Nonadiabatic Atomic Distortion in Low-Energy Electron and Positron Scattering*

W. R. Garrett

Health Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee

(Received 19 August 1968)

A perturbation method is used to obtain equations for the dynamic distortion of the target atom in low-energy electron and positron scattering. In an approximation which is adequately simple for application to heavier systems, the equations for hydrogen are reduced to a form analogous to the perturbation equations of the method of polarized orbitals. After expressing the interaction of the incident particle with an atomic electron in terms of a multipole expansion, the equations are solved for the multipole components of the polarization potential, where the equations governing the distortion are dependent on the energy of the incident particle. Phase-shift results for electron and positron scattering on hydrogen are compared with adiabatic results and with results obtained by other nonadiabatic and variational methods.

I. INTRODUCTION

An important question in the theoretical treatment of low-energy electron or positron scattering from atomic and molecular systems concerns dynamic effects in the distortion of the target system by the incident charged particle. [1-7] If the external charge were completely stationary, then the distortion of the target orbitals could be determined by a perturbation method such as that of Sternheimer, [8] where the polarization of the target is expressed in terms of the induced multipole moments of the target atom. Thus, if the perturbing charge is sufficiently "exterior" to the atom, the interaction potential between the particle and the atom has a leading term $-\alpha_d/r^4$, where α_d is the atomic dipole polarizability, followed by a quadrupole term $-\alpha_q/r^6$, where α_q is the quadrupole polarizability, and so on for higher-order induced moments.

If the perturbing charge is at a distance of the order of the atomic size, the potential function as represented by its multipole components is altered from its asymptotic form (and an added monopole term becomes significant since the perturbing charge is partially inside the charge distribution of the atomic cloud) but is, in any case, still calculable. However, the situation in a real scattering event is more complicated. The distortion of the atomic orbitals does not result from a stationary charge at a fixed distance but from a moving projectile whose coordinates change at a rate dependent on its initial energy and on the attractive polarization force between projectile and target. If one persists in the description of the scattering event through a perturbation technique and describes the atomic distortion by the free projectile at $\vec{r}_f$ through a perturbation term, then the perturbation will depend in some way on the energy of the projectile. Intuitively one can argue that the perturbation $\chi(\vec{r}, \vec{r}_f)$ induced in an atomic orbital by a moving charge at $\vec{r}_f$ will be reduced as compared to that due to a stationary charge at the same distance, since the orbital electrons require a finite time to rearrange themselves in the electric field produced by the projectile (we neglect any relativistic effect which would result from

the use of a retarded potential). Thus one would predict that within the perturbation framework, the distortion χ of the atomic orbital becomes a function of the coordinate and velocity of the incident particle and that this distortion becomes smaller and the resultant polarization potential becomes weaker with more rapidly moving projectiles.

For electron scattering there is an added complication from the effect of exchange on the target distortion. These exchange polarization effects are expected to be small as compared to the direct and nonadiabatic polarization terms[4] and will be neglected in the present investigation.

In Sec. II the equations for the dynamic polarization of atomic hydrogen are derived and the scattering of positrons and electrons are treated in Secs. II and III. The objective here is not to obtain very accurate scattering cross sections for hydrogen atoms, but rather, it is to investigate the importance of the dynamic effect on target distortion utilizing a method which can be adapted to more complicated scattering systems.

II. TARGET DISTORTION; POSITRON-HYDROGEN SCATTERING

We proceed in a manner analogous to the method of polarized orbitals[9, 10] and consider the scattering of positrons from atomic hydrogen. The stationary scattering problem is described by the Schrödinger equation:

$$(H_0 + H_p + W)\Psi = E\Psi, \tag{1}$$

where, in rydberg units,

$$H_0 = -\nabla_1^2 - 2/r_1, \tag{2a}$$

$$H_p = -\nabla_p^2 + 2/r_p, \tag{2b}$$

$$W \equiv W(r_1, r_p) = -2/r_{1p}. \tag{2c}$$

Here $\vec{r}_1$ is the coordinate of the bound electron, $\vec{r}_p$ is that of the incident particle, and W is the

Coulomb interaction between the electron and the incident particle. The total energy $E = E_0 + k_0^2$, where k_0^2 is the kinetic energy of the free particle, and E_0 is the hydrogen ground-state energy defined by

$$H_0 \phi_0(\vec{r}_1) = E_0 \phi_0(\vec{r}_1), \quad , \tag{3a}$$

with $\langle \phi_0, \phi_0 \rangle = 1$. $\tag{3b}$

Without loss of generality the total wave function $\Psi \equiv \Psi(\vec{r}_1, \vec{r}_p)$ can be written in the form

$$\Psi(\vec{r}_1, \vec{r}_p) = \psi(\vec{r}_p)[\phi_0(\vec{r}_1) + \chi(\vec{r}_1, \vec{r}_p)] , \tag{4}$$

with the boundary conditions

$$\langle \phi_0, \chi \rangle = 0 \tag{5}$$

$$\chi(r_1, r_p) \to 0, \quad \text{as } r_1 \text{ or } r_p \to \infty . \tag{6}$$

The term $\chi(\vec{r}_1, \vec{r}_p)$ will later be considered as the perturbation of the ground-state hydrogen wave function $\phi_0(\vec{r}_1)$, due to the scattered particle whose wave function asymptotically is $\psi(\vec{r}_p)$.

