and A. H. A. Moussa, Proc. Phys. Soc. (London) **71**, 38 (1958).

TABLE II. Positron-helium partial-wave phase shifts in radians.

	Adiabatic dipole			Adiabatic total			Extended polarization		
k	η_0	η_1	η_2	η_0	η_1	η_2	η_0	η_1	η_2
0.1	0.0293	0.0026	0.00042	0.0539	0.0027	0.00042	0.0069	0.0025	0.00041
0.2	0.0342	0.0092	0.0016	0.0781	0.0100	0.0017	−0.0068	0.0084	0.0016
0.3	0.0223	0.0178	0.0037	0.0802	0.0203	0.0038	−0.0334	0.0154	0.0036
0.4	−0.00029	0.0268	0.0065	0.0675	0.0317	0.0068	−0.0676	0.0219	0.0062
0.5	−0.0292	0.0348	0.0098	0.0457	0.0430	0.0106	−0.1057	0.0264	0.0092
0.6	−0.0615	0.0409	0.0136	0.0185	0.0528	0.0150	−0.1454	0.0284	0.0123
0.7	−0.0953	0.0446	0.0175	−0.0114	0.0595	0.0198	−0.1852	0.0281	0.0154
0.8	−0.1292	0.0458	0.0213	−0.0422	0.0656	0.0247	−0.2241	0.0238	0.0182
0.9	−0.1624	0.0444	0.0249	−0.0729	0.0670	0.0295	−0.2614	0.0184	0.0205
1.0	−0.1944	0.0408	0.0280	−0.1027	0.0655	0.0339	−0.2968	0.0110	0.0221
1.25	−0.2671	0.0243	0.0330	−0.1710	0.0604	0.0425	−0.3756	−0.0185	0.0226
1.5	−0.3284	0.0012	0.0335	−0.2288	0.0344	0.0465	−0.4402	−0.0441	0.0179

approximation which agrees with a similar calculation by Kestner *et al.*[15]

The adiabatic approximation with dipole polarization potential only yielded a scattering length of $-0.437\ a_0$. Our results in this approximation appear to be in reasonably good agreement with those obtained under similar conditions by Massey, Lawson, and Thompson.[21]

The adiabatic approximation with the three-component-sum polarization potential yielded a scattering length of $-0.697\ a_0$ which is in rough agreement with the value $-0.575\ a_0$ obtained by Kestner *et al.*,[15] in a similar calculation. The most complete calculation performed under a similar approximation is that of Drachman.[22] He used the full Dalgarno-Lynn[2] polarization potential with partial suppression of the monopole component. This monopole suppression was empirically imposed to reduce the large attractive polarization potential near the origin. The use of the present formalism accomplishes this in a less empirical manner, with the distortion potential exactly canceling the polarization potential at the origin. The results from Drachman's calculations were no monopole suppression was imposed are very nearly equal to our adiabatic total results. This is in accord with the conclusions reached by Bransden and Jundi[23] that the multipole components of the polarization potential above $l=2$ are relatively unimportant in scattering calculations.

The extended polarization approximation calculation yielded a scattering length of $-0.202\ a_0$. The total cross section from this calculation displays a Ramsauer minimum at low energies as exemplified in the low-energy insert in Fig. 4. The large differences in the cross sections at low energy between the static, adiabatic, and special dynamic approximations should be resolvable by experiment. The possibility of positronium formation would modify these results somewhat but since the threshold in helium is rather high (17.8 eV) we would not expect large changes to occur in the low-energy region.

We next discuss the calculations for atomic hydrogen.

Hydrogen

The scattering equation for electron-hydrogen scattering is obtained from Eq. (46) by setting $Z=1$, $\epsilon_{1s}=-1$ and appending a ± sign to the right-hand side to account for the two spin symmetries possible in this case (+ for triplet, − for singlet). For positron scattering, all terms on the right-hand side are again set to zero. The resulting equations were solved numerically for the phase shifts in the exact analogy to the helium case.

