PHYSICAL REVIEW A VOLUME 3, NUMBER 3 MARCH 1971

Elastic Scattering of Positrons from Hydrogen: An Optical Potential Calculation*

John J. Matese and Albert C. Fung
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803

(Received 29 July 1970)

The optical potential of Bell and Squires is used to formulate the problem of the elastic scattering of positrons from atoms. An application is made to the scattering of S-wave positrons from hydrogen below the threshold for positronium formation. The single-particle states of the electron are chosen to be the hydrogenic solutions, while the positron states are obtained by using a single-particle potential which includes the Hartree potential plus a model polarization potential. Various models are investigated and a choice is made which effectively maximizes the calculated phase shifts through second order in the perturbation expansion of the optical potential. Phase shifts thus obtained yield approximately 67–80% of the difference between the static Hartree results and the variational results of Schwartz. Higher-order effects are evaluated using the techniques of Kelly. Intermediate states of multipole $l \leq 3$ are included.

I. INTRODUCTION

It is well known that in the scattering of low-energy positrons from atoms the distortion of the atom by the incident positron gives rise to substantial effects on the scattering phase shifts.[1-5] Various attempts have been made to take account of this polarization phenomenon. The case of S-wave positron-hydrogen scattering provides a good test of these approaches since accurate results have been obtained by Schwartz[6] in an extensive many-parameter variational calculation.

One class of approximations is nonvariational in nature. This includes the adiabatic polarized orbital method[1] and the nonadiabatic extended polarization potential method of Callaway *et al.*[5] The former method[1] tends to overestimate the S-wave phase shifts while the latter method[5] tends to underestimate them. Because these nonvariational approaches do not yield a stationary property of the phase shifts, attention has recently shifted to variational methods, some of which yield bounds.[6-8]

The many-parameter variational approaches of Schwartz,[6] Hahn and Spruch,[4] and Burke and Taylor,[8] are capable of yielding reliable results. However, extension to more complicated atoms is a formidable problem. The close-coupling formalism,[9-11] in which the first few lowest-lying states of hydrogen are included, yields poor results, mainly because of the neglect of excitation to the electron continuum which is of great importance in the hydrogen case.

This undesirable feature is partially eliminated by a modification of the close-coupling formalism which introduces localized pseudostates of the atom that effectively represent the continuum.[12-15]

In considering the positron-hydrogen problem, Perkins[14] has coupled pseudo-p and -d states to the $1s$ state of hydrogen. Two adjustable parameters are used to maximize the lower-bound phase shifts. Burke *et al.*[15] have close-coupled pseudo-p and -d states along with the $1s$, $2s$, and $2p$ states of hydrogen in a calculation of electron-hydrogen scattering. The pseudostates used yield the exact values of the polarizabilities $\alpha(1s \rightarrow p \rightarrow 1s)$, $\alpha(1s \rightarrow d \rightarrow 1s)$ and contain no adjustable parameters. The main disadvantage of Perkins's approach[14] over that taken by Burke *et al.*[15] is that his pseudo-p state carries the much heavier burden of providing an adequate representation of the $2p$ state as well as the continuum p states.

One of the most fruitful approaches to the low-energy scattering of positrons from hydrogen has been formulated by Drachman[2] using the lower-bound principle of Gailitis.[16] As discussed in Appendix A, this approach can be viewed in the context of the optical potential formalism of Feshbach.[17] The Hilbert space of the atom is decomposed into the ground state and the first-order perturbed atomic state which implicitly includes *all* excited atomic states. This method has recently been extended to the electron-hydrogen elastic scattering problem by Oberoi and Callaway.[18] The success of these calculations is heartening, although extension to more complicated systems requires approximations which destroy the lower-bound properties.

A completely different formulation of the elastic scattering problem is the optical-potential approach of many-body theory. As shown by Bell and Squires,[19] the optical potential is equivalent to the self-energy of the single-particle Green's function and can be represented by a perturbation expansion. Brueckner[20] and Goldstone[21] have developed techniques for representing these terms in diagrammatic form. The method has been applied by Pu and Chang[22] to the problem of electron-helium scattering and by Kelly[23] to the problem of triplet scattering of S-wave electrons from hydrogen.

The main difficulty of this approach is that the numerical work involved in the calculation is lengthy. However, extension to more complicated systems is straightforward. First-order and second-order diagrams can be readily and accurately evaluated, but higher-order diagrams can only be approximated in practice. For this reason it is desirable to formulate the problem in such a manner as to minimize these higher-order effects.

The objectives of the present calculation include the extension of the many-body formalism to the problem of the elastic scattering of positrons from atoms, consideration of various possible choices of the single-particle potential, and an investigation of the usefulness of this perturbative approach to scattering problems when correlation effects are large. In Sec. II we detail the extension of the formalism to the problem of positron-atom scattering. Section III contains a discussion of the choice of the single-particle potential of the positron, and in Sec. IV we present the results. Conclusions and a summary are contained in Sec. V.

II. FORMALISM

The application of the formal optical potential of Bell and Squires[19] to the scattering of electrons from atoms has been made by Pu and Chang[22] and Kelly.[23] We briefly discuss the extension of this formalism to the scattering of positrons from atoms.

The total Hamiltonian describing an incident positron and an atom of Z electrons is given by

$$H(A, x) = H_A(A) + T_+(x) - \sum_{i=1}^{Z} v(ix), \tag{1}$$

where H_A is the atom Hamiltonian

$$H_A(A) = \sum_{i=1}^{Z} T(i) + \sum_{i>j}^{Z}\sum v(ij). \tag{2}$$

$T(i)$ is the sum of the kinetic energy and the nuclear potential energy of the ith electron, T_+ is the corresponding quantity for the positron, and the two-body interactions are given by

$$v(ij) = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}, \quad v(ix) = \frac{e^2}{|\vec{r}_i - \vec{x}|}. \tag{3}$$

The scattering equation of interest is

$$H(A, x)\Psi(A, x) = (E_A + \epsilon)\Psi(A, x), \tag{4}$$

where E_A is the total energy of the ground state of the atom and ϵ is the energy of the incident positron. The optical potential formalism, described below, replaces this many-particle Schrödinger equation with a single-particle equation,

$$[h(x) + V_{op}]\psi(x) = \epsilon\psi(x), \tag{5}$$

the solution of which yields the exact scattering phase shifts. Here h is a zero-order positron Hamiltonian and V_{op} is the optical potential; these are obtained as follows.

