

(c) Integrals of Products of Spherical Harmonics

The integration of products of several spherical harmonics is easily accomplished by expanding pairs²⁹

$$Y_{l_1 m_1}(\theta, \phi) Y_{l_2 m_2}(\theta, \phi) = \sum_L D(l_1, l_2, L; m_1, m_2) Y_{L, m_1+m_2}(\theta, \phi),$$

where L takes on all values such that $|l_1 - l_2| \leq L \leq l_1 + l_2$ and $l_1 + l_2 + L$ is even. The coefficients may be given in terms of Clebsch-Gordon coefficients as

$$D(l_1, l_2, L; m_1, m_2) = \left[\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2L + 1)} \right]^{1/2} \times C(l_1, l_2, L; m_1, m_2) C(l_1, l_2, L; 0, 0).$$

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¹D. R. Bates and H. S. W. Massey, *Phil Trans. Roy. Soc. (London)* **A239**, 269 (1943).

²M. M. Klein and K. A. Brueckner, *Phys. Rev.* **111**, 115 (1958).

³J. W. Cooper and J. B. Martin, *Phys. Rev.* **126**, 1482 (1962).

⁴A. Temkin, *Phys. Rev.* **107**, 1004 (1957).

⁵A. Temkin and J. C. Lamkin, *Phys. Rev.* **121**, 788 (1961).

⁶I. H. Sloan, *Proc. Roy. Soc. (London)* **A281**, 151 (1964).

⁷R. W. LaBahn and J. Callaway, *Phys. Rev.* **135**, A1539 (1964).

⁸W. R. Garrett, *Phys. Rev.* **140**, A705 (1965).

⁹D. G. Thompson, *Proc. Roy. Soc. (London)* **A294**, 160 (1966).

¹⁰R. J. W. Henry, *Phys. Rev.* **162**, 56 (1967).

¹¹A. Dalgarno and R. J. Moffett, *Proc. Natl. Acad. Sci. India* **A33**, 511 (1963).

¹²D. H. Sampson and R. C. Mjolsness, *Phys. Rev.* **140**, A1466 (1965).

¹³S. Geltman and K. Takayanagi, *Phys. Rev.* **143**, 25 (1966), **138**, A1003 (1965).

¹⁴A. Temkin and K. V. Vasavada, *Phys. Rev.* **160**, 109 (1967).

¹⁵V. M. Martin, M. J. Seaton, and J. B. G. Wallace, *Proc. Phys. Soc. (London)* **72**, 701 (1958).

¹⁶H. W. Joy and R. G. Parr, *J. Chem. Phys.* **28**, 448 (1958).

¹⁷W. Kolos and L. Wolniewicz, *J. Chem. Phys.* **46**, 1426 (1967).

¹⁸G. A. Victor, J. C. Browne, and A. Dalgarno, *Proc. Phys. Soc. (London)* **92**, 42 (1967).

¹⁹M. Adamov, V. Objedkov, and R. Evarestov, *Lietuvos Fiz. Rinkiny, Lietuvos TSR Mosklu Akad., Lietuvos TSR Aukstosios Mokyklos* **3**, 245 (1963).

²⁰S. Weinbaum, *J. Chem. Phys.* **1**, 593 (1933).

²¹N. F. Lane and S. Geltman, *Phys. Rev.* **160**, 53 (1967).

²²D. E. Golden, H. W. Bandel, and J. A. Salerno, *Phys. Rev.* **146**, 40 (1966).

²³A. M. Arthurs and A. Dalgarno, *Proc. Roy. Soc. (London)* **A256**, 540 (1960).

²⁴S. C. Wang, *Phys. Rev.* **31**, 579 (1928).

²⁵E. Gerjuoy and S. Stein, *Phys. Rev.* **97**, 1671 (1955).

²⁶A. I. McIntosh, private communication.

²⁷R. W. B. Ardill and W. D. Davison, private communication.

²⁸E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Cambridge University Press, Cambridge, 1931), pp. 43 and 95.

²⁹M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957), p. 61.

Variational Bounds in Positron-Atom Scattering

Richard J. Drachman

NASA Laboratory for Theoretical Studies, Goddard Space Flight Center, Greenbelt, Maryland

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We have previously applied Dalgarno and Lynn's complete first-order adiabatic correlation function to the problem of low-energy elastic positron scattering by hydrogen and helium atoms. This approach is now extended to yield rigorous lower bounds on the scattering phase shifts in the case of hydrogen and "quasibounds" for helium. In addition, the positron annihilation rate in helium is re-evaluated, and lower values are now found, with the enhancement factor over the Dirac rate varying between 1.5 and 1.8. Some comparisons are made between the present method and other recent work.

I. INTRODUCTION

In two recent papers,^{1,2} the problem of low-energy elastic scattering of positrons from simple atoms (hydrogen and helium) has been treated in a

modified adiabatic approximation. The method consisted in assuming that the optical potential³ is well represented by the position-dependent second-order energy shift in the ground state of the target atom due to the electric field of the positron.⁴

Two novel features were introduced in these calculations. Firstly, the exact second-order potential⁵ was used in place of an approximate form.⁴ Secondly, suppression of the short-range parts of the potential was accomplished by the use of a semi-empirical energy-independent parameter, which served to reduce the spherical (monopole) distortion of the atom which would otherwise dominate as the positron approached the nucleus.

In the case of positron-hydrogen scattering,¹ 90% suppression of the monopole was found to give essentially exact agreement with the definitive S-wave results of Schwartz⁶ from zero energy up to the positronium formation threshold. Higher partial waves gave smaller phase shifts than the best present estimates,⁷ presumably due to the inclusion of insufficient amounts of virtual positronium in the wave function.

The positron-helium calculation² was repeated for various values of monopole suppression, and suffered from the use of the shielded hydrogenic approximation for the atomic ground state. But since no exact results exist, its correctness cannot yet be evaluated.⁸ The only existing experiment⁹ measures the momentum-transfer cross section near the positronium formation threshold, and seems to disagree strongly.

The results for hydrogen¹ seem to imply that the adiabatic wave function contains, to a considerable extent, the significant physics of low-energy positron scattering. Nevertheless, it is disturbing that a semiempirical parameter is required, and also that no extremum principle or bound is contained in the results. The purpose of the present work¹⁰ is to use the adiabatic wave function in such a way as to obtain rigorous lower bounds to the phase shifts for e^+ -H scattering and "quasirigorous" lower bounds in the e^+ -He case.

In Sec. II, the lower-bound principle of Gailitis¹¹ is adapted to the adiabatic type of trial function for e^+ -H scattering. In Sec. III, a simple scale change gives the corresponding equations for e^+ -He scattering, and the e^+ annihilation rate in helium is also calculated. Results for these two cases are given and discussed in Sec. IV. In Sec. V we clarify the relations between the present method and other recent work. Two appendices contain details of the calculation.

II. FORMULATION AND POSITRON-HYDROGEN SCATTERING

We are interested here in obtaining approximate solutions to the positron-atom elastic scattering problem. The energy will be restricted so as to forbid any rearrangement or inelastic processes, the lowest of which is real positronium formation, occurring above 6.8 eV in hydrogen and 17.8 eV in helium. To apply the lower-bound principle of Gailitis,¹¹ it is sufficient in this energy range to use a trial scattering function of the form

$$\Psi_{\vec{k}}(\vec{r}, \vec{x}) = \chi_{\vec{k}}(\vec{x})\phi(r) + \Phi(\vec{r}, \vec{x}). \quad (1)$$

Here \vec{x} is the position vector of the positron, \vec{r} represents the atomic electrons, ϕ is the ground-state wave function of the target atom, and χ is the

scattering function for the positron of momentum \vec{k} , which must approach the correct asymptotic form as $x \rightarrow \infty$. The distortion or polarization of the target by the incoming positron—the closed-channel part of the wave function—is approximately represented by Φ , which satisfies the conditions¹²

$$\int d^3r \phi(\vec{r}) \Phi(\vec{r}, \vec{x}) = 0, \quad \text{for all } x, \quad (2a)$$

$$\text{and } \iint d^3x d^3r [\Phi(\vec{r}, \vec{x})]^2 < \infty. \quad (2b)$$

Then the two functions χ and Φ are to be determined. The resulting form of χ yields partial-wave phase shifts $\delta_L(k)$ which satisfy the inequality $\tan \delta_L(k) \leq \tan \delta_L(k)$ (exact), for all energies below any resonances that might occur.