The functions ψ and χ are to be obtained by solving the appropriate differential equations. To this end we substitute (4) into (1) and get

$$(H_0 + W)(\phi_0 + \chi)\psi + H_p(\phi_0 + \chi)\psi = E(\phi_0 + \chi)\psi . \tag{7}$$

In order to proceed in the usual perturbation manner, we obtain an expression for E by performing a scalar multiplication from the left on (7) by $\psi^* \phi_0^*$ and integrating over $\vec{r}_1$ and $\vec{r}_p$. Utilizing (3a), (3b), and (5), this yields

$$(E - E_0)\langle \psi, \psi \rangle = \langle \psi, H_p \psi \rangle + \langle \psi, [\phi_0, W\phi_0]\psi \rangle$$

$$+ \langle \psi, [\phi_0, W\chi]\psi \rangle . \tag{8}$$

From the stationary behavior of E this leads to

$$E\psi(\vec{r}_p) = E_0 \psi(r_p)$$

$$+ \left(H_p + \int \phi_0^*(\vec{r}_1) \frac{2}{r_{1p}} \phi_0(\vec{r}_1) d\vec{r}_1 \right.$$

$$+ \left. \int \phi_0^*(\vec{r}_1) \frac{2}{r_{1p}} \chi(\vec{r}_1, \vec{r}_p) d\vec{w}_1 \right) \psi(r_p) , \tag{9}$$

In this expression we recognize the energy terms as E_0, the ground state energy of hydrogen, and H_p, the kinetic energy and interaction with the nucleus of the scattered particle. The first integral is just the interaction energy of the positron with the unperturbed target, and the second integral is the interaction energy of the scattered particle

with the perturbation of the target. This is the polarization potential $V_p(r_p)$.

If we now utilize the usual perturbation method, wherein the term W is considered as a perturbing potential with resultant perturbation χ, and substitute Eq. (9) into (7), we get the first-order equation

$$\psi(\vec{r}_p)(H_0 - E_0 - \nabla_p^2)\chi(\vec{r}_1, \vec{r}_p)$$

$$= 2\nabla_p \chi(\vec{r}_1, \vec{r}_p) \cdot \nabla_p \psi(\vec{r}_p)$$

$$+ \psi(\vec{r}_p)(\langle \phi_0, W\phi_0 \rangle - W)\phi_0(\vec{r}_1) . \tag{10}$$

This equation determines the correlation or distortion term $\chi(\vec{r}_1, \vec{r}_p)$ through the static- and kinetic-energy contributions from the incident particle. An analogous equation was given by Obedkov[11] for the electron-hydrogen problem neglecting exchange. Of course the equation is not complete without the scattering equation for the determination of $\psi(\vec{r}_p)$.

Returning to the Schrödinger equation (7) for the scattering, we now perform a scalar multiplication from the left on (7) with $\Psi^*(\vec{r}_1, \vec{r}_p)$ and integrate over the electron coordinate $\vec{r}_1$.

$$\int \psi^*(\vec{r}_p)[\phi_0^*(\vec{r}_1) + \chi^*(\vec{r}_1, \vec{r}_p)]$$

$$\times [H_0(\vec{r}_1) - \nabla_p^2 + 2/r_p + W(\vec{r}_1, \vec{r}_p) - E]$$

$$\times \psi(\vec{r}_p)[\phi_0(\vec{r}_1) + \chi(\vec{r}_1, \vec{r}_p)] d\vec{r}_1 = 0 . \tag{11}$$

With the use of Eqs. (3a), (3b), (5), and some algebra, Eq. (11) becomes

$$- (1 + \langle \chi, \chi \rangle)\nabla_p^2 \psi + (1 + \langle \chi, \chi \rangle)$$

$$\times (2/r_p + \langle \phi_0, W\phi_0 \rangle - k_0^2)\psi$$

$$+ \langle \chi, W\chi \rangle \psi - \langle \chi, \chi \rangle \langle \phi_0, W\phi_0 \rangle \psi + \langle \phi_0, W\chi \rangle \psi$$

$$+ \langle \chi, W\phi_0 \rangle \psi + \langle \chi, H_0 \chi \rangle \psi - \psi \langle \chi, \nabla_p^2 \chi \rangle$$

$$- 2\langle \chi, \nabla_p \chi \cdot \nabla_p \psi \rangle = E_0 \langle \chi, \chi \rangle \psi . \tag{12}$$