The interaction between the particles can be approximated by single-particle electron and positron potentials, V and V_+, respectively. We then define the zero-order Hamiltonians

$$h(x) = T_+(x) + V_+(x), \tag{6a}$$

$$H_A^{(0)}(A) = \sum_{i=1}^{Z}[T(i) + V(i)], \tag{6b}$$

$$H^{(0)}(A, x) = h(x) + H_A^{(0)}(A), \tag{6c}$$

from which one obtains the many-body perturbation

$$\begin{aligned} H'(A, x) &= H(A, x) - H^{(0)}(A, x) \\ &= \sum_{i>j}^{Z}\sum v(ij) - \sum_{i=1}^{Z} v(ix) - \sum_{i=1}^{Z} V(i) - V_+(x). \end{aligned} \tag{7}$$

The only restriction placed on the single-particle potentials is that they be Hermitian so that the single-particle wave functions

$$[T(i) + V(i)]\phi_n(i) = \epsilon_n\phi_n(i), \tag{8a}$$

$$[T_+(x) + V_+(x)]\phi_K(x) = \epsilon_K\phi_K(x) \tag{8b}$$

form an orthonormal set.[24]

The zero-order atomic wave function $\Phi_0^{(0)}(A)$ is chosen to be a Slater determinant formed from Z single-particle states ϕ_n representing the ground state of the atom. We refer to these states as the unexcited states.

Since the atom constitutes a system of identical fermions, it is desirable to use the formalism of second quantization. In this representation the operators defined in Eqs. (6) and (7) become

$$H_A^{(0)} = \sum_{n=1}^{Z} \epsilon_n \eta_n^\dagger \eta_n, \tag{9a}$$

$$h = \sum_K \epsilon_K \lambda_K^\dagger \lambda_K, \tag{9b}$$

$$\begin{aligned} H' = {}& \sum_{pqmn} \langle pq|v|mn\rangle \eta_p^\dagger \eta_q^\dagger \eta_n \eta_m \\ & - \sum_{PqKn} \langle Pq|v|Kn\rangle \lambda_P^\dagger \eta_q^\dagger \eta_n \lambda_K - \sum_{qn} \langle q|V|n\rangle \eta_q^\dagger \eta_n \\ & - \sum_{PK} \langle P|V_+|K\rangle \lambda_P^\dagger \lambda_K. \end{aligned} \tag{9c}$$

The electron operators $\eta^\dagger$ and η satisfy the Fermi-Dirac anticommutation relations as do the positron operators $\lambda^\dagger$ and λ. However η and λ commute; i.e., we are not treating electrons and positrons as antiparticles of one another. In the summations $\sum_{PqKn}$, $\sum_{pqmn}$, only distinct matrix elements are included. For example, $\langle pq|v|mn\rangle$ is not distinct from $\langle qp|v|nm\rangle$ but is distinct from $\langle pq|v|nm\rangle$.

Continuum solutions of the single-particle equations, Eqs. (8), are normalized as follows:

$$\phi = r^{-1} R(r) Y_{lm}(\theta, \phi) \chi_{m_s},$$
$$R(r) \sim \cos[kr + \delta_l - \tfrac{1}{2}(l+1)\pi] \quad \text{as } r \to \infty. \tag{10}$$

With this normalization the summation over continuum states is replaced by $(2/\pi)\int_0^\infty dk$.[25] In this calculation bound states are summed up to principal quantum number $N = 10$. Higher states are included using the estimation formula of Kelly.[25]

The single-particle Green's function can then be constructed and from it one obtains the self-energy or optical potential as shown by Bell and Squires[19]:

$$V_{op} = \langle \Phi_0^{(0)} | \sum_{\substack{m=0 \\ LP}}^{\infty} H' \left(\frac{H'}{E_A^{(0)} + \epsilon_{K_0} - H^{(0)} + i\delta} \right)^m | \Phi_0^{(0)} \rangle . \tag{11}$$

This sum can be represented by a series of diagrams in the standard fashion. The notation LP refers to the fact that only those terms which are linked and proper (as specified by Bell and Squires[19]) are to be retained. The rules for evaluating diagrams need only minor modifications from those used when all the particles are identical.[25] One must distinguish positron lines from electron lines. We use a double bar to indicate a positron. The single-particle interactions are different depending upon whether they are attached to a positron line (V_+) or an electron line (V). Finally, each two-body electron-positron interaction introduces an additional minus sign to the over-all sign of the diagram.

Rather than attempt to solve the scattering equation (5) with the complicated nonlocal optical potential, Eq. (11), or the equivalent radial equation

$$(L - \epsilon_{K_0}) R_{K_0} = \left(-\frac{d^2}{dr^2} + \frac{2z}{r} + \frac{l(l+1)}{r^2} + V_+ + V_{op} - \epsilon_{K_0} \right) R_{K_0}$$
$$= 0, \tag{12}$$

we use the variational principle of Hulthén[26] which yields a stationary property for the phase shift although it does not give a bound. Constructing a trial potential V_t and its scattering solution

$$(L_t - \epsilon_{K_0}) R_{K_0}^t = \left(-\frac{d^2}{dr^2} + \frac{2z}{r} + \frac{l(l+1)}{r^2} + V_t - \epsilon_{K_0} \right) R_{K_0}^t$$
$$= 0, \tag{13}$$

we obtain the variational estimate of the phase shift

$$\delta = \delta_t - \langle R_{K_0}^t | L - \epsilon_{K_0} | R_{K_0}^t \rangle / K_0$$
$$= \delta_t - \langle R_{K_0}^t | L - L_t | R_{K_0}^t \rangle / K_0$$
$$= \delta_t - \langle R_{K_0}^t | V_+ + V_{op} - V_t | R_{K_0}^t \rangle / K_0 . \tag{14}$$

The normalization, Eq. (10), is assumed. One can use different forms for the potentials V_+ and V_t, but since the motivation for choosing each of these potentials is the same, we identify V_t with V_+. The result is then

$$\delta = \delta_t - \langle K_0 | V_{op} | K_0 \rangle / K_0 . \tag{15}$$

In Sec. III we discuss various possible choices for the single-particle potential V_+.

