Here

$$\Xi_A(12,1'2') = i\,\delta(1-2')\delta(1'^{+}-2)V(1-1') - i\,\delta(1-1')\delta(2-2'^{+})V(1-2') \quad (52)$$

is the approximation used in GRPA and RPA, the first term in the expansion of Ξ.

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Generalized Hylleraas Calculation of Positron-Hydrogen Scattering

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A rigorous-bound calculation is performed of positron-hydrogen scattering below the positronium pickup threshold. The correlation function is a generalized Hylleraas function with three nonlinear parameters which includes a virtual-positronium factor explicitly. Phase shifts are calculated as a function of the number of linear parameters using up to 84 terms. Converged phase shifts can be extrapolated to four significant figures. At three of the seven values of k computed, the results are found to disagree slightly but significantly from Schwartz's results. Final phase shifts are estimated to be accurate to $\pm 2\times10^{-4}$ rad.

I. INTRODUCTION

Assuming one has a basis set which is suitably complete, one of the main advantages of a rigorous-bound formulation is that it allows the application of brute-force techniques with considerable confidence that they will converge to the right answer. The case of low-energy positron scattering from atomic hydrogen is an important and interesting case in point. The original application of a bound theorem to the scattering length by Spruch and Rosenberg[1] (SR) yielded a negative (attractive) scattering length, as opposed to previous calculations[2] which were in effect slight perturbations on the repulsive Hartree potential and yielded positive scattering lengths. This immediately showed the importance of a bound principle, and since the SR variational wave function was deliberately chosen to include virtual positronium, it seemed also to imply that virtual positronium was an indispensible element of the dynamical problem. However, subsequently Schwartz[3] using a conventional Hylleraas function obtained a significant lowering of the scattering length. Implicitly the presence of powers of r_{12} does give some virtual positronium, but a key element of the scattering-length calculation was the additional incorporation of the correct description of the long-range polarization part of the wave function – a fact which was previously known in electron-atom scattering and was used to calculate the first correct (triplet) electron-hydrogen scattering length.[4]

Thus, aside from the indisputable value of the bound theorem, the role of virtual-positronium formation was still unclear. However, the situation was accented at nonzero energies where Schwartz's procedure does not correspond to a rigorous bound on the phase shift. It is the purpose of this calculation to settle in a definitive manner the uncertainties with respect to the inclusion of both bound properties and virtual positronium in Schwartz's calculation for nonzero energies.

II. OPTICAL POTENTIAL, BOUNDS, AND SPECTRUM OF *QHQ*

In applying bound techniques to nonzero energies we are again relying fundamentally on the work of the New York University group.[5] The essence of their original paper was to show that the optical potential[6] for a one-particle radial function whose asymptotic form gives the correct phase shift is negative definite below the energy of the lowest resonance or inelastic threshold, thus implying that the phase shift of the full problem is larger than that coming from any approximation which in effect yields a less negative definite potential. Prime examples of this behavior are the natural sequence of close-coupling calculations for electron-hydrogen scattering, as was indicated.[5] A characteristic of these approximations is that the target state is multiplied by an undetermined function which is subsequently determined from an (integro-) differential equation derived from the variational principle:

$$\delta \int \Psi^*(H-E)\Psi\, dt = 0\ , \qquad (2.1)$$

where, to repeat in a form appropriate to e^+-H S-wave scattering,

$$\Psi = [u(r_1)/r_1]\,\varphi_0(r_2) + \Phi(r_1, r_2, r_{12})\ . \qquad (2.2)$$

[Rydberg units will be used throughout; $\vec{r}_1$ and $\vec{r}_2$ are the coordinates of the positron and electron, respectively. $\varphi_0(r_2)$ is the ground-state wave function of the hydrogen atom, and $u(r_1)$ is the S-wave scattering function, which has the well-known asymptotic form $\lim u(r_1) = A \sin(kr_1 + \eta)$ as $r_1 \to \infty$.]

