Positron-Hydrogen Scattering at Low Energies

Jim Mitroy*
Faculty of Science, Northern Territory University, GPO Box 40146, Casuarina, Northern Territory 0811, Australia

Lindsay Berge† and Andris Stelbovics‡
Centre for Atomic, Molecular and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Murdoch, Western Australia 6150
(Received 18 May 1994)

Calculations of positron-hydrogen scattering using the close-coupling approach are reported for incident positron energies below the ionization threshold. The channel space includes nine physical hydrogen and positronium states and, in addition, eleven hydrogen and positronium pseudostates. The accuracy of our model has been validated by computations of elastic phase shifts below the positronium threshold, and elastic and positronium-formation cross sections in the Ore gap. Calculations are performed for sufficient partial waves to obtain converged elastic, positronium, and total cross sections.

PACS numbers: 34.80.–i, 34.90.+q, 36.10.Dr

The positron-hydrogen system is one of the simplest collision systems for which a genuine rearrangement process is possible. For a positron-hydrogen collision, the following classes of reactions are possible:

$$e^+ + \mathrm{H}(1s) \longrightarrow e^+ + \mathrm{H}^*(nl) \quad \text{(excitation)}$$
$$\longrightarrow e^+ + e^- + p \quad \text{(ionization)}$$
$$\longrightarrow \mathrm{Ps}(nl) + p \quad \text{(positronium formation)}.$$

Because of the difficulties in treating collision systems without a single center of symmetry, there have been relatively few calculations of positron-hydrogen scattering that have treated the positronium-formation channels with any degree of realism. Even though the e^+-H system is an important three-body system, the only high-precision calculations that have been done are restricted in scope. At energies below the positronium threshold, numerous variational calculations [1–7] and single-center close-coupling calculations [8,9] have been reported. There are some precise variational calculations [10] and two slightly less accurate close-coupling calculations [11,12] of cross sections in the Ore gap.

Recently, a general expression for the positronium-formation matrix element has been derived that is suitable for large-scale computations [13]. This means that close-coupling (CC) calculations can now be routinely performed on the positron-hydrogen system. This is an important advance, since the CC calculations (unlike the variational calculations) can be performed for enough partial waves to obtain converged cross sections.

The present work represents an improvement over an earlier calculation [12] which coupled six hydrogen and six positronium states. The energy range was extended to the ionization threshold and the basis set enlarged. A total of 20 physical states and pseudostates were included with the expectation that this would result in an accurate set of cross sections. Above the ionization threshold, the presence of resonances [14–17] and possible pseudoresonances complicate the analysis to such an extent that a definitive study in this energy range would require a larger basis set.

To ascertain the degree of convergence, a sequence of successively larger calculations have been compared. These are as follows.

CC($\overline{3},\overline{3}$): This basis includes the hydrogen and positronium ground states. The pseudo H($\overline{2s}$), H($\overline{2p}$), Ps($\overline{2s}$), and Ps($\overline{2p}$) levels were chosen to be identical to those used in an R-matrix calculation [17]. The cross sections reported for this model are taken from an earlier work [12].

CC($\overline{6},\overline{6}$): This basis includes the lowest three physical levels of hydrogen ($1s$, $2s$, $2p$) as well as three pseudolevels ($\overline{3s}$, $\overline{3p}$, $\overline{3d}$). The lowest three physical states of positronium ($1s$, $2s$, $2p$) and three pseudopositronium levels were included ($\overline{3s}$, $\overline{4s}$, $\overline{3p}$).

CC($\overline{12},\overline{8}$): This basis includes the lowest six physical levels of hydrogen ($1s$, $2s$, $2p$, $3s$, $3p$, $3d$) as well as six pseudolevels ($\overline{4s}$, $\overline{5s}$, $\overline{4p}$, $\overline{5p}$, $\overline{4d}$, $\overline{4f}$). The lowest three physical states of positronium (1s, 2s, 2p) and five pseudopositronium levels were included ($\overline{3s}$, $\overline{4s}$, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$).

For our calculations, 40- and 48-point Gaussian quadrature meshes were used to discretize the kernel of the integral equation. (Convergence checks to monitor the numerical accuracy were performed with different quadrature meshes at selected energies.) The Lippmann-Schwinger equations were solved up to $J = 6$ at $E = 0.72$ Ry and $J = 10$ at $E = 1.0$ Ry to ensure convergence of the partial wave sum. The minor contributions from higher partial waves were included by extrapolation.