We have performed two slightly different sets of calculations for electron- and positron-hydrogen scattering. The difference involves the choice of the polarization potential used, the distortion potential being the same in both cases and of the form of the two-component sum ($l=0$, 1) displayed in Fig. 1 and discussed above in connection with the helium calculations. The two polarization potentials were the three-component sum displayed in Fig. 1 (and denoted here as the partial polarization potential) and the completed potential determined by Dalgarno and Lynn.[2]

The phase shifts resulting from these two calculations were nearly the same in all cases and so we display in Table III, IV, V and VI only those from the calculation

TABLE III. Electron-hydrogen *s*-wave phase shifts in radians.

	Singlet		Triplet	
k	Extended polarization	Variational[a]	Extended polarization	Variational[a]
0[b]	7.419	5.965	1.676	1.769
0.01	3.0671		3.1244	
0.05	2.7724		3.0494	
0.1	2.4357	2.553	2.9477	2.9388
0.2	1.9099	2.0673	2.7351	2.7171
0.3	1.5371	1.6964	2.5254	2.4996
0.4	1.2586	1.4146	2.3275	2.2938
0.5	1.0423	1.202	2.1454	2.1046
0.75	0.6891		1.7667	
1.0	0.5258		1.4854	

[a] Reference 24.

[b] The $k=0$ entries are scattering lengths.

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[21] H. S. W. Massey, J. Lawson, and D. G. Thompson, in *Quantum Theory of Atoms, Molecules, and the Solid State*, edited by P. O. Löwdin (Academic Press Inc., New York, 1966), p. 203.

[22] R. J. Drachman, Phys. Rev. 144, 25 (1966).

[23] B. H. Bransden and Z. Jundi, Proc. Phys. Soc. (London) 89, 7 (1966).

TABLE IV. Electron-hydrogen p-wave phase shifts in radians.

	Singlet		Triplet	
k	Extended polarization	Variational[a]	Extended polarization	Variational[a]
0.01	0.0001		0.0001	
0.05	0.0019		0.0024	
0.1	0.0063	0.007	0.0102	0.0114
0.2	0.0150	0.0147	0.0448	0.0450
0.3	0.0160	0.0170	0.1047	0.1063
0.4	0.0076	0.0100	0.1820	0.1872
0.5	−0.0068	−0.0007	0.2607	0.2699
0.75	−0.0404		0.3871	
1.0	−0.0424		0.4119	

[a] Reference 25.

TABLE V. Electron-hydrogen d-wave phase shifts in radians.

k	Singlet Extended polarization	Triplet Extended polarization
0.05	0.0003	0.0003
0.1	0.0013	0.0013
0.2	0.0050	0.0052
0.3	0.0105	0.0119
0.4	0.0163	0.0212
0.5	0.0215	0.0334
0.75	0.0290	0.0713
1.0	0.0316	0.1074

TABLE VI. Positron-hydrogen phase shifts in radians.

	s wave		p wave		d wave
k	Extended polarization	Variational[a]	Extended polarization	Variational[b]	Extended polarization
0[c]	−0.783	−2.10			
0.01	0.0074		0.0001		
0.05	0.0277		0.0020		0.0003
0.1	0.0360	0.151	0.0072	0.009	0.0013
0.2	0.0137	0.188	0.0226	0.033	0.0050
0.3	−0.0352	0.168	0.0370	0.065	0.0109
0.4	−0.0939	0.120	0.0458	0.102	0.0175
0.5	−0.1539	0.062	0.0468	0.132	0.0242
0.6	−0.2112	0.007	0.0408	0.156	0.0299
0.7	−0.2638	−0.054	0.0290	0.178	0.0337
0.8	−0.3036		0.0132		0.0354
0.9	−0.3520		−0.0050		0.0348
1.0	−0.3875		−0.0244		0.0321

[a] Reference 24.
[b] Reference 25.
[c] The $k=0$ entries are scattering lengths.

using the three component sum polarization potential. We have also reproduced in these tables the results from the rigorous variational calculations for s-wave phase shifts by Schwartz[24] and for p-wave by Armstead.[25]

The largest differences obtained from using the complete Dalgarno-Lynn polarization potential were in the scattering lengths. The scattering lengths calculated using the Dalgarno-Lynn form of the polarization potential were; 7.262 a_0 for singlet and 1.643 a_0 for triplet electron-hydrogen scattering and -0.901 a_0 for positron-hydrogen scattering.