Given an arbitrary form of the closed-channel function Φ, Ref. 5 does not really answer the question of how one constructs a bound principle for the phase shifts. A bound on the cotangent of the phase shift was derived in a second paper by the same authors,[7] and it was subsequently used for both positron[8] and electron scattering[9] from hydrogen. The results of these calculations, while valuable, were not definitive, partly we believe because the formulation is not optimum for numerical calculation. A mathematically equivalent but calculationally superior formulation was given by Gailitis.[10] In essence he showed how to compute a bounded optical potential from an arbitrary Φ again starting from the projection operator and optical-potential formalism of Feshbach.[6] For the case in hand, projection operators P and Q are defined as

$$P = \varphi_0(r_2)\rangle\langle\varphi_0(r_2)\ , \qquad (2.3a)$$

$$Q = 1 - P\ , \qquad (2.3b)$$

such that P operating on the wave function does not change its asymptotic form

$$\lim_{r_1\to\infty} P\Psi = \lim_{r_1\to\infty}\Psi\ .$$

This may be easily verified from (2.2), keeping in mind that the bra on the right-hand side in the definition of P means multiplication and integration of $\vec{r}_2$ of all functions standing to its right. (The definition of Φ as a closed-channel function means $\lim\Phi = 0$ as $r_1, r_2 \to \infty$.) Using the idempotency $[P^2 = P,\ Q^2 = Q]$ and orthogonality $[PQ = 0]$, all of which may readily be shown for P and Q defined above, Feshbach[6] has derived a formal expression for the optical potential [which ultimately goes into the equation for $u(r_1)$ of Eq. (2.2)]:

$$\mathcal{V}_{\text{opt}} = PHQ[1/(E - QHQ)]\,QHP\ . \qquad (2.4)$$

Now the point of the recent work mentioned above (which interestingly enough has come from the atomic physics and not nuclear physics) is that $\mathcal{V}_{\text{opt}}$ can be approximated in such a way that it yields bounds on scattering parameters. Specifically, Gailitis[10] has shown that if one substitutes a set of variational approximations of the problem

$$QHQ\,\Phi = \mathcal{E}\,\Phi \qquad (2.5)$$

(the approximate solutions being labeled by Φ_λ and $\mathcal{E}_\lambda$) as intermediate states into $\mathcal{V}_{\text{opt}}$, then one obtains

$$\mathcal{V}_{\text{opt}}^{(\text{bound})} \geq \mathcal{V}_{\text{opt}} \,, \tag{2.6a}$$

which implies

$$\eta \leq \eta_{\text{exact}} \,. \tag{2.6b}$$

Φ_λ and $\mathcal{E}_\lambda$ are calculated from the Rayleigh-Ritz variational principle

$$\delta \frac{\langle \Phi Q H Q \Phi \rangle}{\langle \Phi Q \Phi \rangle} = 0 \,, \tag{2.5$'$}$$

where, as is well known, the number N of eigensolutions, $\lambda = 1, 2, \ldots, N$, is equal to the number of linear parameters in the variational ansatz for Φ.

Given the approximate set of Φ_λ, $\mathcal{E}_\lambda$ one can readily reduce $\mathcal{V}_{\text{opt}}^{(\text{bound})}$ to a transparent and generally calculable form as follows:

$$\mathcal{V}_{\text{opt}}^{(\text{bound})} \equiv \sum_{\lambda} \sum_{\lambda'} PHQ\Phi_\lambda \rangle \langle \Phi_\lambda [1/(E - QHQ)] \Phi_{\lambda'} \rangle \times \langle \Phi_{\lambda'} QHP \,,$$

which, using the orthonormality of the Φ_λ, reduces to

$$\mathcal{V}_{\text{opt}}^{(\text{bound})} = \sum_{\lambda=1}^{N} \frac{PHQ\Phi_\lambda \rangle \langle \Phi_\lambda QHP}{E - \mathcal{E}_\lambda} \,. \tag{2.7}$$

[A nondiagonal form of (2.7) in connection with the construction of bounds was first given by Sugar and Blankenbecler.[11]]

From (2.7) and (2.6) it is easy to see that $\mathcal{V}_{\text{opt}}$ contains no singularities for $E < \mathcal{E}_1 (\leq \mathcal{E}_2 \leq \cdots \leq \mathcal{E}_N)$. If QHQ has no discrete eigenvalues below the first inelastic threshold at which its continuous spectrum begins, then the bound theorem applies right up to that inelastic threshold. We shall find that that is the case in positron-hydrogen scattering right up to the positronium pickup threshold.

In fact the particular suitability of (2.5) for our calculations was occasioned by the fact that we had been searching for eigenvalues of QHQ (i.e., resonances) in the positron-hydrogen system using a generalized Hylleraas function[12]:

$$\Phi = e^{-(\delta r_1 + \gamma r_2 + \alpha r_{12})} \sum_{l,m,n}^{N} C_{lmn} r_1^m r_2^l r_{12}^n \,. \tag{2.8}$$

The nontrivial problem of Q-projecting on the ordinary Hylleraas function has been solved by Bhatia, Temkin, and Perkins[13] in connection with the problem of electron-hydrogen resonances. It turns out that the same techniques are applicable here; on the other hand, the basic trick is necessary even though P and Q are of a simpler unsymmetric form (2.3).