In Table I, phase shifts for the $J = 0$–4 partial waves are presented at energies below the positronium-formation threshold. The variational phase shifts of Bhatia *et al.* [1,2] for the $J = 0$ and $J = 1$ partial waves are generally regarded as the most accurate. This comparison demonstrates that the present calculation is comparable in

 0031-9007/94/73(22)/2966(4)$06.00

TABLE I. Phase shifts for positron-hydrogen scattering as a function of incident momentum (πa_0^{-1}).

k	0.1	0.2	0.3	0.4	0.5	0.6	0.7
Method							
				$J = 0$			
IERM[a]	0.148	0.187	0.167	0.118	0.062	0.004	
CC($\bar{6},\bar{6}$)	0.1404	0.1767	0.1558	0.1105	0.0536	−0.0044	−0.0588
CC($\bar{12},\bar{8}$)	0.1481	0.1870	0.1673	0.1199	0.0620	0.003 31	−0.0519
Variational[b]	0.1483	0.1877	0.1677	0.1201	0.0624	0.0039	−0.0512
Variational[d]	0.1460	0.1849	0.1649	0.1172	0.0593	−0.000 03	−0.0569
				$J = 1$			
IERM[a]	0.009	0.033	0.066	0.102	0.132	0.156	0.185
CC($\bar{6},\bar{6}$)	0.008 76	0.0321	0.0639	0.0974	0.1267	0.1496	0.1732
CC($\bar{12},\bar{8}$)	0.008 85	0.0327	0.0656	0.1002	0.1304	0.1542	0.1786
Variational[c]		0.0338	0.0665	0.1016	0.1309	0.1547	0.1799
Variational[d]	0.005	0.030	0.063	0.097	0.128	0.146	0.169
				$J = 2$			
IERM[a]		0.005	0.013	0.025	0.041	0.062	
CC($\bar{6},\bar{6}$)	0.001 35	0.005 46	0.0127	0.0237	0.0386	0.0580	0.0856
CC($\bar{12},\bar{8}$)	0.001 35	0.005 51	0.0129	0.0241	0.0396	0.0598	0.0885
Variational[d]	0.0013	0.0054	0.0125	0.0235	0.0389	0.0593	0.0863
				$J = 3$			
IERM[a]		0.0018	0.0040	0.0075	0.0126	0.0207	
CC($\bar{12},\bar{8}$)	0.452-3	0.001 80	0.004 07	0.007 52	0.0125	0.0198	0.0307
				$J = 4$			
CC($\bar{12},\bar{8}$)	0.205-3	0.818-3	0.001 82	0.003 28	0.005 29	0.008 05	0.0121

[a]Intermediate energy R matrix (with extrapolation) [9].
[b]Variational, Bhatia *et al.* (1971) [1].
[c]Variational, Bhatia *et al.* (1974) [2]. (It should be noted that the phase of 0.1 was computed using a pure polarization formula and so has been omitted.)
[d]Kohn variational [5].

accuracy with the best calculations and so gives an overall indication of the accuracy of our cross sections. Comparison of the CC($\bar{12},\bar{8}$) and CC($\bar{6},\bar{6}$) phase shifts reveals that the CC($\bar{12},\bar{8}$) phase shifts are larger and close to convergence. The maximum difference from the variational phase shifts is less than 0.002 rad for the $J = 0$ and $J = 1$ partial waves. We estimate the scattering length to be $(-2.09 \pm 0.02)a_0$ in agreement with the value of $(-2.1036 \pm 0.0004)a_0$ of Bhatia *et al.* [1].

For the $J = 2$ and higher partial waves, our phase shifts probably represent the state of the art. At low energies, the CC($\bar{12},\bar{8}$) and CC($\bar{6},\bar{6}$) are almost identical, indicating a high degree of convergence. Only at higher energies, when the positron can penetrate deeper into the centrifugal barrier, does the enlarged channel space of the CC($\bar{12},\bar{8}$) model result in an increased phase shift. For the $J = 2$ wave, our phase shifts are larger than those of Register and Poe [5], as they are for the $J = 0$ and $J = 1$ partial waves. Our results are consistent with those of the intermediate energy R-matrix (IERM) method [9], although we suspect the present calculation may be more precise.

At energies above 0.5 Ry, the Ps($1s$) channel opens and inelastic as well as elastic scattering is possible. Elastic cross sections above 0.5 Ry are listed in Table II and positronium cross sections are listed in Table III. A feature of Table II is the close agreement between the CC($\bar{12},\bar{8}$) and variational calculations [10]. For the $J = 0$ wave, the decrease in the elastic cross section in going from the CC($\bar{6},\bar{6}$) to the CC($\bar{12},\bar{8}$) basis is sufficient to achieve excellent agreement with the variational cross sections. The CC($\bar{12},\bar{8}$) cross sections are closer to the variational cross sections for the $J = 1$ wave as well. The agreement between the two cross section sets is ex-

TABLE II. Elastic cross sections (in units of πa_0^2) for the $J = 0$, 1, and 2 partial waves above the positronium-formation threshold. The summed cross sections are also given.