The Hamiltonian for e^+ -H scattering is

$$H = H_r + H_x + V, \quad (3)$$

$$\text{where } H_r = -(\nabla_r^2 + 2/r), \quad H_x = -\nabla_x^2,$$

$$\text{and } V(\vec{r}, \vec{x}) = 2(1/x - 1/|\vec{x} - \vec{r}|),$$

where we have set $\hbar^2/2m_e = 1$, $e^2 = 2$, with energies in rydbergs and lengths in units of a_0 , the Bohr radius. The correlation function is

$$\Phi(\vec{r}, \vec{x}) = F(\vec{x})G(\vec{r}, \vec{x})\phi(r) \quad (4)$$

where F is to contain short-range nonadiabatic modifications to the adiabatic correlation function G which satisfies the first-order equation⁵

$$[G, H_r]\phi(r) = (V - \langle V \rangle)\phi(r). \quad (5)$$

Throughout this paper the angular-bracket notation will represent expectation value in the ground state, i. e.,

$$\langle V \rangle = \int d^3r \phi(r) V(\vec{r}, \vec{x}) \phi(r). \quad (6)$$

From Eq. (5), the function G is determined to within an arbitrary additive function of x , which may be chosen to make $\langle G \rangle$ vanish. With this choice, Eq. (4) is consistent with Eq. (2a).

If we use standard variational methods¹³ and allow χ and F to undergo free, independent variation, we obtain the following two coupled equations:

$$\langle (H - E)(\chi + FG) \rangle = 0, \quad (7a)$$

$$\langle G(H - E)(\chi + FG) \rangle = 0, \quad (7b)$$

where $E = E_0 + k^2$ and $(H_r - E_0)\phi(r) = 0$. Simple operations, including commutation of H_r and G and use of Eq. (5), yield the following coupled differential equations for χ and F :

$$[\nabla^2 + k^2 - V_1]\chi = V_2 F, \quad (8a)$$

$$[N(\nabla^2 + k^2) + V_2 - V_3 - W - V_N d/dx]F = V_2 \chi. \quad (8b)$$

The "potentials" appearing in Eq. (8) are defined as follows:

$$\begin{aligned}
V_p(x) &= \langle G^{p-1} V \rangle, \quad (p = 1, 2, 3); \\
W(x) &= -\langle G \nabla_x^2 G \rangle; \\
N(x) &= \langle G^2 \rangle; \\
V_N(x) &= -dN/dx.
\end{aligned} \tag{9}$$

Using the exact analytical form of G , given in elliptical coordinates by Dalgarno and Lynn,⁵ we have numerically evaluated¹⁴ all the functions defined in Eq. (9). The evaluation is outlined in Appendix A, and in Table I the potentials are tabulated.

The limiting forms of these potentials can be found analytically for small and large x , and are useful for starting the solutions of Eq. (8) and also to check their numerical evaluation. (See Appendix A) We obtain, for $x \rightarrow 0$,

$$\begin{aligned}
V_1 &\approx 2(1/x-1), \\
V_2 &\approx -1 + O(x^2), \\
V_3 &\approx \frac{3}{4}V_1, \\
N &\approx \frac{3}{4} - \frac{5}{3}x^2, \\
V_N &\approx \frac{10}{3}x, \\
W &\approx 6(1-2x);
\end{aligned} \tag{10}$$

and for $x \rightarrow \infty$

$$\begin{aligned}
V_1 \text{ and } W &\rightarrow 0 \text{ exponentially,} \\
V_2 &\sim -[9/2x^4 + 15/x^6 + \dots], \\
V_3 &\sim -[213/2x^7 + 1773/x^9 + \dots], \\
N &\sim +[43/8x^4 + 107/8x^6 + \dots], \\
V_N &\sim +[43/2x^5 + 321/4x^7 + \dots].
\end{aligned} \tag{11}$$

The solution of the coupled Eqs. (8) is outlined in Appendix B, and the results are discussed in Sec. IV. In Fig. 1 we have plotted the S-wave zero-energy solutions for the two functions χ and $F-\chi$, as well as the "suppression factor," $T(x) = F/\chi$. One can see the natural occurrence of the expected short-range suppression of G . An unexpected small enhancement also occurs for $x > 4$.

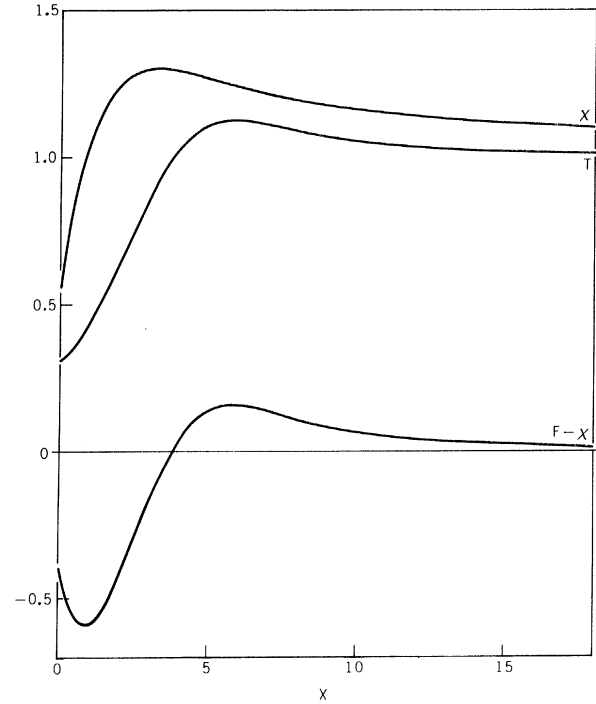


FIG. 1. Zero-energy scattering solutions for $e^+ - H$. The functions χ and F are open-channel and closed-channel functions, and $T = F/\chi$ is the suppression factor. The asymptotic normalization is $\chi = 1 - a/x$, $F = \chi$, and $T = 1$.

TABLE I. Numerical values for the potentials defined in Eq. (9), evaluated using the complete form of G in elliptical coordinates. (Negative exponents appear in parentheses in the usual way.)

x	V_1	$-V_2$	V_3	N	V_N	W
0	$2(1/x-1)$	1	$\frac{3}{4}(1/x-1)$	$\frac{3}{4}$	$\frac{10}{3}x$	$6(1-2x)$
0.5	2.207	6.96(-1)	1.229	5.38(-1)	5.54(-1)	1.913
1.0	5.41(-1)	3.99	1.57(-1)	3.13	3.34	6.42(-1)
1.5	1.66	2.34	-1.40(-2)	1.89	1.79	2.62
2.0	5.49(-2)	1.41	-3.99	1.20	1.07	1.17
2.5	1.89	8.48(-2)	-3.32	7.73(-2)	6.84(-2)	5.25(-2)
3.0	6.61(-3)	5.14	-2.18	4.96	4.41	2.28
3.5	2.34	3.14	-1.29	3.19	2.80	9.61(-3)
4.0	8.39(-4)	1.95	-7.20(-3)	2.06	1.77	3.96
4.5	3.02	1.25	-3.91	1.36	1.11	1.61
5.0	1.09	8.19(-3)	-2.11	9.12(-3)	7.04(-3)	6.43(-4)
6.0	1.43(-5)	3.86	-6.23(-4)	4.43	2.98	1.00
7.0	1.90(-6)	2.03	-2.00	2.36	1.38	1.53(-5)
8.0	2.53(-7)	1.17	-7.18(-5)	1.37	7.00(-4)	2.31(-6)
9.0	3.38(-8)	7.18(-4)	-2.91	8.47(-4)	3.83	3.43(-7)
10.0	4.54(-9)	4.67	-1.31	5.52	2.24	5.06(-8)

III. POSITRON-HELIUM SCATTERING

To extend the results of the preceding section to the case of positron scattering from the ground state of helium, we interpret the correlation function of Eq. (4) as depending on two electronic coordinates, i. e.,

$$\Phi(\vec{r}_1, \vec{r}_2, \vec{x}) = F(\vec{x})G(\vec{r}_1, \vec{r}_2, \vec{x})\phi(\vec{r}_1, \vec{r}_2), \quad (12)$$

where ϕ is the properly antisymmetric ground-state atomic wave function, and G is symmetric in the electronic coordinates.

