Rigorous precision p-wave positron-hydrogen scattering calculation

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Rigorous lower-bound p-wave positron-hydrogen phase shifts are calculated below the positronium pick-up threshold. The wave function is expanded in terms of the two linearly independent D functions each multiplied by an associated Hylleraas-type radial function with two nonlinear parameters. Calculations have been done employing up to a total of 168 linear parameters, so that convergence can be examined and extrapolations in most cases performed to $N = \infty$. In addition, adiabatic and nonadiabatic corrections have been included. Results are found to be larger than Armstead's in all cases, near the upper edge of his estimated uncertainty. The calculation confirms as a byproduct that there are no p-wave Feshbach resonances in this energy range.

I. CALCULATION

This is the second part of a program to calculate definitive positron-hydrogen scattering phase shifts below the positronium pickup threshold. The s-wave scattering was calculated in Paper I,[1] and those results showed some differences with the older calculation of Schwartz,[2] which differences have been confirmed in at least four subsequent calculations.[3] In the present paper we shall be concerned with the p-wave calculation. Here there has been only one previous precision calculation.[4] We shall find here that there are no disagreements with Armstead's results.[4] Rather we shall find, because of greater rigor of our formulation and more extensive nature of our correlation function, greater precision in our phase shifts, which are on the upper edge of Armstead's estimated range of likely final results.

The formulation starts with the $e^+ + \mathrm{H}$ p-wave function

$$\Psi = \frac{u(r_1)}{r_1} Y_{10}(\Omega_1)\phi_0(r_2) + Q\Phi(\vec{r}_1, \vec{r}_2), \tag{1.1}$$

where $u(r_1)$ is the positron scattered orbital, $\phi_0(r_2)$ is the ground state of the electron in the target hydrogen atom, and Φ is a correlation function that can be written[5]

$$\Phi = f_1 \cos(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1+}(\vec{\beta}) + f_2 \sin(\tfrac{1}{2}\theta_{12})\mathfrak{D}_1^{1-}(\vec{\beta}). \tag{1.2}$$

The f_i are taken of the Hylleraas type with two nonlinear parameters:

$$f_i = e^{-(\delta_i r_1 + \gamma_i r_2)} \sum_{l\geq 1} \sum_{m\geq 0} \sum_{n\geq 0} C_{lmn}^{(i)} r_1^l r_2^m r_{12}^n. \tag{1.3}$$

The f_i are linearly independent because the positron ($\vec{r}_1$) and the electron ($\vec{r}_2$) are distinguishable, thus the radial function contains a total of four nonlinear parameters. The $\vec{\beta}$ are the symmetric Euler angles and the $\mathfrak{D}$'s the rotational harmonics that carry the total angular momentum (p-wave) and parity (odd) dependence of the total wave function.[5]

The optical-potential formalism[6] is used to derive an equation for $u(r)$ (rydberg units are used throughout):

$$\left(\frac{d^2}{dr^2} - \frac{2}{r^2} - \mathfrak{V}_{0p} - v_H + k^2\right) u(r) = 0, \tag{1.4}$$

wherein v_H is the Hartree potential

$$v_H = 2e^{-2r}(1 + r^{-1}), \tag{1.5}$$

and $\mathfrak{V}_{pp}$ is the optical potential which is a nonlocal potential

$$\mathfrak{V}_{op} u = r \sum_{\lambda=1}^{2N} \frac{\langle Y_{10}(1)\phi_0(2) PHQ\Phi_\lambda\rangle \langle \Phi_\lambda QHP\Psi\rangle}{E - \mathcal{E}_\lambda}. \tag{1.6}$$

This potential is seen to depend on the projection operators P and Q, which project onto open and closed parts of the wave function

$$P = |\phi_0(r_2)\rangle\langle\phi_0(r_2)|, \tag{1.7a}$$

$$Q = 1 - P. \tag{1.7b}$$

The Φ_λ and $\mathcal{E}_\lambda$ are the eigenfunctions and eigenvalues of QHQ problem in the truncated space of the trial correlation function specified by Eqs. (1.2) and (1.3). Specifically, each function f_i is taken to depend on N parameters, where $N = N(\omega_i)$ is taken in the Perkeris fashion[7] to include all terms such that $(l + m + n) \leq \omega_i$.

The QHQ problem is the variational eigenvalue problem defined by

$$\delta\langle\Phi QHQ\Phi\rangle / \langle\Phi Q\Phi\rangle = 0. \tag{1.8}$$

For Φ of Hylleraas form, the projection problem

TABLE I. Sample of nonlinear parameter search to maximize η for $k=0.2$ and $k=0.7$.