Again we will consider the distortion terms as a perturbation in this equation. However, in Eq. (12) we retain all second-order terms and ignore third-order expressions, e.g., $\langle \chi, \chi \rangle \langle \phi_0, W\phi_0 \rangle \psi$. If we define

$$V_c(r_p) = \langle \phi_0, W\phi_0 \rangle \tag{13}$$

$$V_p(r_p) = \langle \phi_0, W\chi \rangle , \tag{14}$$

divide through by $(1 + \langle \chi, \chi \rangle)$, and drop third-order

terms, Eq. (12) becomes

$$-\nabla_p^2 \psi(\vec{r}_p) + \left(\frac{2}{r_p} + V_c(r_p) + V_p(r_p) - k_0^2\right)\psi(\vec{r}_p)$$

$$= -\psi\langle\chi,\, |H_0 - \nabla_p^2 - E_0|\chi\rangle + 2\langle\chi\nabla_p\chi \cdot \nabla_p\psi\rangle$$

$$-\langle\chi, W\phi_0\rangle\psi + \langle\chi, \langle\phi_0, W\phi_0\rangle\phi_0\rangle\psi \ . \qquad (15)$$

Now we note that the terms on the right-hand side of Eq. (15) are identically equal with those obtained from a scalar multiplication of Eq. (10) by χ. Thus with the use of (10) the right side of (15) is zero. We are then left with

$$-\nabla_p^2 \psi(r_p) + [2/r_p + V_c(r_p)$$

$$+ V_p(r_p) - k_0^2]\psi(r_p) = 0 \ , \qquad (16)$$

which is the desired scattering equation.

The term $V_p(r_p)$ in (16) is the nonadiabatic polarization potential defined by (14) and the solution to Eq. (10). Thus, Eqs. (10) and (16) define the nonadiabatic scattering problem.

Equation (16) is easily solved by partial-wave analysis if V_p is known. However, Eq. (10) presents more of a problem. The presence of the operators ∇_p and ∇_p^2, representing the dynamic effects of the incident particle, seriously complicates the equation for χ. The ordinary adiabatic approximation to χ would obtain if these two terms were dropped in Eq. (10). Thus the description of nonadiabatic effects requires that these terms be retained in some form, though considerable simplification of Eq. (10) must be achieved if solutions are to be found.

First, consider the dynamic term $2\nabla_p\chi(\vec{r}_1, \vec{r}_p)$ $\cdot \nabla_p\psi(r_p)$ of Eq. (10). From Eq. (16) we note that asymptotically $\psi(\vec{w}_p)$ satisfies

$$-\nabla_p^2 \psi(\vec{r}_p) \cong k_0^2 \psi(\vec{r}_p), \qquad (17)$$

with solutions $\psi(\vec{w}_p) \sim \exp(\pm i\vec{k}_0 \cdot \vec{r}_p)$. We then note that it is possible to write the correlation function $\chi(\vec{r}_1, \vec{r}_p)$ in terms of a double sum over the complete set of continuum functions for the incident particle, denoted by $\zeta_\nu(\vec{r}_p)$, and the complete set of hydrogen atom wave functions $\phi_j(\vec{r}_1)$. That is, we could write the expansion

$$\chi(\vec{r}_1, \vec{r}_p) = \int\sum_j a_j(k)\zeta_k(\vec{r}_p)\phi_j(\vec{r}_1)dk. \qquad (18)$$

[From Eq. (5) the $j = 0$ term vanishes: $a_0(k) = 0$.] Thus the correlation function can be formed from a wave packet in $\vec{r}_p$ space and a set of hydrogen solutions $\phi_j(\vec{r}_1)$ in $\vec{r}_1$ coordinates (including continuum).

Now in order to represent the effect of ∇_p on χ we make the observation that over the range of r_p comparable to the atomic radius the dynamic effect due to the transient charged particle should be approximately proportional to the velocity with which it moves through the target system.

This suggests that $(1/\chi)\nabla_p\chi \propto k_0$ over an important part of the range of values of r_p. If we write the set of continuum functions as

$$\zeta_k(r_p) = e^{\pm i\vec{k} \cdot \vec{r}}$$

in Eq. (18), the implication is that the wave packet in r_p centers about k_0. Our approximation is to replace the amplitude function $a_j(k)$ by a narrow packet centered about k_0 which we write as a delta function, i.e., $a_j(k) = a_j\delta(k - k_0)$. Thus, for the purposes of treating the dynamic part of the correlation, we write

$$\chi(\vec{r}_1, \vec{r}_p) = \int\sum_{j=1} a_j\delta(k - k_0)e^{i\vec{k} \cdot \vec{r}_p}\phi_j(\vec{r}_1)dk. \qquad (19)$$

If this approximation is made for χ in the dynamic term on the right-hand side of Eq. (10) and the asymptotic approximation (17) is made for $\psi(r_p)$, the first term on the right hand side of Eq. (10) becomes

$$-2k_0^2\chi(\vec{r}_1, \vec{r}_p)\psi(\vec{r}_p).$$

Having made the approximation (19) for χ in the dynamic term on the right, we do the same in the term $-\nabla_p^2\chi$ which appears on the left side of (10). This leaves Eq. (10) as

$$\psi(\vec{r}_p)(H_0 - E_0 + k_0^2)\chi(\vec{r}_1, \vec{r}_p)$$

$$= -2k_0^2\chi(\vec{r}_1, \vec{r}_p)\psi(\vec{r}_p)$$

$$+ \psi(\vec{r}_p)(\langle\phi_0, W\phi_0\rangle - W)\phi_0(\vec{r}_1). \qquad (10')$$

After cancelling the common factor $\psi(r_p)$ in (10'), the determining equation for the perturbed $\chi(r_1, r_p)$ is reduced to

$$(-\nabla_1^2 - 2/r_1 - E_0 + 3k_0^2)\chi(\vec{r}_1, \vec{r}_p)$$

$$= (\langle\phi_0, W\phi_0\rangle - W)\phi_0(\vec{r}_1), \qquad (20)$$

with boundary conditions (5) and (6).