The Hamiltonian for e^+ -He scattering is

$$H = H_{12} + H_x + V, \quad (13)$$

where

$$H_{12} = -(\nabla_1^2 + \nabla_2^2 + 4/r_1 + 4/r_2) + 2/|\vec{r}_1 - \vec{r}_2|,$$

$$H_x = -\nabla_x^2,$$

and $V = V^{(1)} + V^{(2)}$,

where $V^{(i)} = 2(1/x - 1/|\vec{r}_i - \vec{x}|)$.

The assumption that G is the first-order adiabatic correlation function requires²

$$[G, H_{12}]\phi(\vec{r}_1, \vec{r}_2) = (V - \langle V \rangle)\phi(\vec{r}_1, \vec{r}_2), \quad (14)$$

where the angular-bracket notation of Eq. (6) is extended to include integration over \vec{r}_1 and \vec{r}_2 .

The formal equations to be solved are identical to Eq. (7) where $E = E_0 + k^2$ and $(H_{12} - E_0)\phi(\vec{r}_1, \vec{r}_2) = 0$. Using Eq. (14), one obtains the following coupled equations:

$$(\nabla^2 + k^2 - \langle V \rangle)\chi = \langle GV \rangle F, \quad (15a)$$

$$[\langle G^2 \rangle (\nabla_x^2 + k^2) + \langle GV \rangle - \langle G^2 V \rangle + \langle G \nabla_x^2 G \rangle + \vec{\nabla}_x \langle G^2 \rangle \cdot \vec{\nabla}_x] F = \langle GV \rangle \chi. \quad (15b)$$

If it were possible to solve Eq. (14) exactly, and to evaluate all the angular-bracketed expressions in Eq. (15), the resulting phase shifts would satisfy the rigorous lower-bound theorem. Since no exact solution for the helium-atom ground state is known, one must use an approximate form for $\phi(\vec{r}_1, \vec{r}_2)$. We have used the simple, shielded hydrogenic form $\phi(\vec{r}_1, \vec{r}_2) = \psi(r_1)\psi(r_2)S$, where S is a singlet, antisymmetric spin function, and

$$\psi(r) = \beta^3/2\pi - 1/2 e^{-\beta r}, \quad (16)$$

where β is an effective charge. Since this function is not an exact eigenfunction of H_{12} , the procedure leading to Eq. (15) is itself not really consistent. To the extent that these inconsistencies may be ignored, however, the solutions of Eq. (15) will yield lower bounds to $\tan \delta_L$; we call these "quasi-

bounds."

Using this form of ϕ , it is consistent with Eq. (14) to assume independent distortion of the two electrons.

$$G(\vec{r}_1, \vec{r}_2, \vec{x}) = G(\vec{r}_1, \vec{x}) + G(\vec{r}_2, \vec{x}) \equiv G_1 + G_2. \quad (17)$$

Equation (14) then simplifies to the form

$$[G_i, \nabla_i^2]\psi(r_i) = (\langle V^{(i)} \rangle - V^{(i)})\psi(r_i), \quad (i=1, 2) \quad (18)$$

where angular-bracketed quantities now refer to single integrals, i. e.,

$$\langle V^{(i)} \rangle = \int d^3 r_i \psi(r_i) V^{(i)} \psi(r_i). \quad (19)$$

Again, one must set $\langle G_i \rangle = 0$ to satisfy Eq. (2a). With this condition satisfied, one can immediately rewrite Eq. (15) in terms of single integral quantities:

$$(\nabla^2 + k^2 - 2V_1)\chi = 2V_2 F, \quad (20a)$$

$$[N(\nabla^2 + k^2 - V_1) + V_2 - V_3 - W - V_N d/dx] F = V_2 \chi. \quad (20b)$$

All the "potentials" used in Eq. (20) have the formal definitions of Eq. (9), but with $\phi(r)$ replaced by $\psi(r)$. The factors of 2 appearing in Eq. (20a) are due to the superimposed effects of the two electrons. In Eq. (20b), there is an additional term, $-NV_1$, which did not appear for hydrogen, Eq. (8b). This comes from the third-order term in Eq. (15b),

$$\begin{aligned} \langle G^2 V \rangle &= \langle (G_1 + G_2)^2 (V^{(1)} + V^{(2)}) \rangle \\ &= \langle G_1^2 V^{(1)} \rangle + \langle G_2^2 V^{(2)} \rangle \\ &\quad + \langle G_1^2 \rangle \langle V^{(2)} \rangle + \langle G_2^2 \rangle \langle V^{(1)} \rangle \\ &\quad + 2\langle G_1 \rangle \langle G_2 V^{(2)} \rangle + 2\langle G_2 \rangle \langle G_1 V^{(1)} \rangle. \end{aligned} \quad (21)$$

The last two terms vanish, and the net result is

$$\langle G^2 V \rangle = 2(V_3 + NV_1). \quad (22)$$

It has been noted² that a simple change of scale converts Eq. (18) into its hydrogen equivalent, Eq. (5). Specifically, let $\vec{y} = \beta\vec{r}$ and $\vec{v} = \beta\vec{x}$. Then Eq. (18) becomes

$$[\beta G, \nabla_y^2] e^{-y} = \left[\frac{2}{|\vec{y} - \vec{v}|} - \frac{2}{v} - \bar{V}_1(v) \right] e^{-y}, \quad (23)$$

where $\bar{V}_1(v) = \frac{2}{\pi} \int d^3 y e^{-2y} \left[\frac{1}{v} - \frac{1}{|\vec{y} - \vec{v}|} \right]$.

One sees immediately from Eqs. (23) and (5) that

$$\beta G_{\text{He}}(\vec{r}, \vec{x}) = G_{\text{H}}(\vec{y}, \vec{v}). \quad (24)$$

Also, since $V_{\text{He}}(\vec{r}, \vec{x}) = \beta V_{\text{H}}(\vec{y}, \vec{v})$ and $\psi_{\text{He}}^2(r) d^3 r = \phi_{\text{H}}^2(y) d^3 y$, one can relate all the helium potentials of Eq. (20) to the hydrogen potentials of

Eq. (8) as follows:

$$\begin{aligned} V_p(x) &\rightarrow \beta^{2-p} V_p(v), \quad p = 1, 2, 3 \\ N(x) &\rightarrow \beta^{-2} N(v), \\ V_N(x) &\rightarrow \beta^{-1} V_N(v), \\ W(x) &\rightarrow W(v). \end{aligned} \quad (25)$$

The simplest way to make use of these scaling laws is to change variables throughout Eq. (20):

$$[\nabla^2 + k'^2 - (2/\beta)V_1]\chi = (2/\beta^2)V_2F, \quad (26a)$$

$$\begin{aligned} [N(\nabla^2 + k'^2 - (1/\beta)V_1) + V_2 - (1/\beta)V_3 \\ - W - V_N d/dv]F = V_2\chi. \end{aligned} \quad (26b)$$

Here $k' = k/\beta$, $\nabla^2 \equiv \nabla_v^2$, and all the potentials are the hydrogen functions in terms of v . These equations can be treated just like those appearing in the hydrogen problem, as discussed in Appendix B, and the results are discussed in Sec. IV. As indicated previously,² the value $\beta = \frac{27}{16}$ which minimizes the energy expectation value gives an unsatisfactory value (1.1) for the polarizability of helium. This quantity appears in the present theory as $\lim_{\chi \rightarrow \infty} [2x^4 V_2(x)] = 9\beta^{-4}$. With only a slight change in the energy, one can adjust the polarizability to the experimental value² of 1.376, by setting $\beta = 1.5992$. This value has been used throughout the present work.