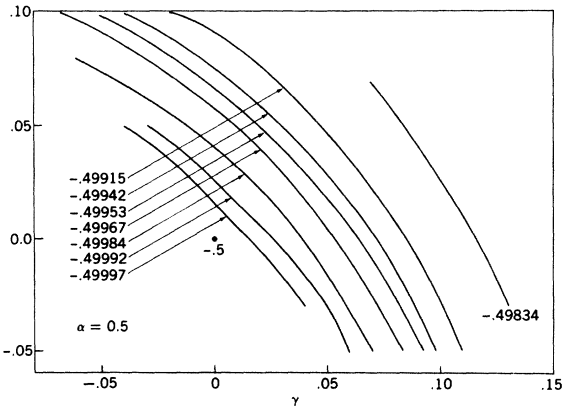

FIG. 1. Contours of $\mathcal{E}$ for $N = 20$ terms as a function of δ and γ ($\alpha = 0.5$).

The results of the search were negative as reported.[12] In Fig. 1 we plot contours of constant $\mathcal{E}$ as functions of δ and γ for $\alpha = \frac{1}{2}$. They are seen to lie above $\mathcal{E} = -0.5$, the energy of ground-state positronium, and to approach that value as γ, $\delta \to 0$ as they should, since that limit represents an unperturbed ground-state positronium at infinity with respect to the fixed proton. We found that we were unable to get nearly as close to the positronium energy unless we included the factor $e^{-\alpha r_{12}}$ explicitly. (For comparison we found a lowest QHQ energy of -0.4636 for $N = 50$ with $\alpha = 0$ and $\gamma = \delta = 0.35$. This leads to the suspicion that $e^{-\alpha r_{12}}$ is also necessary for the desired accuracy of phase shifts near the pickup threshold.) A similar result was calculated by Rotenberg and Stein,[14] who additionally found by extrapolation that only for a fictitious positron mass less than 0.7 of the electron mass would such a resonance arise. These results together with an independent calculation by one of us[14] which, albeit not a rigorous Q-operator calculation, did include the long-range positronium-proton polarization, convince us that there are no Feshbach resonances below the pickup threshold. The absence of any local minima above $\mathcal{E} > -0.5$ also suggests that there are no Feshbach resonances immediately above the pickup threshold,[12] it being understood that all these calculations refer only to total S waves. It should be noted in Fig. 1 that negative values of the parameters α, γ, δ are allowed. The only restriction in order that the integrals be convergent is that the sum of all pairs be positive:

$$\begin{aligned} \alpha + \gamma &> 0 \,, \\ \alpha + \delta &> 0 \,, \\ \gamma + \delta &> 0 \,. \end{aligned} \tag{2.9}$$

This means in particular that no two of the parameters can simultaneously be negative, but nevertheless the fact that one of them at a time can be negative shows that Φ of Eq. (2.7) is a much more flexible correlation function than might at first sight be thought.

TABLE I. Iterative convergence of solutions of Eq. (3.2) for $N=84$.

	$k=0.1$; $\alpha,\delta,\gamma=0.312, 0.128, 0.907$				$k=0.2$; $\alpha,\delta,\gamma=0.2, 0.230, 0.945$			
Iter	$r_{\rm final}$	$u(r)$	η	I_1	$r_{\rm final}$	$u(r)$	η	I_1
1	56.496 09	−21.232 38	−0.057 971 94	0.555 790 6	70.296 09	16.168 15	−0.114 466 0	0.307 762 8
2	31.396 09	− 3.914 446	0.256 315 6	0.431 415 8	39.896 09	8.566 021	0.306 429 8	0.239 502 4
3	34.696 09	− 8.189 429	0.137 256 5	0.444 963 8	45.696 09	1.124 356	0.175 208 7	0.247 177 3
4	35.696 09	− 9.810 514	0.148 721 9	0.443 946 9	45.696 09	0.982 803 9	0.188 469 7	0.246 540 2
5	35.696 09	− 9.806 863	0.147 825 0	0.444 015 2	45.696 09	0.994 273 8	0.187 381 1	0.246 586 6
6	35.696 09	− 9.807 108	0.147 885 7	0.444 010 4	45.696 09	0.993 447 0	0.187 459 8	0.246 583 4
7	35.696 09	− 9.807 091	0.147 881 3	0.444 010 9	45.696 09	0.993 503 8	0.187 454 3	0.246 583 7
	$k=0.6$; $\alpha,\delta,\gamma=0.45, 0.354, 0.914$				$k=0.7$; $\alpha,\delta,\gamma=0.5, 0.415, 0.946$			
1	32.546 09	1.822 719	−0.304 195 4	0.156 711 8	28.646 09	3.146 683	−0.340 019 8	0.118 143 6
2	30.946 09	−0.918 571 8	0.006 804 8	0.131 444 7	27.596 09	1.710 569	0.002 530 7	0.100 681 7
3	30.946 09	−1.188 874	−0.003 823 1	0.134 036 6	26.596 09	−1.033 558	−0.058 129 7	0.102 501 9
4	30.996 09	−1.041 833	0.003 577 6	0.133 815 6	27.621 09	1.530 154	−0.051 858 7	0.102 337 0
5	30.996 09	−1.043 761	0.002 970 4	0.133 832 9	27.621 09	1.526 442	−0.052 376 6	0.102 348 9
6	30.996 09	−1.043 621	0.003 016 6	0.133 831 5	27.621 09	1.526 766	−0.052 344 5	0.102 347 8
7	30.996 09	−1.043 631	0.003 013 2	0.133 831 6	27.621 09	1.526 739	−0.052 346 5	0.102 348 1