This equation is of the same form as that of the method of polarized orbitals, with the important difference that the distortion function χ depends on the energy of the incident particle through the term $3k_0^2$ on the left-hand side. Thus, for a given kinetic energy k_0^2, Eq. (20) may be solved by the usual procedure of decomposition into multipole components.[12,13] Thus we write

$$W = -2/r_{1p}$$

$$= -\sum_\lambda \frac{2r_<^\lambda}{r_>^{\lambda+1}} \frac{4\pi}{2\lambda+1} Y_\lambda^{*m}(\hat{r}_1)Y_\lambda^m(\hat{r}_p), \qquad (21)$$

where $r_<$ is the lesser and $r_>$ the greater of r_1 and r_p. We then write

$$\phi_0(r_1) = P_{1s}(r_1)/r_1\sqrt{4\pi} \qquad (22)$$

and

$$\chi(\vec{r}_1, \vec{r}_p) = \sum_{l,m} \frac{U_l(r_1, r_p)}{r_1}$$

$$\times Y_l^{*m}(\hat{r}_1) Y_l^m(\hat{r}_p) \sqrt{4\pi}/(2l+1). \tag{23}$$

Substitution of (21), (22), and (23) into Eq. (20) leads to the following sets of radial equations for the multipole components U_l of the distortion term χ. Monopole:

$$\left(-\frac{d^2}{dr_1^2} - \frac{2}{r_1} - E_0 + 3k_0^2\right) U_0(r_1, r_p)$$

$$= [-\int P_{1s}(r_1)(2/r_>) P_{1s}(r_1) dr_1$$

$$+ 2/r_>] P_{1s}(r_1); \tag{24}$$

dipole, quadrupole, etc., $(l = 1, 2, \ldots)$:

$$\left(-\frac{d^2}{dr_1^2} - \frac{2}{r_1} + \frac{l(l+1)}{r_1^2} - E_0 + 3k_0^2\right) U_l(r_1, r_p)$$

$$= (2r_<^l/r_>^{l+1}) P_{1s}(r_1); \tag{25}$$

where each of the above are two equations; one for $r_1 < r_p$ and another for $r_1 > r_p$. These must be matched in each case at $r_1 = r_p$ and must satisfy $U_l(r_1, r_p) = 0$ at $r_1 = 0$; also $U_l(r_1, r_p) \to 0$ as $r_1 \to \infty$. The equations (24) and (25) are obviously nonadiabatic extensions of the polarized-orbital equations.[13] Note that the radial equations are independent of the magnetic quantum number m, which has been suppressed in (25). The nonadiabatic polarization potential is given by

$$V_p(r_p) = -\int \Phi_0^*(\vec{r}_1) \frac{2}{r_{1p}} \chi(\vec{r}_1, \vec{r}_p) d\vec{r}_1$$

$$= \sum_l V_p^l, \tag{26}$$

where

$$V_p^l(r_p) = -[2/(2l+1)] \int U_l(r_1, r_p)$$

$$\times (r_<^l/r_>^{l+1}) P_{1s}(r_1) dr_1. \tag{27}$$

As $k_0 \to 0$,

$$V_p^0(r_p) \to 0 \text{ exponentially, as } r_p \to \infty,$$

$$V_p^1(r_p) \to -\alpha/r^4, \quad (\alpha = 4.5a_0^3),$$

$$V_p^2(r_p) \to -\alpha_q/r^6, \quad (\alpha_q = 15a_0^5),$$

where α and α_q are the dipole and quadrupole polarizabilities of hydrogen. We will neglect multipole components higher than quadrupole in $V_p(r_p)$.

Now looking at Eqs. (24) and (25) we note that, since $E_0 < 0$, the term $3k_0^2$ appears in the form of extra binding in the equation for $\chi(r_1, r_p)$. Thus as k_0^2 increases, the magnitude of U_l, and thus χ, decreases though the exact dependence of this decrease with increasing incident energy is not obvious from the equations.[14] We note that the approximation (19) which was used in treating the dynamic part of the correlation function precludes an accurate description of the nonadiabatic contribution to the polarization potential in the limit $r_p \sim \infty$, since the asymptotic form of (19) in r_p coordinates is incorrect. However, since the potential is very weak in this region, this inaccuracy is not necessarily serious.

The set of Eqs. (24) and (25) have been solved for the monopole, dipole, and quadrupole contribution to the nonadiabatic polarization potential for a number of incident energies. The method of solution has been described in Ref. 13. Results for three different incident energies are shown in Fig. 1 where the three multipole components as well as their sum $V_p(r_p)$ are plotted. As expected, the interaction potential obviously decreases with increasing incident energy.