We have previously¹⁵ used the nonvariational e^+ -He wave functions to calculate Z_k , the number of atomic electrons which are effective in annihilating a positron of momentum k . (For plane-wave positrons and omitting atomic distortion, $Z_k = 2$). In terms of our type of wave function,

$$\begin{aligned} \frac{1}{2}Z_k \equiv \int d^3r \int d^3x |\Psi_{\vec{k}}(\vec{r}, \vec{x}, \vec{x})|^2 = \int d^3x \psi^2(x) \\ \times [|\chi + FG(\vec{x}, \vec{x})|^2 + |F|^2 \langle G^2 \rangle]. \end{aligned} \quad (27)$$

Following Ref. 15, we assume that only the $L = 0$ scattering function differs significantly from its plane-wave form, and that for $L > 0$ the ratio of closed-channel to open-channel functions is well approximated by the zero-energy suppression function T . With these approximations, one can write

$$\begin{aligned} \frac{1}{2}Z_k = (2\beta/k)^2 \\ \times \int_0^\infty dv e^{-2v} \{ [U_0 + g_0 G(\vec{v}, \vec{v})]^2 + g_0^2 N(v) \} \\ + 4 \int_0^\infty dv e^{-2v} v^2 M(v) [1 - j_0^2(kv/\beta)], \end{aligned} \quad (28)$$

where $M(v) = [1 + TG(\vec{v}, \vec{v})]^2 + T^2 N(v)$. Here $v = \beta x$, U_0 and g_0 are the S -wave parts of χ and F [see

Eq. (B1)]. The correlation functions used here [$G(\vec{v}, \vec{v})$ and $N(v)$] are scaled appropriately for helium. At $k = 0$, the second integral in Eq. (28) vanishes since no higher L values contribute. For $k \neq 0$, the assumptions made here should be quite good; in Ref. 15 we have estimated that an error of less than 2% is incurred in the values of Z_k . In Table II the results are given for values of the energy up to the positronium threshold, in comparison with the larger values of Z_k previously obtained.¹⁵

The difference between the present results and those obtained previously is traceable partly to the fact that the present calculation gives less attraction than did the nonvariational method,¹⁵ and hence the positron is pulled inward to a smaller degree. A larger effect is the difference between the "correlation function" M defined in Eq. (28) and the monopole-suppressed function Y used in Ref. (15). These two functions are compared in Table III, and one can see that, except at very small distances from the nucleus, $M < Y$. To examine these two effects quantitatively, we have recomputed $\frac{1}{2}Z_k$ at zero energy using both M and Y , as well as both variational and nonvariational scattering functions. By far the largest effect is produced by replacing M by Y , outweighing the effect of interchanging the two forms of U by a factor of 3. Since neither M nor Y is exact, this result constitutes a warning against taking the annihilation results too seriously. It is interesting, however, that the present calculation agrees fairly well at zero energy with the experimental result of Falk *et al.*¹⁶ for thermal positrons of $Z_k = 3.78 \pm 0.17$.

Note added in proof. The zero-energy scattering function derived here can also be used to calculate the angular correlation between the annihilation γ rays. Preliminary results are in reasonable agreement with experiment.

IV. SCATTERING RESULTS AND DISCUSSION

The e^+ -H S -wave scattering phase shifts δ_0 were computed numerically as discussed in Appendix B, where the method of treating the asymptotic behavior of the closed channel is discussed. This

TABLE II. Positron-helium annihilation rate $\frac{1}{2}Z_k$. Column *A* gives the present results, and Column *B* is the nonvariational result of Ref. 15. The Dirac rate is $\frac{1}{2}Z_k = 1$.

<i>E</i> (eV)	<i>A</i>	<i>B</i>
0	1.83	3.16
0.54	1.65	2.79
1.22	1.57	2.58
2.17	1.51	2.43
3.40	1.49	2.35
4.90	1.49	2.31
6.66	1.51	2.30
8.70	1.56	2.33
11.0	1.60	2.38
13.6	1.65	2.44
17.8	1.74	2.54

TABLE III. Correlation functions for e^+ -He annihilation. M is used in the present work and is defined in Eq. (28). $Y = [1 + G(\bar{x}, \bar{x})]^2 + \langle G^2 \rangle$ is used analogously in the nonvariational work (Ref. 15), and employs full monopole suppression in G .

$v = \beta x$	M	Y
0	1.67	1
0.5	1.68	1.91
1.0	1.83	2.78
1.5	2.13	3.50
2.0	2.55	4.07
2.5	3.07	4.53
3.0	3.66	4.92
3.5	4.29	5.25
4.0	4.90	5.55
4.5	5.47	5.82
5.0	5.97	6.06

involves inward integration from a point x_0 in the asymptotic region to an intermediate point \bar{x} . In Table IV the sensitivity of $\tan\delta_0$ to the choice of x_0 and \bar{x} is shown for low and high-energy positrons, confirming the stability of the numerical solutions.

In Table V the e^+ -H S-wave phase shifts (and, at $k=0$, the scattering length) are shown, along with the results of Schwartz.⁶ To assess the quality of the present work, we compute the quantity Δ , the difference between $\tan\delta_0$ and the value of $\tan\delta_0$ obtained with an undistorted atomic wave function. This "Hartree" result is also given in Table V. The figure of merit $Q(k) \equiv \Delta(\text{variational})/\Delta(\text{Schwartz})$ measures how much of the distortion or polarization has been accounted for by our method. It is most interesting that $Q \approx 90\%$, almost independent of energy. The lower-bound results of Hahn and Spruch¹⁷ have somewhat lower

TABLE IV. S-wave e^+ -H results. The sensitivity of $\tan\delta$ to matching radius (\bar{x}) and asymptotic radius (x_0) is shown for two values of positron momentum k .

$\tan\delta$ ($k=0.1$)			
\bar{x}	$x_0=20$	$x_0=25$	$x_0=30$
2	0.12753	0.12804	0.12808
3	0.12747	0.12798	0.12803
4	0.12675	0.12726	0.12731
$\tan\delta$ ($k=0.7$)			
\bar{x}	$x_0=20$	$x_0=25$	$x_0=30$
2	-0.07393	-0.07386	-0.07383
3	-0.07396	-0.07389	-0.07386
4	-0.07440	-0.07433	-0.07430

Q values, as shown in Table V. We consider it a success of the present method that the results compare well with the many-parameter, many- l variational results of Ref. 17. Their method has the considerable advantage, however, of being capable of systematic improvement, by the addition

TABLE V. S-wave e^+ -H scattering results. The entries without subscripts refer to the present work, and are averages over \bar{x} . The other phase shifts are: δ_S - Schwartz (Ref. 6); δ_H - Hartree; and Q_{HS} - Hahn and Spruch (Ref. 16). The figure of merit Q is defined in the text. For $k=0$, scattering lengths are given.

k	$\tan\delta$	$\tan\delta_S$	$\tan\delta_H$	Q	Q_{HS}
0	-1.85	-2.10	0.582	0.91	
0.1	0.128	0.152	-0.058	0.89	
0.2	0.158	0.190	-0.116	0.90	0.87
0.3	0.135	0.170	-0.170	0.90	
0.4	0.089	0.121	-0.222	0.91	0.89
0.5	0.034	0.062	-0.270	0.92	
0.6	-0.022	0.007	-0.314	0.91	0.89
0.7	-0.074	-0.054	-0.354	0.93	

of more terms. The results can also be convincingly extrapolated, and give good agreement with those of Schwartz.⁶

In Table VI the S-wave scattering results for e^+ -He are presented. Along with the "quasirigorous" lower bounds obtained here, we show the "Hartree" results, obtained from a two-term analytic form² approximating the helium ground-state potential, and the nonvariational results.² Since no definitive calculation exists in this case, we have computed the figure of merit Q assuming that δ_{NV} is exact. These Q values are smaller than those obtained for hydrogen, but are also nearly constant. It is not possible to make any further statements about the "correct" values for the S-wave e^+ -He phase shifts from the comparison of the quasivariational and nonvariational results.

The possibility that a bound $e^+ - e^- - p$ exists has been eliminated by an extensive variational calculation¹⁸ which showed that for a "positron" of mass $m > 2.625$

TABLE VI. S-wave e^+ -He scattering results. The entries without subscripts refer to the present work and are averages over \bar{x} . The other phase shifts are: δ_H - Hartree; δ_{NV} - nonvariational (Ref. 2). For $k=0$, scattering lengths are given. Q is computed assuming δ_{NV} to be exact.

k	$\tan\delta$	$\tan\delta_H$	$\tan\delta_{NV}$	Q
0	-0.511	0.420	-0.659	0.86
0.1	0.036	-0.042	0.050	0.85
0.2	0.047	-0.083	0.072	0.84
0.3	0.039	-0.124	0.071	0.84
0.4	0.020	-0.163	0.056	0.84
0.5	-0.007	-0.203	0.032	0.83
0.6	-0.039	-0.240	0.002	0.83
0.7	-0.073	-0.278	-0.031	0.83
0.8	-0.107	-0.313	-0.066	0.83
0.9	-0.142	-0.346	-0.100	0.83
1.0	-0.176	-0.379	-0.134	0.83
1.1	-0.208	-0.409	-0.168	0.83
1.145	-0.223	-0.423	-0.182	0.83

such a bound system does occur. As a further test of the present method, we have calculated this critical mass by looking for the appearance of a node in the S-wave zero-energy scattering function, corresponding to a scattering length $a = \pm\infty$. One modifies Eq. (8) by dividing all terms involving ∇_χ^2 by the positron mass m . This is equivalent to multiplying the potentials V_1 , V_2 , and V_3 by m , and adjusting the asymptotic conditions in an obvious way. We find the critical mass to be 2.79, and since our method gives an upper bound, this agrees with the result of Ref. 18.