		$k=0.2$					$k=0.7$				
$2N$	ω	γ_1	δ_1	γ_2	δ_2	η	γ_1	δ_1	γ_2	δ_2	η
8	2	0.51	0.84	0.75	0.52	0.021 946	0.675	0.75	0.675	0.75	0.089 36
		0.357	0.84	0.75	0.312	0.027 782	0.4725	0.90	0.81	0.75	0.103 41
20	3	0.357	0.84	0.75	0.312	0.030 317	0.4725	0.90	0.81	0.75	0.151 61
		0.4641	0.84	0.75	0.3744	0.030 638	0.52	0.825	0.81	0.825	0.152 96
40	4	0.46	0.8	0.75	0.37	0.031 698	0.52	0.825	0.81	0.825	0.170 453
		0.506	0.8	0.75	0.37	0.031 726	0.468	0.825	0.81	0.825	0.170 276
		0.506	0.8	0.75	0.407	0.031 843	0.559	0.825	0.81	0.825	0.170 459
		0.552	0.8	0.75	0.444	0.031 951	0.559	0.9075	0.81	0.825	0.170 147
		0.598	0.8	0.75	0.444	0.031 945	0.559	0.7425	0.81	0.825	0.170 508
		0.506	0.8	0.75	0.444	0.031 949	0.559	0.7425	0.81	0.9075	0.169 840
		0.552	0.8	0.75	0.481	0.031 968	0.559	0.7425	0.81	0.7425	0.170 818
70	5	0.552	0.8	0.75	0.481	0.032 296	0.559	0.7425	0.81	0.7425	0.174 91
		0.552	0.8	0.75	0.54	0.032 332	0.60	0.7425	0.81	0.7425	0.174 82
		0.552	0.8	0.75	0.58	0.032 311	0.65	0.7425	0.81	0.7425	0.174 66
		0.506	0.8	0.75	0.481	0.032 291	0.559	0.65	0.81	0.65	0.175 05
		0.506	0.8	0.75	0.444	0.032 292	0.559	0.7425	0.70	0.7425	0.174 87
112	6	0.552	0.8	0.75	0.54	0.032 391	0.559	0.65	0.81	0.65	0.176 81
168	7	0.552	0.8	0.75	0.54	0.032 51	0.559	0.65	0.81	0.65	0.177 72

has been solved previously,[8] and when these eigensolutions are used in v_{op} the phase shifts η coming from the asymptotic form of u,

$$\lim_{r_1 \to \infty} u(r_1) = \sin(kr_1 - \tfrac{1}{2}(l\pi) + \eta) \tag{1.9}$$

are guaranteed to be lower bounds,[9] providing the total E,

$$E = -1 + k^2, \tag{1.10}$$

is less than the lowest possible $\mathcal{E}_\lambda$ eigenvalue of Eq. (1.8).

Calculations of Eqs. (1.8) and (1.4) were carried out in a manner completely parallel to Ref. 1. Results are given in Sec. II.

II. RESULTS

Calculations were done first to find whether any $\mathcal{E}_\lambda$ lay below the positronium pickup threshold at $E=-0.5$ Ry. No such eigenvalues were found, which indicates, as in the s-wave case,[1] that no p-wave Feshbach resonances exist below the pickup threshold.

Thereafter, we solved the scattering equation (iteratively as in Ref. 1) as a function of the non-

TABLE II. Optimized η and extrapolation.

	Phase shifts						Extrapolation[a]			
$K/2N(\omega)$	8(2)	20(3)	40(4)	70(5)	112(6)	168(7)	$\omega=5$	$\omega=6$	$\omega=7$	Armstead[b]
0.1	0.007 61	0.008 04	0.008 26	0.008 59	0.008 76	···	0.007 8	0.009 02	···	0.008
							0.007 6	0.008 91		0.009(1)
0.2	0.027 78	0.030 64	0.031 97	0.032 33	0.032 39	0.032 51	0.032 56	0.032 41	···	0.032
							0.032 47	0.032 40		0.033(1)
0.3	0.052 56	0.061 35	0.064 03	0.064 74	0.065 31	0.065 56	0.065 18	0.070 84	0.065 85	0.064
							0.065 00	0.067 52	0.065 76	0.065(1)
0.4	0.074 37	0.092 27	0.097 51	0.098 83	0.099 61	0.100 05	0.099 57	0.101 77	0.101 04	0.099
							0.099 27	0.100 75	0.100 65	0.102(1)
0.5	0.089 84	0.117 99	0.127 31	0.129 21	0.130 10	0.130 27	0.130 02	0.131 45	0.130 33	0.130
							0.129 69	0.130 92	0.130 31	0.132(1)
0.6	0.098 75	0.136 95	0.149 81	0.152 94	0.153 57	0.154 10	0.154 64	0.153 82	···	0.153
							0.153 95	0.153 73		0.156(2)
0.7	0.103 41	0.152 96	0.170 82	0.175 05	0.176 81	0.177 72	0.177 25	0.178 83	0.179 23	0.175
							0.176 36	0.178 07	0.178 68	0.178(3)

[a] Upper entry based on (2.1a) and lower on (2.1b).