Having obtained the polarization potential V_p for a given energy k_0^2, the scattering equation for positrons (Eq. 16) is easily solved by partial-wave analysis. Results for s- and p-wave phase shifts are given in Table I. From the table a comparison can be made between the results obtained from the adiabatic approximation [obtained by ignoring the k_0^2 term in Eqs. (24) and (25); see Ref. 12] and those obtained from the nonadiabatic method of Callaway et al.,[7] the variational method of Schwartz,[15,16] and the present nonadiabatic method.

The variationally obtained phase shifts[15,16] are the results of elaborate calculations and can be assumed to be accurate. Thus we note that the effect of the nonadiabatic terms in the potential
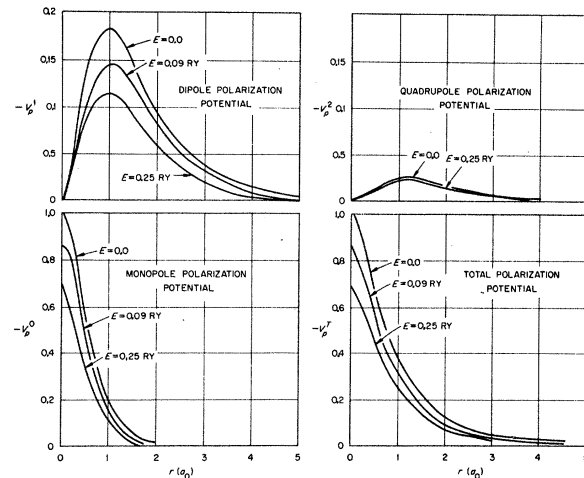

FIG. 1. The multipole components V_p^l and total nonadiabatic polarization potential for three incident energies (potential in rydbergs).

TABLE I. Positron-hydrogen phase shifts as a function of wave vector k_0 (Energy $E = k_0^2$ in rydbergs; η_l in radians).

k_0	Adiabatic $V_p = V_p^0$ $+ V_p^1 + V_p^2$	Extended polari- zation[7]	Present non- adiabatic	Variational[15]
		$l = 0$		
0.0	(-2.540)	(-0.783)	(-2.15)	(-2.10)[a]
0.1	0.160	0.0360	0.150	0.151
0.2	0.208	0.0137	0.162	0.188
0.3	0.196	-0.0352	0.106	0.168
0.4	0.158	-0.0939	0.0292	0.120
0.5	0.111	-0.1539	-0.0520	0.062
0.6	0.0624	-0.2112	-0.120	0.007
0.7	0.0163	-0.2638	-0.182	-0.054
0.8	-0.0261	-0.3036	• • •	• • •
		$l = 1$		Variational[16]
0.1	0.0086	0.0072	0.0083	0.009
0.2	0.030	0.0226	0.0261	0.033
0.3	0.057	0.0370	0.0421	0.065
0.4	0.082	0.0458	0.0489	0.102
0.5	0.101	0.0468	0.0456	0.132
0.6	0.112	0.0408	0.0359	0.156
0.7	0.113	0.0290	0.0209	0.178

[a]The $k_0 = 0$ values are scattering lengths.

function is to reduce the phase shifts from values which are greater than the actual phases to values which are somewhat smaller than the accurate values. The latter behavior is not unexpected, however, since the effects of virtual positronium formation have been neglected herein.[17] This omission causes the phase shifts to lie below the actual values, the discrepancy becoming somewhat greater with increasing incident energy up to the threshold for actual positronium formation.

III. ELECTRON-HYDROGEN SCATTERING

For the electron-scattering problem, we can write the scattering equation in the form of Eq. (1):

$$[H_0(\vec{r}_1) + H_0(\vec{r}_2) + W(\vec{r}_1, \vec{r}_2)]\Psi(\vec{r}_1, \vec{r}_2) = E\Psi(\vec{r}_1, \vec{r}_2), \tag{28}$$

where H_0 is defined in (2a), and $\vec{r}_1$ and $\vec{r}_2$ denote the coordinates of the two electrons. The term $W(\vec{r}_1, \vec{r}_2) = 2/r_{12}$ is opposite in sign to (2c). The total wave function is written as in (4), but is now anti-symmetrized.

$$\Psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2)[\phi_0(\vec{r}_1) + \chi(\vec{r}_1, \vec{r}_2)] \pm \psi(\vec{r}_1)[\phi_0(\vec{r}_2) + \chi(\vec{r}_1, \vec{r}_2)]. \tag{29}$$