The present method is not expected to be as good for $L > 0$ as for $L = 0$, since even the nonvariational results¹ underestimate the P - and D -wave phase shifts at the higher energies. This defect seems to be associated with a lack of sufficient virtual positronium in the wave function. Support for this is the success of Bransden's P -wave results¹⁹ at high energy. More recent results²⁰ indicate that just above the threshold for positronium formation, P waves dominate over S waves in the pick-up process, implying that below threshold neglect of positronium is less serious for S waves. In any case, we show our $L = 1$, e^+ -H results in Table VII, where they are compared with the lower-bound and extrapolated results of Kleinman *et al.*²¹

V. COMPARISON WITH OTHER METHODS

We will now describe briefly some other methods which resemble the present work, hoping that some clarification will result. The field of low-energy positron scattering suffers from some lack of precision in terminology and some overlapping of approximations, which may make it difficult to evaluate the work reported here without a description of the competing methods. The following short review is not complete, but it may aid the orientation of the reader.

1. The nonvariational (polarized-orbital) method¹ uses the form of scattering function given in Eqs. (1) and (4) with the additional restriction $F(\vec{x}) = \chi(\vec{x})$. Since it is nonvariational, however, the single unknown function χ is determined by simply projecting the Schrödinger equation onto the open-channel part of Ψ :

$$\langle (H-E)(1+G)\chi = 0. \quad (29)$$

TABLE VII. P -wave e^+ -H scattering results. The present results (corrected for long-range effects as described in Appendix B) are compared with the lower bounds (LB) and extrapolated values (ext), obtained in Ref. 21. The estimated error in the last digit is shown in parentheses.

k	$\tan\delta_1$	$\tan\delta_1(\text{LB})$	$\tan\delta_1(\text{ext})$
0.1	0.0073(1)	0.0082	0.0086(1)
0.2	0.0263(2)	0.0289	0.032(1)
0.3	0.0518(5)	0.0548	0.066(4)
0.4	0.0764(9)	0.0801	0.11(1)
0.5	0.0952(14)	0.0994	0.14(1)
0.6	0.106(2)	0.112	0.17(2)
0.7	0.109(2)	0.119	0.19(2)

This leads to the differential equation

$$(\nabla^2 + k^2)\chi - (V_1 + V_2)\chi = 0, \quad (30)$$

whose solutions give the phase shifts. In the absence of an applicable lower-bound principle, it is difficult to gauge the error in the phase shifts obtained from Eq. (30).

2. The same polarized-orbital wave function can be employed variationally. The same procedure which leads to Eq. (7) when χ and F are independently varied, leads now to

$$\langle (1+G)(H-E)(1+G)\chi = 0 \quad (31)$$

since $F \equiv \chi$. This gives the differential equation

$$(\nabla^2 + k^2)\chi - (1+N)^{-1}(V_1 + V_2 + V_3 + W + V_N d/dx)\chi = 0, \quad (32)$$

whose solutions provide approximate phase shifts which are lower bounds to the exact ones. Unfortunately, these approximate phase shifts are very low ($\alpha \approx -1.0$), since the large, short-range repulsion represented by W , and the reduction in V_2 caused by the factor $(1+N)^{-1}$ more than overcome the attraction added by V_3 . It is likely that removing some or all of the monopole part of G , as was done nonvariationally in Ref. 1, would improve the results considerably. If G were replaced by $G - (1-\alpha)G_0$, the potentials appearing in Eq. (32) would be modified as follows:

$$\begin{aligned} N &\rightarrow N - (1-\alpha^2)N_0, \\ W &\rightarrow W - (1-\alpha^2)W_0, \\ V_N &\rightarrow V_N - (1-\alpha^2)V_{N0}, \\ V_1 &\rightarrow V_1, \\ V_2 &\rightarrow V_2 - (1-\alpha)^2V_{20}, \\ V_3 &\rightarrow V_3 - (1-\alpha^2)V_{30} - 2(1-\alpha)P, \end{aligned} \quad (33)$$

where, for example, $N_0 \equiv \langle G_0^2 \rangle$, and $P \equiv \langle G_0(G-G_0)(V-V_0) \rangle$. In Eq. (33), the parameter α represents the fraction of adiabatic monopole distortion being retained; $\alpha = 0$ is what we have called "full monopole suppression." The best value of α , for each L and k , is to be determined variationally. Equation (32) is integrated for several values of α , and the value which maximizes the phase shifts is retained. The monopole terms (with subscript 0) are easily evaluated in spherical coordinates, while the remaining terms are known in elliptical coordinates, except for the last term in V_3 . The quantity P is difficult to compute in either set of coordinates, but it might be approximated using the multipole expansions for G and V . This method has not been used up to the present time.

3. Callaway *et al.*²² have made some modifications to Eq. (32) and arrive at another optical potential which they call the extended polarization potential. Although the results obtained are poor, the new

potential has considerable physical interest.

To derive the result of Ref. (22), one first neglects all terms which are formally of higher than second order in the perturbation V . This eliminates from Eq. (32) all reference to N and V_3 , and leaves us with Eq. (30) modified by the addition of the two second-order nonadiabatic potentials $W + V_N d/dx$. Further arguments in Ref. (22) are used to justify a certain normalization of the scattering function, but in essence one next introduces a new function $\bar{\chi}$ by the definition

$$\chi = (1 - \frac{1}{2}N)\bar{\chi}, \quad (34)$$

and a differential equation for $\bar{\chi}$ is derived by direct substitution. Again neglecting terms higher than second order, one obtains the equation

$$[\nabla^2 + k^2]\bar{\chi} - [V_1 + V_2 + V_D]\bar{\chi} = 0, \quad (35)$$

where V_D is the "distortion potential" $\langle (\vec{\nabla}_x G)^2 \rangle$ appearing in Appendix A. From Eqs. (A4) and (10) we find that $V_D = 1$ at $x = 0$. Thus, as Callaway *et al.*²² have emphasized, the distortion potential cancels the polarization potential V_2 at the origin, and hence its inclusion seems to serve the same purpose as does monopole suppression.¹ Unfortunately V_D is fairly long range, decreasing like x^{-6} for large x , while V_{20} exponentially decreases. The equivalence of these two ways of suppressing excessive attraction is limited to small x , and consequently Eq. (35) gives far too much repulsion; the scattering length is²² $a = -0.783$, even worse than the result of Eq. (32).

4. We have previously reported^{10a} a method of obtaining lower bounds to the phase shifts, which is simpler than that of the present work and not much different in its results. In essence it is a hybrid between the present method, which independently varies two functions and obtains coupled differential equations, and the method of Eq. (31) which varies only one function.

In this method, one again uses a trial function of the type represented by Eqs. (1) and (4), with

$$F(\vec{x}) = \chi_{\mathbf{K}}(\vec{x})T(x), \quad (36)$$

where $T(x)$ is some function which approaches unity for large x and decreases for small x . It is to contain adjustable constants,²³ and is designed to suppress the short-range correlation. Variation on χ leads to the following equation, analogous to Eq. (31):

$$\langle (1 + TG)(H - E)(1 + TG) \rangle \chi = 0. \quad (37)$$

The optical potential of Eq. (32) is modified, and the lower-bound phase shifts are solutions of the differential equation

$$\begin{aligned} & [\nabla^2 + k^2]\chi - [1 + T^2N]^{-1} \left[V_1 + (2T - T^2)V_2 \right. \\ & \quad \left. + T^2(V_3 + W) + (T^2V_N - 2TT'N)d/dx \right. \\ & \quad \left. + (T\nabla^2T)N + TT'V_N \right] \chi = 0, \end{aligned} \quad (38)$$

which is seen to reduce to Eq. (32) if $T = 1$. For $k = 0$, $L = 0$ scattering, the optimum form of T would be that shown in Fig. 1, where $T = F/\chi$, while F and χ were numerically obtained. For $k \neq 0$, however, χ and F both are oscillatory but their zeros do not generally coincide, and one must use a smoothed approximate form for T , as has been done for the annihilation problem in Sec. III. It is also possible to combine the monopole suppression method with the present method. In that case, the constant α would measure the amount of monopole correlation retained, while the function T would be capable of making adjustments in the remaining parts of the correlation function.