III. CHOICE OF SINGLE-PARTICLE POTENTIALS

The positron-atom problem has a computational advantage over the associated electron-atom problem in that exchange diagrams involving the scattered particle do not occur because the Pauli principle does not enter. A serious disadvantage is that correlation effects are generally larger for the positron than for the electron. Therefore one must judiciously choose the positron single-particle potential to include as much as possible of the correlation effects and minimize the higher-order correlations. In particular, it is desirable to choose V_+ such that it includes the screening effect of all the atomic electrons and also includes a model potential which approximates the polarization effects. The electron single-particle potential V should be chosen to represent the screening of $Z - 1$ electrons (generally the lowest-lying electrons). Such a choice gives rise to both bound and continuum excited electron states. Pu and Chang[22] and Kelly[23] chose a single-particle electron potential which did not give rise to bound excited states. Kelly[23] then found that second-order effects accounted for about 70% of the full correlation effect in triplet S-wave electron-hydrogen scattering and about 60% of the dipole polarizability. By estimating higher-order effects he was able to obtain good agreement with the exact results.

For the application considered here, the scattering of S-wave positrons from hydrogen, we choose $V = 0$. The excited electron states ϕ_k are just the hydrogenic functions. Diagrams which then arise, through third order, are shown in Fig. 1. Only the two terms of H' in Eq. (9c) which contain positron operators will contribute. The perturbation expansion of the matrix element $\langle K_0 | V_{op} | K_0 \rangle$ gives the following terms through third order:

$$-\langle K_0 | V_+ | K_0 \rangle , \tag{16a}$$

$$-\langle K_0 n | v | K_0 n \rangle = \langle K_0 | V_H | K_0 \rangle , \tag{16b}$$

$$\sum_{Kk} \frac{\langle K_0 n | v | Kk \rangle \langle Kk | v | K_0 n \rangle}{\epsilon_n + \epsilon_{K_0} - \epsilon_k - \epsilon_K} , \tag{16c}$$

$$-\sum_{\substack{KK' \\ kk'}} \frac{\langle K_0 n | v | K'k' \rangle \langle K'k' | v | Kk \rangle \langle Kk | v | K_0 n \rangle}{(\epsilon_n + \epsilon_{K_0} - \epsilon_{K'} - \epsilon_{k'})(\epsilon_n + \epsilon_{K_0} - \epsilon_K - \epsilon_k)} , \tag{16d}$$

$$-\sum_{KK'k} \frac{\langle K_0 n | v | K'k \rangle \langle K' | V_+ | K \rangle \langle Kk | v | K_0 n \rangle}{(\epsilon_n + \epsilon_{K_0} - \epsilon_{K'} - \epsilon_k)(\epsilon_n + \epsilon_{K_0} - \epsilon_K - \epsilon_k)} . \tag{16e}$$

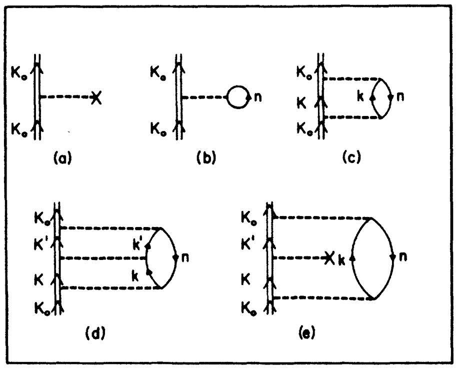

FIG. 1. Contributing diagrams to $\langle K_0 | V_{\text{op}} | K_0 \rangle$ through third order.

Here we denote the hydrogenic 1s state by n and V_H is the (attractive) Hartree potential

$$V_H = -\langle n | v | n \rangle . \tag{17}$$

The standard choice of V_+ is such as to make the first-order corrections, Eq. (16a) plus Eq. (16b), vanish. However, the second-order correlation effect, Eq. (16c), is large in this case, and we choose V_+ in such a manner as to partially compensate for this polarization effect. Preliminary calculations including first- and second-order diagrams with intermediate states restricted to the multipoles $l \leq 3$ were performed using four choices of V_+: (i) $V_+ = V_H$, (ii) $V_+ = V_H + V(\text{Bethe})$ where V(Bethe) is the adiabatic dipole polarization potential,[27] (iii) $V_+ = V_H + V(\text{Bethe}) + V(\text{Reeh})$ where V(Reeh) is the adiabatic quadrupole polarization potential,[28] (iv) $V_+ = V_H + V(\text{Buckingham})$ where

$$V(\text{Buckingham}) = -4.5/(r^2 + \Delta^2)^2 \tag{18}$$

and Δ is used as an adjustable parameter.[29] A value of $\Delta \approx 1.85$ was found to maximize the second-order results.

Choices (ii), (iii), and (iv) (with $\Delta = 1.85$) were found to give essentially the same second-order phase shifts, with $V_+ = V_H + V(\text{Bethe})$ giving slightly larger values. However, choosing $V_+ = V_H$ gives decidedly inferior results at low energies. This is illustrated in Fig. 2 where we plot δ_t(Hartree), δ_t(Hartree + Bethe), δ (Hartree), δ(Hartree + Bethe) and Schwartz's values for δ.[6] The agreement of the second-order phase shifts for all model potentials at the high-energy portion of the spectrum implies that the variational method of computing the phase shifts should be quite good away from threshold. The results discussed in Sec. IV were computed using the choice $V_+ = V_H + V(\text{Bethe})$. However, we shall refer to the difference between the Schwartz result and the Hartree result as the full correlation correction to the phase shift. The zero-energy scattering solution to Eq. (8b) was found to have no zeros other than at the origin, and therefore there exist no bound states of the zero-order positron Hamiltonian h.