III. SCATTERING PROBLEM

The form of the scattering equation as given by Gailitis[10] is

$$[PHP+\mathcal{V}_{\rm opt}^{(\rm bound)}-E]\Psi=0 \ . \qquad (3.1)$$

Given the form of Ψ [Eq. (2.2)], the projection operators [Eq. (2.3)], $\mathcal{V}_{\rm opt}^{(\rm bound)}$ [Eq. (2.7)], and the complete set of eigenfunctions Φ_λ and $\mathcal{E}_\lambda$ associated with Eq. (2.5), one may straightforwardly reduce (3.1) to the one-dimensional *integro*differential equation

$$\left[\frac{d^2}{dr_1^2}-2e^{-2r_1}\left(1+\frac{1}{r_1}\right)+k^2\right]u(r_1)$$
$$-\sum_{\lambda=1}^{N}\frac{V_\lambda(r_1)\langle V_\lambda u\rangle}{E-\mathcal{E}_\lambda}=0 \ . \qquad (3.2)$$

The kernels V_λ are defined by

$$V_\lambda(r_1)=\int[Q\Phi(\vec{r}_1,\vec{r}_2)](-2/r_{12})\varphi_0(r_2)\,d^3r_2 \ . \qquad (3.3)$$

Using the device of Ref. 13 to evaluate $Q\Phi_\lambda$ with Φ_λ of the form of Eq. (2.8), we find that V_λ can be reduced to

$$V_\lambda(r_1)=\sqrt{8}\sum_{l,m,n}C_{lmn}^{(\lambda)}r_1^m e^{-\delta r_1}\{I_{l,n-1}(r_1)$$
$$-[r_1^{-1}-e^{-2r_1}(1+r_1^{-1})]I_{l,n}(r_1)\}, \qquad (3.4)$$

where

$$I_{l,n}(r_1)=\int_0^\infty dr_2\int_{|r_1-r_2|}^{r_1+r_2}dr_{12}\,e^{-(1+\gamma)r_2-\alpha r_{12}}\,r_2^{l+1}\,r_{12}^{n+1} \ . \qquad (3.5)$$

$I_{l,n}(r_1)$ can be and is evaluated in closed form for machine purposes.

Since the optical potential is a sum of separable terms, one could in principle reduce it to a set of uncoupled ordinary differential equations. However, the number of such equations is formidable ($N+1$) when going to large N, and thus we chose to solve it by iteration, with the expectation that the vast number of terms would in fact aid the convergence. That this expectation was borne out is shown in Table I wherein the convergence for an

TABLE II. Search results to find optimized α,δ,γ; $N=10$.