5. Two interesting modifications of the close-coupling approximation have been introduced recently. They are quite close in approach to the present coupled-equation method.

(a.) Damburg and Karule,²⁴ noticing that the close-coupling method fails to give the correct asymptotic dipole polarizability, have proposed a trial function which is equivalent to our Eqs. (1) and (4), with a different form for G :

$$\begin{aligned} G_{DK}(\vec{r}, \vec{x}) &= (r + \frac{1}{2}r^2)P_1(\cos\eta), \\ \cos\eta &= \hat{r} \cdot \hat{x}. \end{aligned} \quad (39)$$

The motivation for this choice is clear: comparing Eq. (39) with Eq. (A8), one sees that G_{DK} correctly describes the asymptotic form of the adiabatic correlation function, as far as the coordinates of the electron (r, η) are concerned, and since $F(\vec{x})$ can be freely varied, the solutions of the resulting coupled equations will be identical, for large x , to those of Eq. (8). Eq. (39) is separable in r , η , and x , however, and hence does not give the same short-range dipole correlation as does the Dalgarno-Lynn function G . In addition, each multipole term in the correlation function would require another coupled equation (as is the case for ordinary close coupling). In return, one gains enormously in the simplicity of the potentials which must be used; all the potentials in this method can be evaluated analytically, while some reduce trivially to constants. The method is promising, but no numerical results are available yet.

(b.) Perkins²⁵ has made a modification starting from a conventional close-coupling expansion containing $1s - 2p - 3d$ states. Noting that, since only one term of each angular symmetry is retained, the orthogonality of closed and open channels [Eq. (2a)] is assured, he has modified the forms of the $2p$ and $3d$ functions as follows

$$\begin{aligned} \phi_{2p'} &= r e^{-\delta r} P_1, \\ \phi_{3d'} &= r^2 e^{-\eta r} P_2. \end{aligned} \quad (40)$$

The usual coupled differential equations of close coupling are solved numerically, but now two additional nonlinear parameters, δ and η , are adjusted to maximize the phase shifts. The results are much better than the corresponding unmodified close-coupling results, although the exact asymptotic polarizability is not achievable. The method

can be extended to include higher l values with the usual difficulty that more coupled equations are then required. Without generalizing the basis functions considerably, one would not expect the procedure to converge toward the exact wave function, but the lower-bound theorem holds and offers the usual estimate of quality.

6. An interesting general formulation was recently presented,²⁶ which uses numerical solutions of the two-center problem in the adiabatic approximation, and which may prove applicable to positron scattering. Similarities with our method include generalizations of our V_N and W . The binding energy of the $e^+ - e^- - e^+$ molecule was computed as an example, but no scattering results were given.

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APPENDIX A. EVALUATION OF THE POTENTIALS

The analytic solution of Eq. (5) was given by Dalgarno and Lynn⁵ and has the form

$$G = A(x)(\lambda + \mu) + (1 + 2A/x) \ln(1 + \lambda) + (1 + 1/x)Q(x, \mu) + \bar{G}(x), \quad (\text{A1})$$

$$A(x) = \frac{1}{2}[(x+1)e^{-2x} - 1], \quad \text{and } \text{Ei}(-Z) = -\int_Z^\infty dy e^{-y}/y,$$

where $Q(x, \mu) = \text{Ei}[x(\mu-1)] - \ln(1-\mu) - e^{-2x} \{ \text{Ei}[x(\mu+1)] - \ln(1+\mu) \}$.

In terms of these elliptical coordinates, $r = \frac{1}{2}x(\lambda + \mu)$ and $\cos\eta = (1 + \lambda\mu)/(\lambda + \mu)$, where η is the angle between \vec{x} and \vec{r} . The potential $V = (2/x)[1 + 2/(\mu - \lambda)]$; the angular-bracket notation takes the form

$$\langle f(x, \lambda, \mu) \rangle = \frac{1}{2\pi} \int_0^\pi d\lambda \int_{-1}^1 d\mu e^{-x(\lambda + \mu)} (\lambda^2 - \mu^2) f(x, \lambda, \mu), \quad (\text{A2})$$

and we may determine $\bar{G}(x)$ by requiring $\langle G \rangle = 0$, obtaining

$$\bar{G}(x) = (2/x)[\ln 2 - \text{Ei}(-2x)] + e^{-2x} [2(1 + 1/x) \ln \gamma x + x - \frac{1}{2}], \quad (\text{A3})$$

where $\ln \gamma = 0.5772\dots$, Euler's constant. The solubility of Eq. (5) depended on its additive separability in elliptical coordinates. For the same reason, it is possible to evaluate most of the potentials defined in Eq. (9) in terms of one-dimensional integrals. Since, however, the important function W cannot be reduced in this way, we have numerically evaluated all the potentials uniformly by the use of Gaussian quadrature in two dimensions. We have confirmed the accuracy of this procedure in three ways: We have evaluated $\langle V \rangle$, $\langle G \rangle$, and $\langle GV \rangle$ in elliptical coordinates, using our numerical method, and compared the results with the known values, obtaining excellent agreement. In particular, $\langle G \rangle$ never differs from zero by more than about 10^{-7} , and we feel that this figure measures the accuracy of the two-dimensional integrals.

The two nonadiabatic terms, V_N and W , present additional problems. To evaluate W directly would involve the operation $\nabla_x^2 G$, which would give a very intricate analytic expression. Instead, we have rewritten the expression for W in the form

$$W = V_D - \frac{1}{2} \nabla^2 N = V_D + (1/x + \frac{1}{2} d/dx) V_N, \quad (\text{A4})$$

where $V_D \equiv \langle (\vec{\nabla}_x G)^2 \rangle$ is the "distortion potential" employed in Ref. 22, and discussed here in Sec. V. The function V_D involves both x and η components of the gradient (with r held fixed), while V_N only requires the x component. Both components were found analytically and inserted into the numerical double integration, while the first derivative of V_N needed in Eq. (A4) was gotten by numerical differentiation of V_N . All three terms in Eq. (A4) have asymptotic inverse-power behavior, with x^{-6} as the leading term; these all cancel leaving short-range (exponential) terms dominant.

In Sec. III we require the value of $G(\vec{x}, \vec{x})$, i. e., $G(\vec{r}, \vec{x})$ evaluated at $\vec{r} = \vec{x}$. In elliptical coordinates this relation becomes $\lambda = \mu = 1$, since then $r = x$ and $\cos\eta = 1$. Care is required in evaluating $Q(x, 1)$, since its first two terms are singular. Letting $\mu = 1 - \epsilon$ and expanding the exponential integral about $\epsilon = 0$, we have

$$Q(x, 1 - \epsilon) \approx \ln(\gamma \epsilon x) - \epsilon x - \ln \epsilon - e^{-2x} [\text{Ei}(2x) - \ln 2], \quad (\text{A5})$$

and the limit $\epsilon \rightarrow 0$ can be taken. The final result is

$$G(\vec{x}, \vec{x}) = (1 + 1/x) [\ln(2\gamma x) + e^{-2x} [2 \ln(2\gamma x) - \text{Ei}(2x)]] - 1 - (2/x) \text{Ei}(-2x) + e^{-2x} (\frac{1}{2} + 2x). \quad (\text{A6})$$

This is the function which, properly scaled, is used in the e^+ -He annihilation and forms the basis for Table III.

To obtain the long-range asymptotic forms shown in Eq. (11), we expand V in Legendre polynomials (for $x > r$):

$$V(\vec{r}, \vec{x}) \sim -\frac{2}{x} \sum_{l=1}^{\infty} \left(\frac{r}{x}\right)^l P_l(\cos\eta). \quad (\text{A7})$$

Then a particular solution of Eq. (5) is (for $x > r$)

$$G = \frac{1}{x} \sum_{l=1}^{\infty} \left(\frac{r}{x}\right)^l \left(\frac{1}{l} + \frac{r}{l+1}\right) P_l(\cos\eta), \quad (\text{A8})$$

which is the correct asymptotic form of G . By inserting these expressions into the definitions, Eq. (9), one can carry out the integrations in spherical coordinates and obtain the leading terms, (in x^{-1}) for each potential. Since V has no long-range $l=0$ term, V_1 is short-ranged. To show that W is also, one notes that $\nabla_x^2 x^{-(l+1)} P_l(\cos\eta) = 0$, for $l > 0$. To illustrate, let us compute the asymptotic form of N :

$$N \equiv \langle G^2 \rangle \sim (2/x^4) \int_0^{\infty} dr r^2 e^{-2r} r^2 (1+r/2)^2 \int_{-1}^1 d(\cos\eta) [P_1(\cos\eta)]^2, \quad (\text{A9})$$

$$\text{or } N \sim 43/8x^4. \quad (\text{A10})$$

The expansion can be carried to any desired order in l , and represents an asymptotic expansion, since we have set the upper limit of the integral equal to ∞ rather than x . Care is required in evaluating the asymptotic form of V_3 , since more than one value of l contributes to the same order in x^{-1} , because *three* Legendre polynomials appear.