IV. RESULTS

With the choice $V_+ = V_H + V(\text{Bethe})$ the first-order contribution becomes

$$\langle K_0 | V_{\text{op}}^{(1)} | K_0 \rangle = -\langle K_0 | V(\text{Bethe}) | K_0 \rangle , \tag{19}$$

which is the sum of Eqs. (16a) and (16b). This partially cancels the second-order matrix element Eq. (16c). In Table I we list the various contributions to δ through second order. These results are subdivided into the multipole of the intermediate states, and further subdivided into contributions from bound excited states $k(b)$ and from continuum excited states $k(c)$. Bound f states are not included since their contribution is small. We estimate that an error of about 1% of the difference between the static results and the exact results is made when one neglects multipoles $l \geq 4$ *in second-order*. The second-order phase shifts are also plotted in Fig. 2. One observes that approximately 67–80% of the total correlation effect is accounted for in second order. This is to be compared with the results of Hahn and Spruch[4] who obtain 85–89% of the full correlation effect

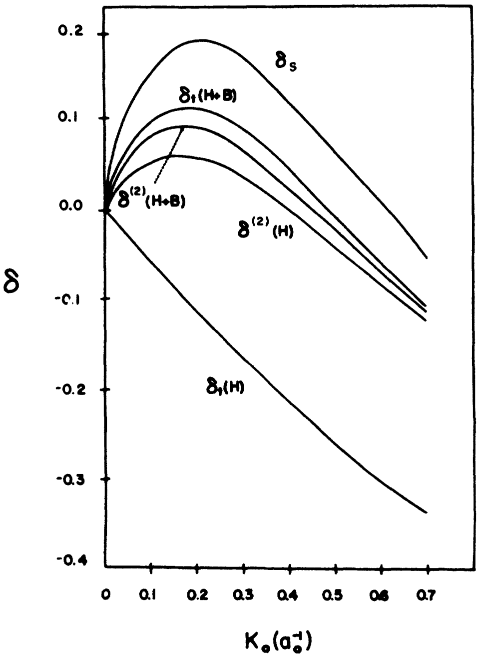

FIG. 2. S-wave positron-hydrogen phase shifts (in rad). δ_s = Schwartz results, δ_t = zero-order results, and $\delta^{(2)}$ = second-order results. H = Hartree single-particle potential, and $H + B$ = Hartree plus Bethe single-particle potential.

TABLE I. Contributions to the second-order S-wave phase shift (in rad) for positron-hydrogen scattering using the single-particle positron potential $V_+ = V_{\mathrm{Hartree}} + V_{\mathrm{Bethe}}$. The l value is the multipole of the bound (b) or continuum (c) excited electron states.

K_0	0.0[a]	0.1	0.2	0.3	0.4	0.5	0.6	0.7
δ_t	-1.4587	0.0982	0.1139	0.0870	0.0415	-0.0102	-0.0622	-0.1115
$V_{\mathrm{op}}^{(1)}$	2.7803	-0.2094	-0.2836	-0.2964	-0.2868	-0.2697	-0.2509	-0.2327
$V_{\mathrm{op}}^{(2)}(kl=c0)$	-0.0544	0.0048	0.0080	0.0104	0.0125	0.0147	0.0171	0.0198
$V_{\mathrm{op}}^{(2)}(kl=b0)$	-0.0950	0.0083	0.0139	0.0179	0.0214	0.0250	0.0291	0.0345
$V_{\mathrm{op}}^{(2)}(kl=c1)$	-0.6956	0.0545	0.0785	0.0871	0.0890	0.0883	0.0860	0.0826
$V_{\mathrm{op}}^{(2)}(kl=b1)$	-1.4705	0.1038	0.1283	0.1230	0.1106	0.0953	0.0814	0.0705
$V_{\mathrm{op}}^{(2)}(kl=c2)$	-0.1877	0.0158	0.0233	0.0255	0.0251	0.0235	0.0214	0.0191
$V_{\mathrm{op}}^{(2)}(kl=b2)$	-0.0250	0.0020	0.0025	0.0022	0.0018	0.0013	0.0010	0.0007
$V_{\mathrm{op}}^{(2)}(kl=c3)$	-0.0494	0.0042	0.0062	0.0068	0.0066	0.0060	0.0053	0.0046
$\delta^{(2)}$	-1.2561	0.0822	0.0910	0.0635	0.0218	-0.0258	-0.0719	-0.1123

[a] $K_0 = 0$ entries are contributions to the scattering length.

using multipoles $l \leq 3$ and including all orders of interactions.

The radial integrals were performed using $R_{\max} = 45$. The trial phase shift δ_t and the first-order matrix element, Eq. (19), were extended to infinity using the technique of Levy and Keller.[30] A check on the numerical accuracy of the second-order p and d multipole contributions was made by simultaneously computing the adiabatic matrix elements which are obtained by setting ϵ_K equal to ϵ_{K_0} in the denominator of Eq. (16c). The results were compared to the matrix elements of the Bethe potential and the Reeh potential and were found to agree to approximately 0.5%. The latter figure then serves as our estimate of the numerical accuracy of the second-order results.

Higher-order correlations involving multipoles $l \leq 3$ are estimated using the third-order diagrams according to the techniques devised by Kelly.[23,25] The most important intermediate electron states of the second-order matrix element are $2s$, $2p$, $ks \approx 0.5s$, $kp \approx 0.5p$, $kd \approx 0.75d$, and $kf \approx 1.0f$. Similarly we find that the most important intermediate positron states are given by $ks \approx 0.75s$, $Kp \approx (0.25 + 0.8K_0)p$, $Kd \approx (0.75 + 0.6K_0)d$, and $Kf \approx (1.25 + 0.6K_0)f$.

For a particular l value of the excited states K, k in Fig. 1(c), with K, k chosen to be the typical excitations of importance just given, the ratios

$$t(K,k) = \sum_{K'k'} \frac{\langle K_0 n | v | K'k' \rangle \langle K'k' | v | Kk \rangle}{\epsilon_n + \epsilon_{K_0} - \epsilon_{K'} - \epsilon_{k'}} \Big/ \langle K_0 n | v | Kk \rangle , \tag{20}$$

$$a(K,k) = -\sum_{K'} \frac{\langle K_0 n | v | K'k \rangle \langle K' | V_+ | K \rangle}{\epsilon_n + \epsilon_{K_0} - \epsilon_{K'} - \epsilon_k} \Big/ \langle K_0 n | v | Kk \rangle \tag{21}$$

are constructed. The motivation for forming these ratios becomes clear when one compares the third-order matrix elements, Eqs. (16d) and (16e), with the second-order matrix element, Eq. (16c). The ratio t has been found by Kelly[23,25] to be a reasonably accurate approximation for the ratio of the ladder diagram, Fig. 1(d), to the second-order diagram, Fig. 1(c). Similarly, a approximates the ratio of Fig. 1(e) to Fig. 1(c).