The electron-hydrogen s-wave phase shifts are also displayed in Fig. 5 (EP) in comparison with Schwartz's variational values (VAR) and the exchange-adiabatic (AED) and polarized-orbital (PO) phase shifts of Temkin and Lamkin.[4] The Temkin and Lamkin exchange-adiabatic calculations correspond to using only the dipole polarization potential to represent the distortion interaction. In their polarized-orbital calculation, they include some distortion effects in the exchange interaction in addition to the dipole polarization potential.

The positron-hydrogen s-wave phase shifts are displayed in Fig. 6 (EP) in comparison with Schwartz's[24] variational values (VAR) and the adiabatic (AC) phase shifts of Drachman.[26] The Drachman adiabatic phase shifts correspond to using the complete Dalgarno and Lynn[2] polarization potential to represent the distortion interaction.

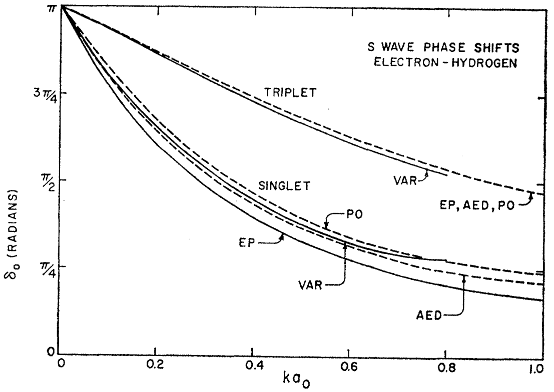

FIG. 5. Electron-hydrogen s-wave phase shifts: AED, adiabatic exchange with dipole polarization potential; PO, polarized orbital (Temkin and Lamkin, Ref. 4); VAR, variational (Schwartz, Ref. 24); EP, present calculation with extended polarization potential.

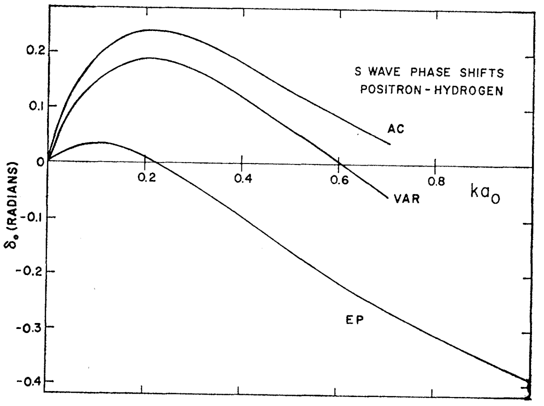

FIG. 6. Positron-hydrogen s-wave phase shifts: AC, adiabatic with complete polarization potential (Drachman, Ref. 26); VAR, variational (Schwartz, Ref. 24); EP, present calculation with extended polarization potential.

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[24] C. Schwartz, Phys. Rev. **124**, 1468 (1961).

[25] R. L. Armstead, Lawrence Radiation Laboratory Report No. UCRL-11628, 1964 (unpublished).

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

[27] Further discussion of electron- and positron-hydrogen scattering including experimental data can be found in the review by P. G. Burke and K. Smith [Rev. Mod. Phys. **34**, 458 (1962)].