	α	δ	γ	η
$k=0.2$	0.24	0.272 09	0.726 958 7	0.176 270 2
	0.264	0.272 09	0.726 958 7	0.177 218 5
	0.264	0.227 929 9	0.726 958 7	0.177 740 7
	0.264	0.227 929 9	0.799 654 6	0.179 148 7
	0.288	0.248 650 8	0.872 350 4	0.181 310 9
	0.312	0.248 650 8	0.872 350 4	0.181 506 9
	0.312	0.269 371 7	0.872 350 4	0.181 366 6
	0.312	0.227 929 9	0.872 350 4	0.181 523 8
	0.312	0.227 929 9	0.945 046 3	0.181 941 3
$k=0.4$				
	0.215 625	0.300 680 8	0.802 515 6	0.106 163 5
	0.237 187 5	0.300 680 8	0.802 515 6	0.107 794 3
	0.237 187 5	0.330 748 9	0.802 515 6	0.108 518 8
	0.237 187 5	0.330 748 9	0.882 767 2	0.112 487 2
	0.258 75	0.360 817 0	0.963 018 7	0.112 441 5
	0.280 312 5	0.360 817 0	0.963 018 7	0.112 513 1
	0.280 312 5	0.390 885 0	0.963 018 7	0.111 515 2
	0.280 312 5	0.330 748 9	0.963 018 7	0.113 222 5
	0.280 312 5	0.330 748 9	1.043 270	0.109 816 2
	0.280 312 5	0.330 748 9	0.882 767 2	0.113 382 4
	0.323 437 5	0.330 748 9	0.882 767 2	0.113 311 9
	0.345	0.330 748 9	0.882 767 2	0.113 030 5
	0.301 875	0.330 748 9	0.882 767 2	0.113 441 3
	0.301 875	0.360 817 0	0.882 767 2	0.112 813 1
	0.301 875	0.300 680 8	0.882 767 2	0.113 787 9

84-term expansion is exhibited. The integration is automatically stopped as a function of r when the phase shift is suitably constant as a function of r. Table I shows that the value of r as well as the radial function $u(r)$ and a typical integral I_1 all do converge after seven interations.

The phase shifts are of course functions of the nonlinear parameters. The same search routine which was used to minimize the energies $\mathcal{E}_\lambda$ could be easily adapted to maximize the phase shifts as a function of α, γ, δ. Table II gives the results of the search for two values of k with ten linear parameters ($N=10$). Such searches were too time consuming for larger N, therefore,we fixed the value of γ and δ from ten-term searches and varied on α to get a maximum. Figures 2–4 show the results for four different k's; they demonstrate that although the optimum value of α remains essentially the same for $k=0.1$ as one increases N, it can vary quite substantially for the higher values of k. Clearly, then, even for 84 linear terms, one achieves much higher accuracy with the presence of the $e^{-\alpha r_{12}}$ term. Final results are given in Table III.

As a valuable check of the numerical accuracy we evaluated both sides of the following easily derivable identity:

$$\sin(\eta-\eta_0)=\frac{1}{AA_0k}\sum_{\lambda=1}^{N}\int_0^\infty u_0(r)V_\lambda(r)\,dr$$

$$\times\int_0^\infty u(r')V_\lambda(r')\,dr'(E-\mathcal{E}_\lambda)^{-1}. \qquad (3.6)$$

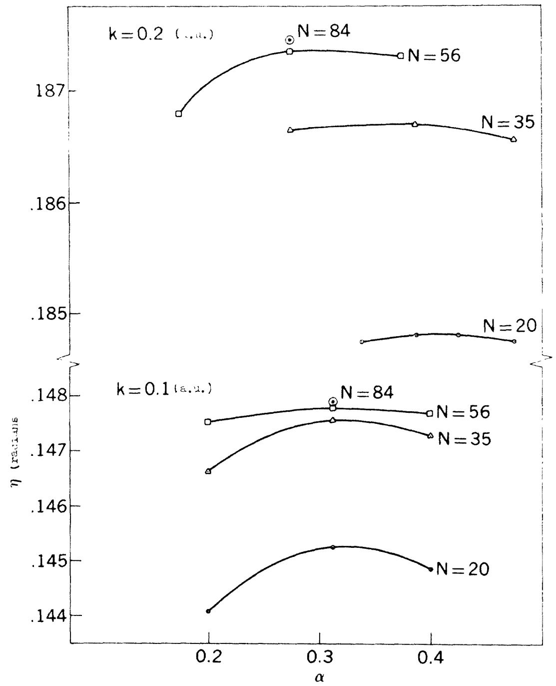

FIG. 2. Curves of η (rad) for $k=0.1$ and $k=0.2$ (a.u.) as a function of α. Values of γ and δ are those which optimized η for the $N=10$ expansion. Note the change in optimum α as N increases for $k=0.2$ (a.u.).