In order to facilitate the discussion we subdivide the contributions to the ladder approximation, $t(K, k)$, into its diagonal part and its nondiagonal parts. For a given k the diagonal parts considered, $t_D(k)$, are as follows:

$$\begin{aligned} &k = 2s \rightarrow k' = 2s, \quad k = ks \rightarrow k' = \text{continuum } s, \\ &k = 2p \rightarrow k' = 2p, \quad k = kp \rightarrow k' = \text{continuum } p, \\ &k = kd \rightarrow k' = \text{continuum } d, \end{aligned} \tag{22}$$

while the nondiagonal parts considered, $t_{ND}(k \rightarrow k')$, are

$$\begin{aligned} &k = 2s \rightarrow k' = \text{all } s \ (\neq 2s); \quad k = ks \rightarrow k' = \text{bound } s; \\ &k = 2p \rightarrow k' = \text{all } s, \quad \text{all } p \ (\neq 2p), \quad \text{all } d, \quad \text{all } f; \\ &k = kp \rightarrow k' = \text{all } s, \quad \text{bound } p, \quad \text{all } d, \quad \text{all } f; \\ &k = kd \rightarrow k' = \text{bound } d. \end{aligned} \tag{23}$$

We have not considered diagonal third-order corrections for intermediate f and bound d states since their contribution is small. Similarly, some (presumably small) nondiagonal third-order effects have not been included [e.g., $t(s \rightarrow d)$].

In evaluating Eq. (21) the intermediate matrix element, $\langle K' | V_+ | K \rangle$, diverges for $K' = K$ if we let $R_{\max}$ approach infinity.[25] However, the integration over K' removes this infinity. A similar phenomenon occurs for $t_D(k)$. Further, there is substantial cancellation between $t_D(k)$ and $a(k)$. The third-order ratios have been computed for the energies of interest. In Table II we list the results for the single case $K_0 = 0.3$.

Higher-order corrections are estimated in the following manner. Diagonal ladder diagrams can be summed to all orders since the ratio of the $(n+1)$th-order diagram to the nth-order diagram is approximately given by $t_D(k) + a(k)$. The net effect is to modify the second-order diagram associated with the state k by the factor

$$[1 - t_D(k) - a(k)]^{-1}. \tag{24}$$

Nondiagonal third-order diagrams contribute a factor

$$[1 - t_D(k) - a(k)]^{-1}\, t_{ND}(k \to k')[1 - t_D(k') - a(k')]^{-1}. \tag{25}$$

The transitions considered are given in Eq. (23). A factor of 2 should be included for the l changing third-order nondiagonal diagrams to account for both $k \to k'$ and $k' \to k$. We also estimate some small fourth-order diagrams of the type $k \to k' \to k$ which give rise to a factor

$$[1 - t_D(k) - a(k)]^{-1}\, t_{ND}^2(k \to k')[1 - t_D(k) - a(k)]^{-1}. \tag{26}$$

Using these estimates we compute a "coefficient of enhancement," C_e, for each of the second-order contributions listed in Table I. We have set $C_e = 1$ for bound d and continuum f contributions. The C_e value for s and d states includes only the l nonchanging transitions as indicated in Eq. (23). The l changing corrections have been included in the p-state C_e value. These results are listed in Table III. Explicit expressions for the C_e values are given in Appendix B.

TABLE II. Third-order ratios for $K_0 = 0.3$. Transitions included are listed in Eqs. (22) and (23).

$t_D(2s) + a(2s)$	-0.5487
$t_D(ks) + a(ks)$	-0.2808
$t_D(2p) + a(2p)$	-0.0478
$t_D(kp) + a(kp)$	-0.0017
$t_D(kd) + a(kd)$	0.0627
$t_{ND}(2s \to s)$	0.1188
$t_{ND}(ks \to s)$	0.1461
$t_{ND}(2p \to s)$	-0.0398
$t_{ND}(2p \to p)$	0.0818
$t_{ND}(2p \to d)$	0.0660
$t_{ND}(2p \to f)$	0.0184
$t_{ND}(kp \to s)$	0.0053
$t_{ND}(kp \to p)$	0.0742
$t_{ND}(kp \to d)$	0.0343
$t_{ND}(kp \to f)$	0.0054
$t_{ND}(kd \to d)$	0.0139

TABLE III. C_e values.

K_0	$C_e(b0)$	$C_e(c0)$	$C_e(b1)$	$C_e(c1)$	$C_e(c2)$
0.0	0.7262	0.8735	1.1260	0.9956	1.0646
0.1	0.7265	0.8733	1.1521	1.0646	1.0754
0.2	0.7216	0.8713	1.1649	1.1181	1.0811
0.3	0.7115	0.8675	1.1644	1.1561	1.0817
0.4	0.6968	0.8620	1.1475	1.1755	1.0755
0.5	0.6758	0.8544	1.1237	1.1859	1.0679
0.6	0.6425	0.8442	1.1031	1.1963	1.0627
0.7	0.5989	0.8316	1.0822	1.2036	1.0585

The final value of the phase shift is then obtained from

$$\delta = \delta_t - [\langle K_0 | V_{\mathrm{op}}^{(1)} | K_0 \rangle + \textstyle\sum_i C_e(i) \langle K_0 | V_{\mathrm{op}}^{(2)}(i) | K_0 \rangle]/K_0, \tag{27}$$

where the summation runs over those contributions to the second-order optical potential listed in Table I. Table IV contains the results of our calculation and compares them with the variational calculation of Hahn and Spruch.[4] The Hahn and Spruch results include multipoles $l \leq 3$ and constitute an accurate estimate of the best results one can obtain with just these multipoles. (This is an intermediate stage of their calculation. They extend the analysis to multipoles $l \leq 5$ and successfully extrapolate the contributions from the remaining multipoles.)

The present calculation, which includes only intermediate s, p, d, and f states contains about 8% less of the full correlation effect than the corresponding calculation of Hahn and Spruch. Subsidiary calculations were performed in which only s, p, d, and only s, p states were included. The differences with the corresponding calculations of Hahn and Spruch were 4 and 1%, respectively.