[b] Upper entry is his actual results and lower entry his estimate of converged result with uncertainty in last figure given in parenthesis (Ref. 4).

linear parameters to maximize the phase shifts.

Table I gives a sample of such results. For the lower ω a full search in the nonlinear parameter space was made. However, this was much too time consuming for larger ω and a selective search was continued thereafter, in which those parameters that seemed to have the least effect on the phase shifts were frozen.

The lowest results for all k as a function of N are given in Table II. On the right of the table we give the extrapolated values using the two extrapolation formulas derived from $\eta_\omega - \eta_{\omega-1} = c\omega^{-p}$ and $\eta_\omega - \eta_{\omega-1} = c'a^\omega$, respectively:

$$\eta_{\text{extrap}} = \eta_\omega + c(p-1)^{-1}\omega^{1-p} - \tfrac{1}{2}c\omega^{-p} + \tfrac{1}{12}c\omega^{-p-1} + O(\omega^{-p-2}), \quad (2.1a)$$

$$\eta_{\text{extrap}} = \eta_{\omega-1} + c'a^\omega(1-a)^{-1}. \quad (2.1b)$$

When the differences do not get smaller or get smaller slowly, one cannot make sensible extrapolations. Such cases have been omitted in the extrapolation part of the table. Of those that remain, the agreement between the various results, associated with the largest ω that was included in Eq. (2.1), is not always good. This indicates that the $\omega = 5$ results are certainly insufficient for extrapolation purposes.

Another source of difficulty in the extrapolation process is the fact that the long-range polarization effects are not well included in a Hylleraas-type correlation function. As in Ref. 1 these can be added in an approximate way by seeing where the phase shift as a function of r_1 for large r_1 no longer augments itself as it should, due to these long-range potentials. In the present case, we have included both the dipole adiabatic[10] ($\alpha = \frac{9}{2}$ is the polarizability of H)

$$\Delta\eta_d = \frac{\alpha}{k}\int_{r_0}^{R} \frac{\{kr[j_1(kr)\cos\eta(r_0) - n_1(kr)\sin\eta(r_0)]\}^2}{r^4}\,dr \quad (2.2)$$

and the quadrupole adiabatic plus nonadiabatic terms[11]

$$\Delta\eta_q = -\frac{69/4}{k} \times \int_{r_0}^{R} \frac{\{kr[j_1(kr)\cos\eta(r_0) - n_1(kr)\sin\eta(r_0)]\}^2}{r^6}\,dr, \quad (2.3)$$

TABLE III. Final results (p-wave phase shifts in radians).

k	η_{extrap}[a]	$\Delta\eta_d$	$\Delta\eta_q$	η_f
0.1	0.009	...	...	0.0094[b]
0.2	0.0325	0.001 3	-0.13×10^{-4}	0.0338
0.3	0.0659	0.000 70	-0.56×10^{-5}	0.0665
0.4	0.1010	0.000 61	-0.59×10^{-5}	0.1016
0.5	0.1303	0.000 59	-0.66×10^{-5}	0.1309
0.6	0.1541	0.000 61	-0.72×10^{-5}	0.1547
0.7	0.1792	0.000 73	-0.11×10^{-4}	0.1799

[a]Confer, text for the manner in which these were obtained for different k.

[b]Computed from formula (2.5).

where R has been extended to a large enough value so that the integrals converge. r_0 then is the value of r where the phase shift coming directly from the solution of (1.4) as a function of r no longer augments itself as the sum of (2.2) and (2.3). In practice we found $r_0 \sim 15$ for most of the values of k, and R was taken to be 100 in all cases.

Final results are given in Table III. As in Ref. 1 we add the long-range corrections to the extrapolated values from Table II,

$$\eta_f = \eta_{\text{extrap}} + \Delta\eta_d + \Delta\eta_q. \quad (2.4)$$

We have used the larger of the $\omega = 7$ extrapolated values from Table II in those cases where it is given ($k = 0.3, 0.4, 0.5, 0.7$). For $k = 0.2, 0.6$ we use the unextrapolated $\omega = 7$ results For $k = 0.1$ the polarization is so dominant that our results are not more reliable (but consistent with) the long-range-polarization formula of Spruch *et al.*[12]

$$\tan\eta_l = \left.\frac{\pi\alpha k^2}{(2l-1)(2l+1)(2l+3)}\right|_{l=1}. \quad (2.5)$$

The major uncertainty comes from the differences in extrapolated values, where they can be made, or from the lack of reasonable extrapolations elsewhere. In all cases these uncertainties appear to us to be bounded by 0.0005 rad. Compared to this, the uncertainties in $\Delta\eta_d$ and $\Delta\eta_q$ are negligible. Thus we estimate our η_f to be correct to this uncertainty (5×10^{-4} rad) with a slightly greater probability that our values lie on the low side.

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