The short-range behavior of the potentials (Eq. 10) is due to the small $-l$ parts of the distortion function G . In Ref. 1 the $l=0$ solution of Eq. (5) is exhibited. Near $x=0$ it becomes

$$G_0 \approx \frac{3}{2} - r + \frac{2}{3}x^2(1-x) [\ln(2\gamma r) + r - 1/2r - \frac{5}{2}], \quad (\text{A11})$$

$$\text{and } \nabla_x^2 G_0 \approx 4(1-2x) [\ln(2\gamma r) + r - 1/2r - \frac{5}{2}]. \quad (\text{A12})$$

Since, for small x , all the integrals have limits of 0 and ∞ , one finds

$$N_0 \equiv \langle G_0^2 \rangle \approx \frac{3}{4} - 2x^2, \quad W_0 \equiv -\langle G_0 \nabla_x^2 G_0 \rangle \approx 6(1-2x), \quad V_{N0} \equiv -(d/dx)N_0 \approx 4x. \quad (\text{A13})$$

The constant terms in Eq. (A13) are unaffected by the neglect of higher l values, but the second term in N and, hence, the leading term in V_N , is modified by the $l=1$ part of the expansion. One finds

$$G_1 \approx P_1(\cos\eta) [x + O(x^3)], \quad (\text{A14})$$

and $N_1 \equiv \langle G_1^2 \rangle \approx \frac{1}{3}x^2$. No higher terms contribute to order x^2 , and we obtain the results given in Eq. (10). The $l=0$ and $l=1$ parts of V_D can now be found from Eq. (A4). The result is $V_{D0} \approx 0$ and $V_{D1} \approx 1$ near $x=0$, and no higher terms contribute.

APPENDIX B. SOLUTION OF THE SCATTERING EQUATIONS

The numerical integration of Eq. (8), in partial-wave decomposition, would be straightforward were it not for difficulties connected with the asymptotic form of the closed-channel part of the trial function, Eq. (1). The problem is very similar to those arising in the close-coupling method with closed channels, and our treatment follows the review by Burke and Smith²⁷ fairly closely.

Since we are dealing here with a set of two coupled second-order differential equations, four linearly independent solutions can be found, with each solution consisting of a pair of functions (χ, F) . We will see later that only two of these solutions are sufficiently regular at $x=0$ to be admissible. The general solution of Eq. (8) is thus a linear combination of these two solutions, and our problem is to determine such a combination which is sufficiently regular as $x \rightarrow \infty$. Making partial wave expansions as follows

$$\chi(\vec{x}) = \sum_{L=0}^{\infty} x^{-1} U_L(x) P_L(\cos\theta), \quad F(\vec{x}) = \sum_{L=0}^{\infty} x^{-1} g_L(x) P_L(\cos\theta), \quad (\text{B1})$$

one can write the partial wave equivalent of Eq. (8):

$$U_L'' + [k^2 - L(L+1)x^{-2} - V_1]U_L = V_2 g_L, \quad (\text{B2a})$$

$$g_L'' + [k^2 - L(L+1)x^{-2} + N^{-1}(V_2 - V_3 - W + V_N x^{-1})]g_L - N^{-1}V_N g_L' = N^{-1}V_2 U_L. \quad (\text{B2b})$$

From Eq. (10) we obtain the dominant terms of the potentials near $x=0$. Representing each linearly independent solution as a vector $\psi = (U, g)$, we find two linearly independent regular solutions near zero:

$$\psi_L^{(a)}(x) = (t_L, 0), \quad \psi_L^{(b)}(x) = (0, t_L), \quad (\text{B3})$$

where $t_L \approx x^{L+1}[1 + x/(L \neq 1)]$, plus higher powers of x . Eq. (B2) is numerically integrated, using these starting forms, up to a point $x = \bar{x}$, and the general solution there is

$$\psi_L(\bar{x}) = A\psi_L^{(a)}(\bar{x}) + B\psi_L^{(b)}(\bar{x}), \quad (\text{B4})$$

where A and B are constants to be determined. For large distance, we can rewrite Eq. (B2) using the asymptotic expressions in Eq. (11). Retaining terms which fall off less rapidly than x^{-3} we find

$$U_L'' + [k^2 - L(L+1)x^{-2}]U_L = 0, \quad (\text{B5a})$$

$$g_L'' - (4/x)g_L' + \{k^2 - \frac{36}{48} + [4 - L(L+1)]x^{-2}\}g_L = -\frac{36}{48}U_L. \quad (\text{B5b})$$

[We will discuss the $L=0, k=0$ case below.] Taking $x \geq 20$ as a typical "asymptotic" distance, we see that the x^{-2} term is not negligible for small k (≈ 0.1) in Eq. (B5a), but is negligible in Eq. (B5b). Of the four solutions to Eq. (B5), three are well-behaved for $x \rightarrow \infty$. If we set $U_L = 0$ in Eq. (B5b) and neglect x^{-2} terms, we find that the closed-channel function g_L has two solutions,

$$S_{\pm} \equiv e^{\pm\gamma x} [1 \mp (\gamma x) + \frac{1}{3}(\gamma x)^2], \quad \gamma = (\frac{36}{48} - k^2)^{1/2} \quad (\text{B6})$$

The asymptotic regularity condition, Eq. (2b), requires

$$\int_0^{\infty} dx g_L^2(x) N(x) < \infty, \quad (\text{B7})$$

and since $N \sim x^{-4}$, g_L must increase slower than $x^{3/2}$ for large x . Thus we are forced to drop the rising exponential form S_+ of Eq. (B6). The nonzero linearly independent solutions of Eq. (B5a) are composed of the spherical Bessel functions:

$$U_L = x^j j_L(kx) \quad \text{or} \quad xn_L(kx). \quad (\text{B8})$$

Corresponding to these open-channel solutions one finds a slowly converging²⁸ series of inverse powers for g_L . The three solutions for large x are thus:

$$\psi_L^{(c)}(x) = (0, S_-), \quad \psi_L^{(d)}(x) = (x^j j_L, p_{Lj}), \quad \psi_L^{(e)}(x) = (xn_L, p_{Ln}), \quad (\text{B9})$$

where $p_{Lj} = x^j j_L \left(1 + \frac{a}{x^2} + \frac{b}{x^4} + \dots\right) + xn_L \left(\frac{c}{x} + \frac{d}{x^3} + \dots\right)$, $p_{Ln} = xn_L \left(1 + \frac{\bar{a}}{x^2} + \frac{\bar{b}}{x^4} + \dots\right) + x^j j_L \left(\frac{\bar{c}}{x} + \frac{\bar{d}}{x^3} + \dots\right)$.

$$(\text{B10})$$

The coefficients in Eq. (B10) can be obtained directly by use of Eq. (B5b) and equating like powers of x . The result for $L=0$ is, for example,

$$p_{0j} = \sin kx \left[1 - \frac{3}{2} \left(\frac{43k}{9x}\right)^2 + \dots\right] - \cos kx \left(\frac{43k}{9x} + \dots\right),$$

$$p_{0n} = \cos kx \left[1 - \frac{3}{2} \left(\frac{43k}{9x}\right)^2 + \dots\right] + \sin kx \left(\frac{43k}{9x} + \dots\right). \quad (\text{B11})$$

Eq. (B2) is numerically integrated *inward* from some "asymptotic" point $x = x_0$, using these starting forms, down to the matching point $x = \bar{x}$, where the general solution is

$$\psi_L(\bar{x})_> = C\psi_L^{(c)}(\bar{x}) + \psi_L^{(d)}(\bar{x}) - \tan\delta_L \psi_L^{(e)}(\bar{x}). \quad (\text{B12})$$

Setting $\psi_L(\bar{x})_< = \psi_L(\bar{x})_>$ and $(d/dx)\psi_L(\bar{x})_< = (d/dx)\psi_L(\bar{x})_>$ gives four linear equations in the unknowns A , B , C , and $\tan\delta_L$. We have tested the stability and consistency of the numerical procedure by comparing the results obtained for $x_0 = 20, 25$, and 30 , and $\bar{x} = 2, 3$, and 4 ; and we find essentially no variation in the phase shifts for $L = 0$ (see Table IV). (An empirical correction for $L = 1$, obtained from our previous non-variational work was applied to account for the increase produced by the long-range x^{-4} potential beyond $x = 20$. For very low energies, exact analytic expressions exist²⁹ and are superior to our numerical results.)