TABLE IV. Positron-hydrogen phase shifts (in rad).

K_0	Hartree	This work[a]	Hahn and Spruch[a]	Schwartz
0.0[b]	0.5822	-1.4091		-2.10
0.1	-0.0580	0.0996		0.151
0.2	-0.1145	0.1187	0.142	0.188
0.3	-0.1682	0.0938		0.168
0.4	-0.2181	0.0488	0.076	0.120
0.5	-0.2635	-0.0043		0.062
0.6	-0.3042	-0.0540	-0.029	0.007
0.7	-0.3400	-0.1038		-0.054

[a] Including multipoles $l \leq 3$.

[b] $K_0 = 0$ entries are scattering lengths.

The good agreement of the results when only s, p states are included suggests that the variational approximation used here, Eq. (14), is sufficient if the single-particle potential is properly chosen. We believe the growing discrepancy with increasing multipoles is due partly to the techniques used for estimating the higher-order effects and partly to the total neglect of fourth-order diagrams of the type $s \to p \to d$, $p \to d \to f$, and $p \to p' \to s, d$ where the first transition is nondiagonal.

V. SUMMARY AND CONCLUSIONS

We have calculated phase shifts for the S-wave scattering of positrons from hydrogen using a many-body optical potential. A single-particle positron potential has been chosen which effectively minimizes third- and higher-order correlations. These higher-order effects are still large, and present techniques seriously underestimate their contribution. In the model problem where only s, p, and d intermediate states are allowed to enter, the present formulation agrees to within 5% of the "exact" answer.[4] This is consistent with the results of the triplet S-wave electron-hydrogen scattering calculation of Kelly[23] where only these multipoles are important.

The contribution from multipoles $l \geq 3$ is known to be large.[4] Second-order contributions from these multipoles have been found to be small in this calculation. Attempts to estimate their contribution in third and higher orders give substantially smaller corrections than can be inferred from the calculation of Hahn and Spruch.[4] For this reason we have not attempted to include multipoles $l \geq 4$.

Virtual positronium formation is implicitly contained in the many-body formalism used here. Calculations of real positronium formation above threshold[31] indicate that the main contribution comes from the P channel. We find little unusual behavior of our S-wave results as we approach threshold. The rapid rise of $t_D(2s) + a(2s)$ toward the value -1 at threshold is the only sign of the importance of virtual positronium formation in the S channel.

The optical potential calculation of Drachman[2] (see Appendix A) in which all multipoles are included in a nonadiabatic manner gives excellent results for the positron-hydrogen problem. However, extension of this formalism to the positron-helium problem necessitated an approximation and the results are somewhat poorer. We anticipate that an application of the present many-body formalism to the positron-helium problem would give better results than those obtained here for the positron-hydrogen case. The substantially smaller polarizability of helium implies that higher-order correlations will be smaller and therefore any errors made in estimating them would be reduced.

ACKNOWLEDGMENTS

The authors gratefully acknowledge some informative correspondence with Dr. R. J. Drachman concerning the Gailitis formalism. We also wish to thank the Lousiana State University Computing Center for the use of the IBM 360 computer.

APPENDIX A: OPTICAL POTENTIAL OF DRACHMAN

In this Appendix we recast the variational formulation of Drachman[2] into an optical potential formalism to facilitate comparison with the method presented in this paper.[32] The starting point is the Hamiltonian of the interacting positron-atom system, Eq. (1), which is separated in a different fashion from the many-body formalism. Here we write

$$H(A, x) = H_A(A) + h(x) + h'(A, x), \tag{A1}$$

where H_A is the exact atom Hamiltonian, Eq. (2), h is the zero-order positron Hamiltonian, Eq. (6a), and h' is the perturbation

$$h'(A, x) = -\sum_{i=1}^{z} v(ix) - V_+(x), \tag{A2}$$

which contains the two-body electron-positron interactions and the single-particle positron potential, which is chosen here to be the Hartree potential

$$V_+ = V_H = -\sum_{i=1}^{z} \langle \Phi_0(A) | v(ix) | \Phi_0(A) \rangle . \tag{A3}$$

Φ_0 is the exact ground state of the unperturbed atom,

$$H_A(A)\Phi_0(A) = E_A \Phi_0(A). \tag{A4}$$

The optical potential formalism of Feshbach[17] introduces the projection operator

$$P = | \Phi_0(A) \rangle \langle \Phi_0(A) | \tag{A5}$$

and its complement

$$Q = 1 - P. \tag{A6}$$

We write the exact scattering equation, Eq. (4), in the form

$$P(H - E_A - \epsilon)(P + Q)\Psi = 0, \quad Q(H - E_A - \epsilon)(P + Q)\Psi = 0. \tag{A7}$$

Eliminating $Q\Psi$ we obtain for $P\Psi$

$$(H_{\text{op}} - E_A - \epsilon) P\Psi = 0, \tag{A8}$$

where

$$H_{\text{op}} = P\{H - HQ[Q(E_A + \epsilon - H)Q]^{-1} QH\} P. \tag{A9}$$

Equation (A8) is effectively a one-body scattering equation for the function

$$\psi(x) = \langle \Phi_0(A) | \Psi(A, x) \rangle \tag{A10}$$

whose solution yields the exact phase shifts.

In the manner of Gailitis[16] we consider now a projection onto a subspace of the full space

$$R = P + \hat{Q}\,, \tag{A11}$$

where we choose

$$\hat{Q} = \frac{|w(A, x)\rangle\langle w(A, x)|}{N(x)}\,. \tag{A12}$$

Here $w(A, x)$ is the first-order perturbed atomic wave function which is the solution to

$$[H_A(A) - E_A]w(A, x) = -h'(A, x)\Phi_0(A) \tag{A13}$$

and is made orthogonal to $\Phi_0(A)$. The function N is given by

$$N(x) = \langle w(A, x)|w(A, x)\rangle\,. \tag{A14}$$

Gailitis[16] has shown that the approximate optical Hamiltonian

$$\hat{H}_{\text{op}} = P\{H - H\hat{Q}[\hat{Q}(E_A + \epsilon - H)\hat{Q}]^{-1}\hat{Q}H\}P \tag{A15}$$

will yield lower bounds to the true scattering phase shifts for energies which lie below the lowest eigenvalue of QHQ.