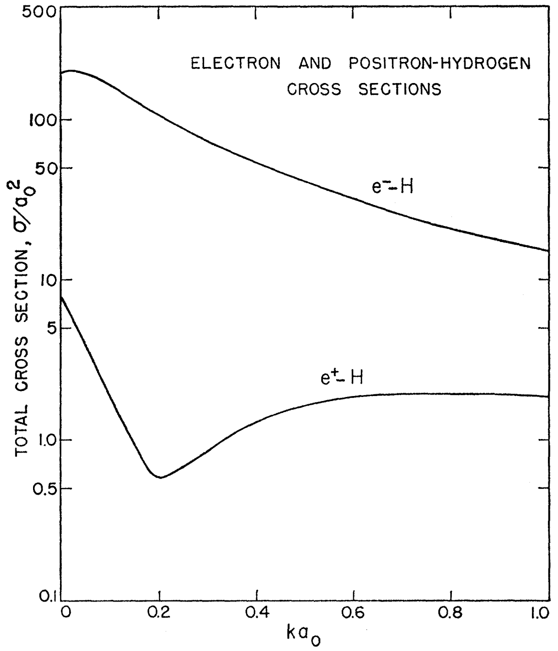

FIG. 7. Electron- and positron-hydrogen total scattering cross sections computed with the extended polarization potential.

Finally, in Fig. 7 we display the total cross sections for scattering of electrons and positrons by hydrogen using the extended polarization method.[27]

VI. CONCLUSIONS

An extended polarization potential for atomic scattering has been derived and applied to the scattering of electrons and positrons by hydrogen and helium. This work stems from earlier studies of electron scattering from helium[9] wherein it was found that significant improvements scattering calculations including distortion interaction effects were obtained when some of the nonadiabatic interaction effects were included. The present work has extended the formalism to the point where the previous nonadiabatic, or specifically velocity-dependent, interactions are replaced by an additional central distortion potential.

A general conclusion which had been reached in numerous other atomic scattering calculations is that it is reasonable to include only the dipole polarization potential to describe the distortion interactions in calculations of the type described above. The major reason for this conclusion was two fold; first, the monopole component which has a comparatively large value at the origin produces too much attraction, and second, the higher multipoles are relatively small and hence unimportant. The results of the present work supports the conclusion that the monopole polarization potential is too attractive near the origin but corrects this by the addition of a distortion potential, the dipole component of which exactly cancels the monopole polarization potential at the origin. The resulting combination of polarization potential plus distortion potential thus vanishes at the origin and also presents a slight repulsion for small R to account for the nonadiabatic effects. (The velocity dependence of this effect is only implicit in that the higher the velocity of the scattering particle, the deeper it can penetrate into the atom and hence "see" more of the repulsive distortion interaction.)

The applications of this formalism to electron scattering by helium has produced results closely resembling our previous calculations[9] using the explicit velocity-dependent interaction. The application to positron-helium scattering has no direct parallel and awaits experimental comparison.

The application of this formalism to electron- and positron-hydrogen scattering has not produced encouraging results. The effect of adding the new distortion potential seriously lowers the phase shifts for positron scattering and singlet electron scattering. The combination of polarization and distortion potentials now apparently contains too much repulsion. This difficulty might be corrected if the effects of distortion on the exchange interaction in electron scattering and virtual positronium formation in the positron case were included. These ideas are supported by the previous calculation of Temkin and Lamkin[4] and Sloan[28] using the method of polarized orbitals which indicated that the exchange distortion interaction has an over-all attractive effect in the singlet state. The calculations by Cody, Lawson, Massey, and Smith[29] and Bransden[30] indicate that the inclusion of positronium formation also has an over-all attractive effect. Thus it is possible that a proper inclusion of distortion in the electron-exchange interaction and including positronium formation will yield better results.

Note added in proof. A numerical calculation of the distortion potential using the full Dalgarno-Lynn[2] perturbed orbital has recently been completed.[31] The resulting "complete" form of V_d is found to be only slightly different from the two component sum displayed in Fig. 1.

ACKNOWLEDGMENTS

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

[29] W. J. Cody, J. Lawson, H. S. W. Massey, and K. Smith, Proc. Roy. Soc. (London) **A278**, 479 (1964).

[30] B. H. Bransden, Proc. Phys. Soc. (London) **79**, 190 (1962).

[31] R. J. Drachman (private communication).