For $L = 0$ and $k = 0$ the long-range potential V_2 is not negligible in Eq. (B2a), even for $x \geq 20$, so it is not correct to use the asymptotic form Eq. (B5a). Instead, one has

$$U_0'' = -(9/2x^4)g_0, \quad (\text{B13a})$$

$$g_0'' - (4/x)g_0' - \frac{38}{43}g_0 = -\frac{38}{43}U_0. \quad (\text{B13b})$$

Solution $\psi_0^{(c)}$ is unchanged from the form given in Eqs. (B9) and (B6), but the other two asymptotic solutions are now

$$\psi_0^{(d)} = (x - 9/4x, x - 253/36x), \quad \psi_0^{(e)} = (1 - 3/4x^2, 1 - 3/4x^2), \quad (\text{B14})$$

and the linear combination shown in Eq. (B12) is unchanged except that $\tan\delta_0$ is replaced by the scattering length a .

- ¹R. J. Drachman, Phys. Rev. **138**, A1582 (1965).
²R. J. Drachman, Phys. Rev. **144**, 25 (1966).
³H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958).
⁴A. Temkin and J. C. Lamkin, Phys. Rev. **121**, 788 (1961).
⁵A. Dalgarno and N. Lynn, Proc. Phys. Soc. (London) **A70**, 223 (1957).
⁶C. Schwartz, Phys. Rev. **124**, 1468 (1961).
⁷C. J. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. **140**, A413 (1965).
⁸A similar calculation [N. R. Kestner, J. Jortner, M. H. Cohen, and S. A. Rice, Phys. Rev. **140**, A56 (1965)] with a less complete form of the potential gives qualitatively similar results.
⁹S. Marder, V. W. Hughes, C. S. Wu, and W. Bennett, Phys. Rev. **103**, 1258 (1956); W. B. Teutsch and V. W. Hughes, Phys. Rev. **103**, 1266 (1956).
¹⁰Preliminary versions of this work have been reported previously: (a) Bull. Am. Phys. Soc. **12**, 70 (1967) and (b) *Abstracts of the Fifth International Conference on the Physics of Electronic and Atomic Collisions* (Nauka, Leningrad, 1967), pp. 106-108.
¹¹M. Gailitis, Zh. Eksperim. i Teor. Fiz. **47**, 160 (1964) [English transl.: Soviet Phys. - JETP **20**, 107 (1965)].
¹²P. G. Burke and A. J. Taylor [Proc. Phys. Soc. (London) **88**, 549 (1966)] have shown that the orthogonality requirement [Eq. (2a)] can be weakened.
¹³T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., 1962), pp. 57-68.
¹⁴The potentials V_1 and V_2 are expressible in closed form (Ref. 5). Their numerical evaluation thus served as a check on the accuracy of our computation.
¹⁵R. J. Drachman, Phys. Rev. **150**, 10 (1966).
¹⁶W. R. Falk, Ph. D. dissertation, University of British Columbia, 1965 (unpublished); see also W. R. Falk, P. H. R. Orth, and G. Jones, Phys. Rev. Letters **14**, 447 (1965). Other experimental values of Z_k are: T. B. Daniel and R. Stump, Phys. Rev. **115**, 1599 (1959) [$Z_k = 3.2$]; B. G. Duff and F. F. Heymann, Proc. Roy. Soc. (London) **A270**, 517 (1962) [$Z_k = 3.25 \pm 0.22$]; P. E. Osmon, Phys. Rev. **138**, B216 (1965) [$Z_k = 2.46$]; T. M. Kelly and L. O. Roellig, private communication to P. Fraser [$Z_k = 3.96 \pm 0.04$].
^{16a}C. V. Briscoe, S.-I. Choi, and A. T. Stewart, Phys. Rev. Letters **20**, 493 (1968).
¹⁷Y. Hahn and L. Spruch, Phys. Rev. **140**, A18 (1965).
¹⁸A. A. Frost, M. Inokuti and J. P. Lowe, J. Chem. Phys. **41**, 482 (1964).
¹⁹B. H. Bransden, Proc. Roy. Soc. (London) **A79**, 190 (1962).
²⁰B. H. Bransden and Z. Jundi, Proc. Phys. Soc. (London) **92**, 880 (1967); M. F. Fels and M. H. Mittleman, Phys. Rev. **163**, 129 (1967).
²¹C. J. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. **140**, A413 (1965).
²²J. Callaway, R. W. LaBahn, R. T. Pu, and W. M. Duxler, Phys. Rev. **168**, 12 (1968).
²³A simple form which has proven to give fairly good results is $T(x) = 1 - B \exp(-mx^2)$, with $B \approx 0.8$ and $m \approx 0.15$. This function does not, however, reproduce the maximum at $x = 6$ shown in Fig. 1.
²⁴R. Damburg and E. Karule, Proc. Phys. Soc. (London) **90**, 637 (1967).
²⁵J. F. Perkins, Phys. Rev. **173**, (1968).
²⁶L. I. Ponomarev, Zh. Eksperim. i Teor. Fiz. **52**, 1549 (1967) [English transl.: Soviet Physics - JETP **25**, 1031 (1967)].
²⁷P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962), see especially pp. 477-479.

²⁸Experience shows that problems of this type are not very sensitive to the detailed form of the closed-channel function, provided that the regularity condition (Eq. B7) is satisfied. In fact, if all the coefficients ($a, b, \dots, \bar{a}, \bar{b}, \dots$) in Eq. (B10) are omitted, the phase shifts are

unaffected, although the asymptotic oscillations of g_L are not correctly represented.

²⁹T. F. O'Malley, L. Rosenberg, and L. Spruch, Phys. Rev. 125, 1300 (1962).

Faddeev Equations for Atomic Problems and Solutions for the (e, H) System*

James S. Ball[†]

*Department of Physics,
University of California, Los Angeles, California*

and

Joseph C. Y. Chen

*Department of Physics and Institute for Pure and Applied Physical Sciences,
University of California, San Diego, La Jolla, California*

and

David Y. Wong

*Department of Physics,
University of California, San Diego, La Jolla, California*
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Solutions of the Faddeev equations for Coulomb potentials are investigated. A method which is of practical use for solving the Faddeev equations below the three-particle breakup threshold is developed. As an example, the method is applied to the (e, H) system in which the H^- bound state and the lowest members of the resonances in both the singlet and the triplet $J=0$ series are calculated. The results are in good agreement with the experimental measurements and previous calculations which used conventional methods.

I. INTRODUCTION

The nonrelativistic three-body problem with two-body interactions has been formulated by Faddeev^{1,2} in a way that allows straightforward computations. For short-range forces, the Faddeev equations have been applied successfully to a number of problems.³⁻¹³ It is the purpose of this paper to show that the Faddeev equations are equally applicable to atomic problems as long as the total energy is below the three-body breakup threshold – for example, the calculation of three-body bound states and resonance energies and wave functions below the ionization energy. The significant advantage of the Faddeev equation over conven-

tional methods is that the wave functions are calculated systematically along with the energy levels. No trial wave function is needed in the computation. Although this paper only contains a few illustrative examples all dealing with the $e-H$ problem, we believe that the Faddeev equation has a considerably wider range of applicability. A brief account of this work was presented recently at the Leningrad Conference.¹⁴

In Sec. II, we give a simple derivation of the Faddeev equation, and review the method of reduction with respect to angular momentum. The method of solution is presented in Sec. III and applied to the H^- problem in Sec. IV. A discussion of possible extensions is given in Sec. V.

II. THE FADDEEV EQUATIONS

A. Formal Derivation

The scattering matrix $T(s)$ for the three-particle system with two-body interactions is a solution of the equation

$$T(s) = V + VG_0(s)T(s), \quad (2.1)$$

$$\text{with } V = \sum_i V_i \quad (V_i \equiv V_{jk}), \quad (2.2)$$

$$G_0(s) = (s - H_0)^{-1}, \quad (2.3)$$