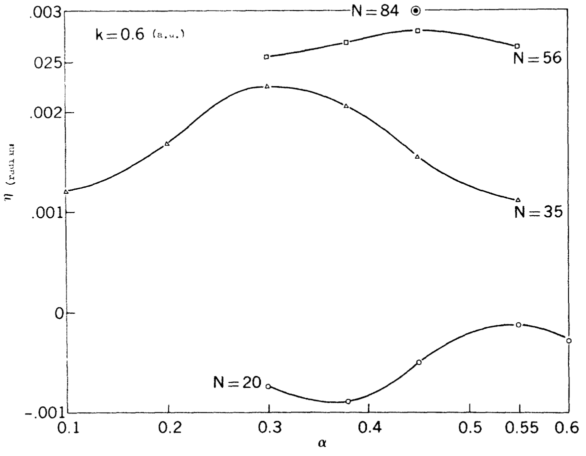

FIG. 3. Same as Fig. 2 for $k=0.6$ (a.u.).

The $u_0(r)$ and η_0 are the radial functions and well-known phase shifts of the Hartree approximation, respectively. The latter are listed under the column labeled 0 in Table III. The η and $u(r)$ to be used in (3.6) correspond to the subsequent columns of Table III for whatever N one wants to make the check. A and A_0 are the amplitudes of the asymptotic solutions:

$$\lim_{r\to\infty}\left\{\begin{array}{l} u=A\sin(kr+\eta)\,, \\ u_0=A_0\sin(kr+\eta_0)\ . \end{array}\right.$$

The last two columns give the left- and right-hand sides of (3.6) for the 35-term expansion. For larger N the check tended to be less accurate owing to large cancellations of terms in the right-hand side of Eq. (3.6). That such cancellations could not be present in the optical potential itself follows from the iterative convergence of $u(r)$ for all N, exhibited in Table I for $N=84$.

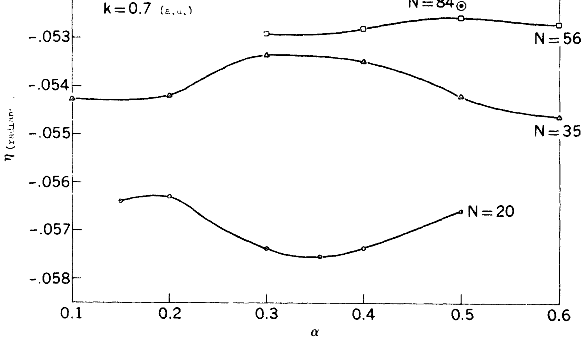

FIG. 4. Same as Fig. 2 for $k=0.7$ (a.u.).

TABLE III. Phase shifts vs number of linear parameters.[a]

								Check $N=35$	
$k \backslash N$	0	4	10	20	35	56	84	Left-hand side of (3.6)	Right-hand side of (3.6)
0.1	−0.057 97	0.124 16	0.141 58	0.145 53	0.147 56	0.147 77	0.147 88	0.204 09	0.204 10
0.2	−0.114 47	0.163 92	0.181 94	0.184 81	0.186 83	0.187 35	0.187 45	0.296 59	0.296 60
0.3	−0.168 17	0.142 03	0.161 63	0.165 41	0.166 45	0.166 94	0.167 15	0.328 29	0.328 29
0.4	−0.218 09	0.090 67	0.113 79	0.117 71	0.118 95	0.119 46	0.119 61	0.330 35	0.330 36
0.5	−0.263 53	•••	•••	0.059 67	0.060 99	0.061 81	0.061 92	0.318 42	0.318 42
0.6	−0.304 20	−0.026 23	−0.002 45	−0.000 12	0.002 26	0.002 81	0.003 01	0.301 01	0.301 31
0.7	−0.340 02	−0.079 64	−0.058 63	−0.056 30	−0.053 37	−0.052 59	−0.052 35	0.281 91	0.282 11

[a] The nonlinear parameters are approximately optimized for each N and k.

We found it necessary to go to $N=84$, in order that we might make extrapolations reliably to the fourth figure after the decimal point in η. Such reliability could be established by using two alternate assumptions about the differences

$$\eta_\omega - \eta_{\omega-1} = c\omega^{-p}\,, \tag{3.7a}$$

$$\eta_\omega - \eta_{\omega-1} = c'a^\omega\,. \tag{3.7b}$$

Here ω is the Pekeris index; it is the integer such that N of Eq. (2.7) includes all triples l, m, n of Φ [Eq. (2.7)], such that $l+m+n \leq \omega$. The difference formulas lead to extrapolation formulas

$$\eta_{\text{extrap}} = \eta_\omega + c(p-1)^{-1}\omega^{1-p} - \tfrac{1}{2}c\omega^{-p} + \tfrac{1}{12}\,cp\omega^{-p-1} + O(\omega^{-p-2})\,, \tag{3.8a}$$

$$\eta_{\text{extrap}} = \eta_{\omega-1} + c'a^\omega(1-a)^{-1}\,. \tag{3.8b}$$

The coefficients $c(c')$, p, and a were determined from the 35-, 56-, and 84-term results. The η_{extrap} are listed in Table IV and they are seen to agree with each other to four significant figures.