The plus and minus signs refer to the singlet and triplet states of the two-electron system.
We obtain the scattering equation from the variational principle

$$\delta \int \Psi^*(\vec{r}_1, \vec{r}_2)(H - E)\Psi(\vec{r}_1, \vec{r}_2)d\vec{r}_1 d\vec{r}_2 = 0 \tag{30}$$

where H is the total Hamiltonian and E the total energy of the system. In (30) we will apply a limited variation, that is, variation with respect to the continuum function ψ of Eq. (29), considering the bound state functions as being predetermined. After substituting (29) into (30), this operation results in the equation

$$\int [\phi_0^*(\vec{r}_1) + \chi^*(\vec{r}_1, \vec{r}_2)](H - E)\{\psi(\vec{r}_2)[\phi_0(\vec{r}_1) + \chi(\vec{r}_1, \vec{r}_2)]$$

$$\pm \psi(\vec{r}_1)[\phi_0(\vec{r}_2) + \chi(\vec{r}_1, \vec{r}_2)]\}d\vec{r}_1 = 0. \tag{31}$$

We will consider the direct and exchange terms separately in Eq. (31), these being, respectively, the term preceding the $\pm$ inside the curly bracket and the exchange term, that associated with the product following the $\pm$ in Eq. (31).

First we note that apart from the change in sign in the Coulomb terms, the direct part of (31) is identical to Eq. (11) for the positron with r_2 replacing r_p in that equation. Thus the treatment of the direct part has been done previously where we retained terms through second order in the perturbation.

In Eq. (31) it is necessary to treat the exchange term in a lower approximation than that of the direct part. First, in the exchange integrals we retain terms only through first order in the perturbation. With the aforementioned analysis on the direct terms, the scattering equation reduces to

$$[-\nabla_2^2 - 2/r_2 + V_c(r_2) + V_p(r_2) - k_0^2]\psi(\vec{r}_2) \pm \{(E_0 - k_0^2)\int \phi_0(\vec{r}_1)\psi(\vec{r}_1)d\vec{r}_1 \phi_0(\vec{r}_2)$$

$$-k^2[\int\phi_0(\vec{r}_1)\psi(\vec{r}_1)\chi(\vec{r}_1,\vec{r}_2)d\vec{r}_1 + \int\chi(\vec{r}_1,\vec{r}_2)\psi(\vec{r}_1)d\vec{r}_1\phi_0(\vec{r}_2)]$$

$$+\int\chi(\vec{r}_1,\vec{r}_2)(-\nabla_1^2 - 2/r_1)\psi(\vec{r}_1)d\vec{r}_1\phi_0(\vec{r}_2) + \int\phi_0(\vec{r}_1)(-\nabla_2^2 - 2/r_2)\psi(\vec{r}_1)\chi(\vec{r}_1,\vec{r}_2)d\vec{r}_1$$

$$+\phi_0(\vec{r}_2)\int\phi_0(\vec{r}_1)W(\vec{r}_1,\vec{r}_2)\psi(\vec{r}_1)d\vec{r}_1\} = 0. \tag{32}$$

The term $V_p(r_2)$ is the nonadiabatic polarization potential due to the incident electron. This term arises here in the treatment of the direct terms in the scattering equation as mentioned above, and results from the solutions to Eq. (10) with r_2 replacing r_p and with a change in sign of W. The phase of χ is changed by π as compared to the positron case; thus the polarization potential[14] is still attractive as it must be.

Thus in the electron-scattering problem the exchange distortion terms are neglected in determining $\chi(\vec{r}_1,\vec{r}_2)$. In order to further simplify the scattering, Eq. (32), and to be consistent with the analysis of the target distortion, we will neglect the dynamic polarization exchange terms in Eq. (32), these being the terms in the curly bracket which contain the perturbation $\chi(\vec{r}_1,\vec{r}_2)$. These are in any case small for two reasons. At large distances the perturbation χ rapidly vanishes. For small distances the second and fourth terms almost exactly cancel, since $(-\nabla_1^2 - 2/r_1)\psi(\vec{r}_1) \sim k^2\psi(\vec{r}_1)$, and from (31) the first and third terms are proportional to the monopole component of χ as $r \to 0$.

Thus neglecting the exchange distortion terms, the scattering equation becomes

$$-\nabla_2^2\psi(\vec{r}_2) + [V_c(r_2) + V_p(r_2) - 2/r_2 - k_0^2]\psi(\vec{r}_2)$$

$$= \pm[(k_0^2 - E_0)\int\phi_0(\vec{r}_1)\psi(\vec{r}_1)d\vec{r}_1 - \int\phi_0(\vec{r}_1)W\psi(\vec{r}_1)d\vec{r}_1]\phi_0(\vec{r}_2). \tag{33}$$

Partial-wave analysis of this equation leads to the set of radial equations

$$\frac{d^2}{dr_2^2}f_l(r_2) + \left(\frac{2}{r_2} - \int\phi_0(r_1)\frac{2}{r_{12}}\phi_0(r_1)d\vec{r}_1 - V_p(r_2) + k_0^2\right)f_l(r_2)$$

$$= \pm P_{1s}(r_2)\{(E_0 - k_0^2)\delta_{l0}\int_0^\infty f_0(r_1)P_{1s}(r_1)dr_1$$

$$+ [2/(2l+1)][r_2^l\int_0^\infty f_l(r_1)P_{1s}(r_1)r_1^{-(l+1)}dr_1 + r_2^{-(l+1)}\int_0^{r_2}f_l(r_1)P_{1s}(r_1)r_1^l dr_1$$

$$- r_2^l\int_0^{r_2}f_l(r_1)P_{1s}(r_1)r_1^{-(l+1)}dr_1]\}, \tag{34}$$

where $\quad \psi(\vec{r}_2) = \sum_{l=0}^\infty \frac{f_l(r_2)}{r_2}P_l(\cos\theta_2); \quad \phi_0(\vec{r}_2) = \frac{P_{1s}(r_2)}{r_2}\frac{1}{\sqrt{4\pi}}$

and $\quad f_l(r_2) \sim k_0^{-1}\sin(k_0 r_2 - \tfrac{1}{2}l\pi + \eta_l), \quad$ as $r_2 \to \infty$. $\tag{35}$