Evaluation of $\hat{H}_{\text{op}}$ using the choice $\hat{Q}$ of Eq. (A12) is straightforward when Eqs. (A13) and (A14) are used. The result is

$$\hat{H}_{\text{op}} = |\Phi_0\rangle\{h + E_A + V_P[N(\epsilon - h) + V_P - W - \vec{\mathrm{V}}_n\cdot\vec{\nabla} - V_3]^{-1}V_P\}\langle\Phi_0|\,, \tag{A16}$$

where the potentials are defined as follows:

$$V_P(x) = \langle w(A, x)|h'(A, x)|\Phi_0(A)\rangle\,, \tag{A17}$$

$$W(x) = \langle w(A, x)| -\nabla^2(x)|w(A, x)\rangle\,, \tag{A18}$$

$$V_3(x) = \langle w(A, x)|h'(A, x)|w(A, x)\rangle\,, \tag{A19}$$

$$\vec{\mathrm{V}}_n(x) = \langle w(A, x)| -2\vec{\nabla}(x)|w(A, x)\rangle\,. \tag{A20}$$

V_P is the well-known polarization potential, W and $\vec{\mathrm{V}}_n$ are nonadiabatic potentials, and V_3 is a third-order potential. Using Eqs. (A10) and (A16), the approximate one-body equation which yields a lower bound on the phase shift is

$$\{h + V_P[N(\epsilon - h) + V_P - W - \vec{\mathrm{V}}_n\cdot\vec{\nabla} - V_3]^{-1}V_P\}\psi(x) = \epsilon\psi(x)\,, \tag{A21}$$

which can be reduced to a set of coupled equations

$$\begin{aligned}&(h - \epsilon)\psi = -V_P F\,,\\ &[N(h - \epsilon) - V_P + W + \vec{\mathrm{V}}_n\cdot\vec{\nabla} + V_3]F = -V_P\psi\,.\end{aligned} \tag{A22}$$

These are identical to the coupled equations obtained by Drachman[2] who also projected onto the space $R = P + \hat{Q}$ and used a variational technique.

An approximate nonadiabatic equation can be obtained by formally expanding the integral operator in Eq. (A21) about V_P, i.e.,

$$[N(\epsilon - h) + V_P - W - \vec{\mathrm{V}}_n\cdot\vec{\nabla} - V_3]^{-1} \to 1/V_P - (1/V_P)[N(\epsilon - h) - W - \vec{\mathrm{V}}_n\cdot\vec{\nabla} - V_3](1/V_P)\,, \tag{A23}$$

from which one obtains

$$[h + (1 + N)^{-1}(V_P + V_3 + W + \vec{\mathrm{V}}_n\cdot\vec{\nabla})]\psi = \epsilon\psi\,. \tag{A24}$$

This is just the dynamic polarization equation of LaBahn and Callaway[33] (neglecting the higher-order terms N and V_3).

The case of positron-hydrogen elastic scattering provides a good test of this approximation. The perturbed orbital w has been obtained analytically[34] and all the potential functions, Eqs. (A17)–(A20), have been evaluated numerically.[2] One obtains that the nonadiabatic function W dominates at short ranges. Therefore the expansion does not give an adequate representation of the short-range behavior of the optical potential. The approximation, Eq. (A24), will be valid only when short-range effects are known to be unimportant.

We now show how a similar nonadiabatic expansion of the second- and third-order optical potential of many-body theory[35] also yields Eq. (A24) which provides the desired link with the optical potential used by Drachman. We consider positron-hydrogen scattering and choose $V_+ = V_H$, which causes the first-order diagrams to cancel. Denoting the scattering solution to the optical Hamiltonian by ψ (which is not an eigenstate of h), we construct the second-order term $V_{\text{op}}^{(2)}\psi(x)$ as in Eq. (16c) and expand the energy denominator, treating $\epsilon_K - \epsilon_{K_0}$ as a small number,

$$V_{\text{op}}^{(2)}\psi(x) \approx \sum_{Kk} |K(x)\rangle\langle n(i)|v(ix)|k(i)\rangle\langle Kk|v|\psi n\rangle \times\left(\frac{1}{\epsilon_n - \epsilon_k} + \frac{\epsilon_K - \epsilon_{K_0}}{(\epsilon_n - \epsilon_k)^2}\right). \tag{A25}$$

For the third-order terms we make the full adiabatic approximation

$$V_{\text{op}}^{(3)}\psi(x) \approx -\sum_{\substack{KK'\\kk'}} \frac{|K'(x)\rangle\langle n(i)|v(ix)|k'(i)\rangle\langle K'k'|v|Kk\rangle\langle Kk|v|\psi n\rangle}{(\epsilon_n - \epsilon_{k'})(\epsilon_n - \epsilon_k)} - \sum_{\substack{KK'\\k}} \frac{|K'(x)\rangle\langle n(i)|v(ix)|n(i)\rangle\langle K'|V_H|K\rangle\langle Kk|v|\psi n\rangle}{(\epsilon_n - \epsilon_k)^2}\,. \tag{A26}$$

The closure relations

$$\textstyle\sum_K |K(1)\rangle\langle K(2)| = \delta(1-2), \qquad \text{(A27)}$$

$$\textstyle\sum_k |k(1)\rangle\langle k(2)| + |n(1)\rangle\langle n(2)| = \delta(1-2), \qquad \text{(A28)}$$

and the corollary relation

$$\textstyle\sum_K (\epsilon_K - \epsilon_{K_0})|K(1)\rangle\langle K(2)| = [h(1) - \epsilon_{K_0}]\delta(1-2), \qquad \text{(A29)}$$

along with the eigenfunction expansion of the perturbed orbital

$$w(1,2) = \sum_k \frac{|k(1)\rangle\langle k(3)|v(32)|n(3)\rangle}{\epsilon_k - \epsilon_n}, \qquad \text{(A30)}$$

can be used in a lengthy but straightforward calculation to demonstrate that the resulting approximate optical potential $V_{\mathrm{op}}^{(2+3)}\psi$ given in Eqs. (A25)–(A26) reduces to precisely Eq. (A24) and therefore establishes the connection with the optical potential of Drachman.