At this point, it is appropriate to compare these extrapolated values to those of Schwartz given in the first column of Table IV. The first observation to be made is that by and large his values do stand up even after nine years. In somewhat finer detail there are some discrepancies which should be mentioned. Since his estimated accuracy is one in the last figure,[3] there are seen to be discrepancies at $k=0.1$, 0.6, and 0.7. At the lower k, since our values are below his, the bound theorem cannot be used to disprove his results; but, since our correlation function includes his (when $\alpha=0$, $\gamma=\delta$), we can confidently rely on our value. Secondly, the results of the following paper[15] strongly suggest that Kohn-Hulthén-type methods do not necessarily yield a lower bound at nonzero energies. This, we believe, is basically the case here too. At $k=0.6$ the discrepancy is a factor of 2; but the absolute value of the difference from our value is only slightly greater than at $k=0.1$, so that this may also reflect the lack-of-a-bound principle. At $k=0.7$ our value exceeds Schwartz's, so that his value is ruled out by the lower-bound principle. Dynamically this probably comes from the explicit inclusion of a positronium factor in our calculation which was discussed in connection with the QHQ calculation in Sec. II.

One can gain some confidence in the superiority of these phase shifts by comparing them and Schwartz's to those calculated by Drachman[16] using a quite different (and less accurate) lower-bound technique. Originally introduced to measure the quality of the latter results as compared with Schwartz's, a quality factor is defined as

TABLE IV. Final values of S-wave e^{+}-H phase shifts.[a]

		η_{extrap}		$\Delta\eta$	η_{final}
k	Schwartz (Ref. 3)	This calculation Eq. (3.8a)	This calculation Eq. (3.8b)		
0.1	0.151	0.148 085	0.147 999	0.000 223	0.1483
0.2	0.188	0.187 496	0.187 490	0.000 200	0.1877
0.3	0.168	0.167 407	0.167 310	0.000 306	0.1677
0.4	0.120	0.119 724	0.119 685	0.000 420	0.1201
0.5	0.062	0.061 934	0.061 934	0.000 429	0.0624
0.6	0.007	0.003 191	0.003 126	0.000 689	0.0039
0.7	−0.054	−0.052 183	−0.052 160	0.000 980	−0.0512

[a] A definitive value of the scattering length is calculated in the following paper (Ref. 15).

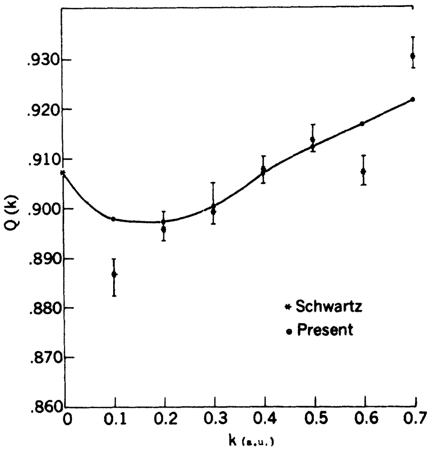

Fig. 5. Quality factor Q as a function of k for two different sets of "exact" η. See text for further comments.

$$Q(k)\equiv\frac{\eta_D-\eta_0}{\eta-\eta_0}\ ,$$

where η_D are the phase shifts of Ref. 16. $Q(k)$ varies with energy, but one does not expect anything but smooth variations since Drachman's method does not distinguish strongly between different energies. In Fig. 5 we display $Q(k)$ for two values of the "exact" phase shift η; the smoother curve corresponds to the present results. Including the scattering-length values[15] at $k=0$, we see that at exactly those three points where a disagreement was found, Schwartz's results produce abrupt deviations.

In order to evaluate phase shifts correct to four significant figures, it is necessary to include a correction for the long-range polarization potential even at nonzero k.[4,17] The correction formula used is

$$\sin(\Delta\eta)$$

$$=\frac{4.5}{k}\int_{r_0}^{\infty}\frac{\sin[k+\eta(r)]\sin[kr+\eta(r)+\Delta\eta(r)]}{r^4}\,dr\,. \tag{3.9}$$

In (3.9), $\Delta\eta(r)$ is the value of $\Delta\eta$ with the upper limit taken at the variable point r. Thus we have

$$\Delta\eta=\lim_{r\to\infty}\Delta\eta(r)\,.$$

The value of r_0 was determined by seeing at what value of r the contributions to $\eta(r)$ coming directly from (3.2) were exceeded by those coming from (3.9). Comparison showed that the point at which the respective increments began to differ significantly from each other depended inversely on k. For $k=0.1$ the optical potential simulated the polarization potential out to $r=25$, whereas for $k=0.7$ differences were large beyond $r=10$. This inverse relationship accounts for the fact that net increment coming from (3.9), listed as $\Delta\eta$ in Table IV, actually increases as k increases.