Equations (32) and (33) are identical in form to the equations of the adiabatic exchange approximation,[13] with the difference that $V_p(r_2)$ is no longer the adiabatic polarization potential. Solutions to (23) were obtained by an iterative technique described earlier.[18]

In Tables II and III the $l=0$ and $l=1$ phase shifts for singlet (η_l^+) and triplet (η_l^-) scattering are tabulated for electrons with wave numbers $k_0 = 0.1$ to 0.8, where $k_0^2 = E$ (Ry). In Tables II and III a comparison is made between the present results for s- and p-waves and those obtained by other methods. The first column contains results from the adiabatic approximation. These were obtained by setting the dynamic term, $3k_0^2$, equal to zero in Eqs. (24) and (25), including all contributions through the quadrupole term in V_p. In columns 2 and 3 the nonadiabatic results of Temkin[3] and of Callaway et al.[7] are given with the

W. R. GARRETT

TABLE II. Electron-hydrogen singlet and triplet s-wave phase shifts $(l=0)$ (Energy $E=k_0^2$ in rydbergs; η_l in radians).

k_0	Adiabatic $V_p = V_p^0 + V_p^1 + V_p^2$	Temkin[3]	Extended[7] polarization	Present nonadiabatic	Variational[15]
		Singlet (η_0^+)			
0.0	$\cdots$	(5.6)	(7.419)	(5.18)	(5.95)[a]
0.1	2.617	2.59	2.436	2.612	2.553
0.2	2.165	2.11	1.910	2.141	2.067
0.3	1.808	1.74	1.537	1.757	1.696
0.4	1.534	1.45	1.259	1.452	1.415
0.5	1.324	1.23	1.042	1.215	1.202
0.6	1.166	$\cdots$	$\cdots$	1.029	1.041
0.7	1.051	$\cdots$	$\cdots$	0.887	0.930
0.8	0.970	0.87	$\cdots$	0.786	0.886
		Triplet (η_0^-)			
0	$\cdots$	(1.76)	(1.676)	(1.57)	(1.769)
0.1	2.957	2.942	2.948	2.955	2.939
0.2	2.752	2.723	2.735	2.733	2.717
0.3	2.547	2.516	2.525	2.529	2.500
0.4	2.354	2.301	2.327	2.321	2.294
0.5	2.177	2.112	2.145	2.129	2.105
0.6	2.017	$\cdots$	$\cdots$	1.956	1.933
0.7	1.875	$\cdots$	$\cdots$	1.800	1.780
0.8	1.750	1.647	$\cdots$	1.662	1.643

[a]The $k_0=0$ values are scattering lengths.

present nonadiabatic results in column 4. The variational results, which are again taken as the true phase shifts, are given in column 5. The entries for $k_0 = 0$ are scattering lengths obtained by use of the expansion based on the low-energy effective-range theory.[19] The effect of the nonadiabatic terms in the polarized-orbital results can best be seen by comparing the phase shifts of columns 1 and 4. The reduction in the magnitude of the polarization potential through the dynamic terms is reflected in the reduction of the corresponding phase shifts. This reduction increases with increasing incident velocities over the energy range below the inelastic threshold.

Comparing the present results with those of Schwartz,[15] we see that the nonadiabatic method investigated herein yields rather reliable phase shifts for low-energy electron-hydrogen collisions.

IV. DISCUSSION

As we noted earlier, the objective here has not been to obtain very accurate hydrogen cross sections. Instead, the objectives were, first, to examine the magnitude of dynamic effects on the distortion of the target system and on the resulting polarization potential as provided by the conventional perturbation procedure and, second, to develop a method which might find application in problems involving more complicated scattering systems.

From the results illustrated in the figure, we see that within the approximations made in the present analysis, the dynamic effect on the polarization potential is appreciable. As one would expect,[14] the various multipole components of the distortion χ are not reduced in the same proportion for a given incident energy. For an incident kinetic energy equal to half the average kinetic energy of the bound electron, the monopole component is reduced by a little less than half, the dipole and quadrupole component by a little more than half as compared to the corresponding adiabatic values.