APPENDIX B: ENHANCEMENT COEFFICIENTS

In this appendix we give the explicit forms used for the C_e values. The transitions included are given in Eqs. (22) and (23):

$$C_e(b0) = \{1 + t_{ND}(2s\to s)[1 - t_D(ks) - a(ks)]^{-1} + t_{ND}^2(2s\to s)[1 - t_D(2s) - a(2s)]^{-1}\}[1 - t_D(2s) - a(2s)]^{-1}, \qquad \text{(B1)}$$

$$C_e(c0) = \{1 + t_{ND}(ks\to s)[1 - t_D(2s) - a(2s)]^{-1} + t_{ND}^2(ks\to s)[1 - t_D(ks) - a(ks)]^{-1}\}[1 - t_D(ks) - a(ks)]^{-1}, \qquad \text{(B2)}$$

$$\begin{aligned} C_e(b1) = \{1 &+ t_{ND}(2p\to p)[1 - t_D(kp) - a(kp)]^{-1} + t_{ND}^2(2p\to p)[1 - t_D(2p) - a(2p)]^{-1} + 2t_{ND}(2p\to s)[1 - t_D(2s) - a(2s)]^{-1} \\ &+ t_{ND}^2(2p\to s)[1 - t_D(2p) - a(2p)]^{-1} + 2t_{ND}(2p\to d)[1 - t_D(kd) - a(kd)]^{-1} + t_{ND}^2(2p\to d)[1 - t_D(2p) - a(2p)]^{-1} \\ &+ 2t_{ND}(2p\to f)\}[1 - t_D(2p) - a(2p)]^{-1}, \end{aligned} \qquad \text{(B3)}$$

$$\begin{aligned} C_e(c1) = \{1 &+ t_{ND}(kp\to p)[1 - t_D(2p) - a(2p)]^{-1} + t_{ND}^2(kp\to p)[1 - t_D(kp) - a(kp)]^{-1} + 2t_{ND}(kp\to s)[1 - t_D(2s) - a(2s)]^{-1} \\ &+ t_{ND}^2(kp\to s)[1 - t_D(kp) - a(kp)]^{-1} + 2t_{ND}(kp\to d)[1 - t_D(kd) - a(kd)]^{-1} + t_{ND}^2(kp\to d)[1 - t_D(kp) - a(kp)]^{-1} \\ &+ 2t_{ND}(kp\to f)\}[1 - t_D(kp) - a(kp)]^{-1}, \end{aligned} \qquad \text{(B4)}$$

$$C_e(c2) = \{1 + t_{ND}(kd\to d)\}[1 - t_D(kd) - a(kd)]^{-1}. \qquad \text{(B5)}$$

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*Work supported in part by the Office of Naval Research.

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PHYSICAL REVIEW A VOLUME 3, NUMBER 3 MARCH 1971

Collisional Ionization Rates for Lithium- and Beryllium-Like Ions[*]

H.-J. Kunze

Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742

(Received 29 October 1970)

Collisional ionization rates for C iv, N v, and O vi as well as for O v and Ne vii are deduced from the time history of spectral lines emitted by these ions in a hot plasma. The plasma (in the electron temperature range 100–260 eV) is produced in a 15-kJ theta-pinch device, and it is analyzed using the light-scattering technique. The results are consistent with theoretical calculations for O vi and with a semiempirical formula based on theoretical calculations for hydrogenic ions but smaller by factors 1.5–2.

I. INTRODUCTION

Cross sections for ionization by electron impact have been measured now for many neutral and some singly ionized atoms.[1] The technique usually employed is the crossed-beam method. With increasing charge, such measurements become very difficult. Not only then are the cross sections decreasing rapidly, but it also is more difficult to obtain suitable high-current ion beams. The cross sections for ionization of some doubly ionized atoms[2,3] appear, at present, to be the only ones measured for higher ionization stages. Multiply ionized atoms, however, are important in many laboratory and astrophysical plasmas. In most of these applications only the corresponding rate coefficients are needed. Such ionization-rate coefficients can be deduced from the spectroscopic analysis of a well-diagnosed plasma, as was shown for neon ions in a stellarator discharge[4] and for heliumlike C v in a theta-pinch plasma.[5] (Excitation coefficients have been obtained by this method as well and will be the subject of another paper.) In Sec. II we present ionization rates for ions of the lithiumlike and berylliumlike isoelectronic sequences obtained with a theta-pinch device.

II. THEORETICAL IONIZATION RATES

Theoretical cross sections for ionization from the ground state, specifically of lithiumlike and berylliumlike ions, have been calculated by Trefftz and Malik for O vi and O v using the Coulomb-Born-Oppenheimer method[6] and the distorted-wave approximation.[7] Recently, Schwartz[8] calculated the ionization cross sections for O vi for ionization from the ground state as well as from the $2p$ excited level in the Coulomb-Born II approximation. The calculations include distortion, which was found to increase the cross section by about 22% at 1.5 times the threshold energy and, to a lesser extent, at lower and higher impact energies (for example, only 13% at 5 times threshold).

The reduced cross section of Schwartz for the ionization from the $2s$ level of O vi agrees to within 10% with the reduced cross section for ionization from the $1s$ level of a hydrogenic ion of charge $Z = 128$ as calculated by Rudge and Schwartz[9] in the Born-exchange approximation. The reduced cross section for O vi as given by Trefftz[6] shows essentially the same maximum value; however, the peak is shifted to lower energies and her cross section is smaller at higher energies (e.g., by 30% at four times threshold.) Finally, the reduced cross section for ionization from the $2p$ level as obtained by Schwartz[8] is somewhat larger than that for ionization from the $2s$ level (by ~31% at 1.125 times threshold and by ~20% at 5 times threshold).

Using an empirical formula with three free parameters, Lotz[10] approximated all experimentally determined cross-section curves to within 10% and predicted many unknown cross sections. For ions four and more times ionized, his formula reduces to one with a single free parameter, and then essentially agrees with the calculations of Rudge and Schwartz[9] for a hydrogenlike ion with high Z number. Rate coefficients derived from the predicted cross sections[10] have been computed and are tabulated in Ref. 11.

For many applications a simple expression of general validity for the ionization rates would be more desirable. A good starting point[12] is the well-known effective Gaunt-factor excitation rate, where the averaged Gaunt factor must now allow, of course, for all electric multipole transitions.