The scattering-length calculation of the accompanying paper also included a dipole term variationally. Since a variationally included dipole term carries with it an associated nonadiabatic term which is effectively r^{-6} in character,[16] it might be thought that the nonadiabatic term, which is not contained in (3.9), is also an important correction. But the subsequent inclusion of the quadrupole term in the accompanying calculation[15] had absolutely no effect to this accuracy. Since the longest-range part of this correction is an adiabatic quadruple polarization potential[17] of order r^{-6}, and since our correlation function makes no distinction between any angular multipole factors, we can confidently expect that *all* corrections of over r^{-6} (and shorter range) are in fact well contained in Φ.

However, an examination shows that the r^{-4} effect described by $\Delta\eta$ would probably require hundreds of terms in Φ of Eq. (2.7) to be adequately described. This is the reason why that correction cannot be expected to affect the convergence pattern on η_{extrap} and must be added on separately. This circumstance is a nice reminder that convergence arguments must always be subordinated to physical arguments.

Our final error is based on the estimate that residual effects could not alter $\Delta\eta$ by more than 25% and by an additional uncertainty of one unit in the fourth place coming from the extrapolations. We therefore believe η_{final} of Table IV is correct within ± 0.0002 rad.

Note added in manuscript. Dr. Schwartz has sent us a more detailed statement of the error in his e^+-H calculation; his assigned phase-shift error was found to vary from ± 0.0005 to ± 0.0018 with the uncertainties being largest at $k=0.1$, 0.6, and 0.7. He concludes that the discrepancy from our results is minimal, but that our results are certainly more accurate.

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Positron-Atom Scattering by the Kohn and Harris Methods

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The S-wave scattering parameters have been calculated for the e^+-H and e^+-He systems below the positronium-formation threshold. The phase shifts were computed using the Harris variational method, while at zero energy the scattering lengths were obtained by the Kohn variational method. For hydrogen, a generalized Hylleraas wave function with three nonlinear parameters was used, giving an upper-bound scattering length $a \leq -2.10278$, agreeing with Schwartz's result $a \leq -2.10$. An extrapolation procedure gives an estimate of $a = -2.1036 \pm 0.0004$. At nonzero energies, agreement with the lower-bound results of Bhatia, Temkin, Drachman and Eiserike, to better than 0.004 rad is achieved. Since the exact atomic-helium wave function is not known, the situation for helium is less clear; various model-target wave functions are examined using a generalized Hylleraas function with two nonlinear parameters. For the exponential model used by Drachman, the scattering is in close agreement with previous results, but the annihilation-rate parameter Z_{eff} is higher by 15% in poorer agreement with experiment at zero energy.

I. INTRODUCTION

In the study of positron interaction with atoms at low energies, the positron-hydrogen system is most tractable theoretically, while the positron-helium system is much more accessible to experiment. Enough similarity between these two systems exists for the calculational techniques that succeed in the former to be expected to succeed also in the latter. It is thus useful to test proposed theoretical methods in the e^+-H system, and then to apply them to the e^+-He system.

In recent years this has been done several times, using different methods.[1-4] None of these methods was both simple enough to apply to helium and really accurate enough, as judged by comparison with the most definitive work in hydrogen. In addition, the serious problem of the inexactness of the atomic-helium wave function remained unresolved. Nevertheless, the best of these calculations[1,4] are now roughly in agreement with the best recent measurements,[5-7] and there is considerable interest in more extensive and exact calculations of cross sections and annihilation rates.

In this paper we report some new results for positron-atom scattering systems, calculated variationally. In Sec. II, the generalized Hylleraas type of scattering function is described and applied to Kohn variational calculations for zero energy and Harris calculations for higher energies. In Sec. III, S-wave scattering from atomic hydrogen below the positronium threshold is considered, and the results are compared with previous ones. In Sec. IV, the corresponding problem for helium is treated. Since the helium ground state is not known exactly, ambiguities in the formulation of scattering approximations exist. A technique is described which involves a model Hamiltonian corresponding to the approximate ground-state wave function assumed. Using this technique, the S-wave scattering parameters are computed and compared with previous results; at zero energy only, the annihila-