Though the approximations made in arriving at the equations for the orbital distortion were somewhat drastic and difficult to quantify, the results indicate that a useful description survived. An alternative approach to the treatment on nonadiabatic effects has been employed LaBahn and Callaway[4] and Callaway et al.,[7] wherein the adiabatic perturbation χ and resulting polarization potential are used to describe the target with additional dynamic terms appearing in the scattering equation. Agreement with the variational phase shifts is somewhat better in the present investigation than in the extended polarization potential method[7] for both electron- and positron-hydrogen scattering. The inclusion of the dynamic effects in the equations determining the distortion χ, as in the present treatment, also has some advantage in that the solving of bound-state equations is in general less troublesome than solving complicated continuum equations containing the correlation functions. In addition, for heavier systems where the complete solutions for a given incident energy might become very time consuming,[20] the present

TABLE III. Electron-hydrogen singlet and triplet p-wave phase shifts $(l=1)$ (Energy $E=k_0^2$ in rydbergs; η_l in radians).

k_0	Adiabatic	Extended[7] polarization	Present	Variational[16]
		Singlet $(\eta_1{}^+)$		
0.1	0.0087	0.0063	0.0071	0.007
0.2	0.0217	0.0150	0.0181	0.0147
0.3	0.9336	0.0160	0.020	0.0170
0.4	0.0398	0.0076	0.0095	0.0100
0.5	0.0422	−0.0068	−0.0080	−0.0007
0.6	0.0446		−0.028	−0.099
0.7	0.0508		−0.043	−0.013
0.8	0.0623		−0.052	−0.010
		Triplet $(\eta_1{}^-)$		
0.1	0.0143	0.0102	0.0118	0.0114
0.2	0.0585	0.0448	0.0523	0.0450
0.3	0.146	0.1047	0.122	0.106
0.4	0.265	0.182	0.207	0.187
0.5	0.388	0.261	0.288	0.270
0.6	0.488		0.351	0.341
0.7	0.555		0.398	0.393
0.8	0.595		0.423	0.427

method offers the possibility of a simple scaling of the effective interaction potential for various incident energies once the solutions have been obtained for a few cases.

Since the method of polarized orbitals[9,10] in the usual adiabatic approximation has provided a very useful technique for studying low energy collisions involving many-electron systems,[13,21,22] a similar technique which includes nonadiabatic effects should provide a useful extension, particularly for systems which are very highly polarizable. These include many atoms, e.g., the alkalis, and a large number of molecules. The present method can be employed on a Hartree-Fock (H.F.) target system in a manner similar to the above treatment, yielding somewhat more complex equations for the dynamically perturbed H.F. orbitals. These quations are presently under investigation.

Regarding the study of dynamic effects in low-energy atomic collision phenomena, one final comment seems appropriate concerning the availability of experimental data. There is particular need of very accurate cross-section data on a system which is both simple and highly polarizable. The Li atom should be a likely candidate for this purpose.

[1]M. H. Mittleman and K. M. Watson, Phys. Rev. 113, 198 (1959).

[2]M. H. Mittleman, Ann. Phys. (N.Y.) 14, 74 (1961).

[3]A. Temkin, Phys. Rev. 126, 130 (1962).

[4]R. W. LaBahn and J. Callaway, Phys. Rev. 113, 198 (1959).

[5]R. Pu and E. S. Chang, Phys. Rev. 151, 31 (1966).

[6]C. J. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. 165, 53 (1968).

[7]J. Callaway, R. W. LaBahn, R. T. Pu, and W. M. Duxler, Phys. Rev. 168, 12 (1968).

[8]R. M. Sternheimer, Phys. Rev. 96, 951 (1954); 115, 1198 (1959).

[9]A. Temkin, Phys. Rev. 107, 1004 (1957); 116, 358 (1959).

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

[11]V. D. Obedkov, Zh. Eksperim. i Teor. Fiz. 43, 649 (1962) [English transl.: Soviet Phys. − JETP 16, 463 (1963)].

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

[13]W. R. Garrett, Phys. Rev. 140, A705 (1965).

[14]The first term on the right side of Eq. (10) behaves as $\sim r_p^{-3}\, d\Psi/dr_p$ for $r \to \infty$. Thus the leading dynamic term in the asymptotic polarization potential goes as

$r_p^{-5}\,(d/dr_p)f_l(r_p)$, where f_l is the lth partial-wave component of ψ. See Refs. 2 and 6.

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

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

[17]A wave function of the form (4) can describe the formation of virtual positronium; however, the second-order terms which were dropped in Eq. (10) must be retained for this description. The present polarization potential is the same for positive or negative incident charges. The complete perturbation equation does not behave similarly.

[18]See Ref. 13. The radial equation of Ref. 13 is misprinted. It should have the form (34).

[19]T. F. O'Malley, L. Spruch, and L. Rosenberg, Phys. Rev. 125, 1300 (1962).

[20]The solutions for the multipole components of V_p required about 3 minutes each for a given kinetic energy, thus about 9 minutes for complete scattering cross sections on the IBM 360/75 at the Oak Ridge National Laboratory. Because of the short word length on the 360/75, all calculations were done in double precisions (16 decimals).

[21]W. R. Garrett and H. T. Jackson, Phys. Rev. 153, 28 (1967).

[22]R. J. W. Henry, Phys. Rev. 162, 56 (1967).