Energy (Ry)	0.5041	0.5625	0.64	0.7225
Model				
		$J = 0$		
CC($\bar{3},\bar{3}$)[a]	0.0511	0.0711	0.0946	0.1157
CC($\bar{6},\bar{6}$)[a]	0.0324	0.0504	0.0730	0.0937
CC($\overline{12},\bar{8}$)	0.0245	0.0427	0.0651	0.0844
Variational[b]	0.026	0.043	0.065	0.085
		$J = 1$		
CC($\bar{3},\bar{3}$)[a]	0.627	0.570	0.490	0.428
CC($\bar{6},\bar{6}$)[a]	0.756	0.684	0.589	0.517
CC($\overline{12},\bar{8}$)	0.801	0.725	0.625	0.551
Variational[b]	0.789	0.724	0.622	0.547
		$J = 2$		
CC($\bar{3},\bar{3}$)[a]	0.265	0.349	0.382	0.374
CC($\bar{6},\bar{6}$)[a]	0.319	0.418	0.455	0.447
CC($\overline{12},\bar{8}$)	0.341	0.446	0.486	0.477
Variational[b]	0.323	0.403	0.423	0.413
		Total		
CC($\bar{3},\bar{3}$)[a]	1.004	1.071	1.081	1.059
CC($\bar{6},\bar{6}$)[a]	1.177	1.245	1.248	1.220
CC($\overline{12},\bar{8}$)	1.238	1.309	1.311	1.281

[a]Reference [12].
[b]Variational [10].

cellent with the maximum difference between them for the $J = 0$ and $J = 1$ waves being only $0.012\pi a_0^2$.

The comparison for the $J = 2$ wave is not quite so good. There are differences of $0.06\pi a_0^2$ between the CC($\overline{12},\bar{8}$) and variational cross sections [10]. Just above threshold, the CC($\overline{12},\bar{8}$) cross section is $0.341\pi a_0^2$, whereas the variational cross section is $0.323\pi a_0^2$. Since a larger cross section implies a larger phase shift, this indicates that the variational flexibility of the CC($\overline{12},\bar{8}$) basis is greater than the variational trial function for $J = 2$. Because of the incomplete optimization of the nonlinear parameters in the variational trial function [10], a notional error bound of 10% was attributed to these cross sections. Consequently, the CC($\overline{12},\bar{8}$) cross sections should be adopted as the preferred cross-section set.

Partial and total cross sections for ground-state positronium formation for several incident energies are presented in Table III. The discrepancy between the CC($\bar{6},\bar{6}$) and variational calculation for the $J = 0$ wave has been largely removed by the use of the larger CC($\overline{12},\bar{8}$) basis. For both the $J = 0$ and $J = 1$ partial waves, the agreement between the CC($\overline{12},\bar{8}$) and variational cross sections is excellent. The largest difference between the two calculations occurs for the $J = 1$ wave at $k = 0.7225$ Ry and is only $0.006\pi a_0^2$. This close agreement does not extend to the $J = 2$ cross section. Since a theoretical uncertainty of 10% is attributed to the variational calculation and the [CC($\bar{3},\bar{3}$), CC($\bar{6},\bar{6}$), and CC($\overline{12},\bar{8}$)] calculations show a reasonable degree of convergence, we conclude that present calculation is more accurate for this partial wave.

At energies above the hydrogen $n = 2$ threshold, other excitation processes are possible. Since the main emphasis of this work is to present elastic, positronium, and total cross sections, separate cross sections are not reported for these other transitions. In the energy range to 1.0 Ry, they make a minor contribution to the summed positronium and total cross sections.

In Fig. 1, the summed elastic cross section from zero to the ionization threshold is shown. Also shown is the total cross section, which is the sum total of all elastic and inelastic processes (including positronium formation). In preparing these graphs, we have avoided doing calculations at energies located close to resonances since a detailed description of the cross section would involve some massive

TABLE III. Ground-state positronium-formation cross sections (in units of πa_0^2) for the $J = 0$, 1, and 2 partial waves. The summed cross sections are also given.

Energy (Ry)	0.5041	0.5625	0.64	0.7225
Model				
		$J = 0$		
CC($\bar{3},\bar{3}$)[a]	0.283^{-2}	0.317^{-2}	0.329^{-2}	0.354^{-2}
CC($\bar{6},\bar{6}$)[a]	0.349^{-2}	0.382^{-2}	0.428^{-2}	0.506^{-2}
CC($\overline{12},\bar{8}$)	0.415^{-2}	0.436^{-2}	0.490^{-2}	0.567^{-2}
Variational[b]	0.41^{-2}	0.44^{-2}	0.49^{-2}	0.58^{-2}
		$J = 1$		
CC($\bar{3},\bar{3}$)[a]	0.244^{-1}	0.349	0.474	0.548
CC($\bar{6},\bar{6}$)[a]	0.262^{-1}	0.364	0.485	0.562
CC($\overline{12},\bar{8}$)	0.266^{-1}	0.366	0.483	0.567
Variational[b]	0.27^{-1}	0.365	0.482	0.561
		$J = 2$		
CC($\bar{3},\bar{3}$)[a]	0.628^{-3}	0.290	0.794	1.085
CC($\bar{6},\bar{6}$)[a]	0.664^{-3}	0.311	0.843	1.139
CC($\overline{12},\bar{8}$)	0.682^{-3}	0.320	0.859	1.159
Variational[b]	0.62^{-3}	0.335	0.812	1.057
		Total		
CC($\bar{3},\bar{3}$)[a]	0.0279	0.677	1.563	2.35
CC($\bar{6},\bar{6}$)[a]	0.0304	0.716	1.639	2.46
CC($\overline{12},\bar{8}$)	0.0314	0.729	1.663	2.512

[a]Reference [12].
[b]Variational [10].

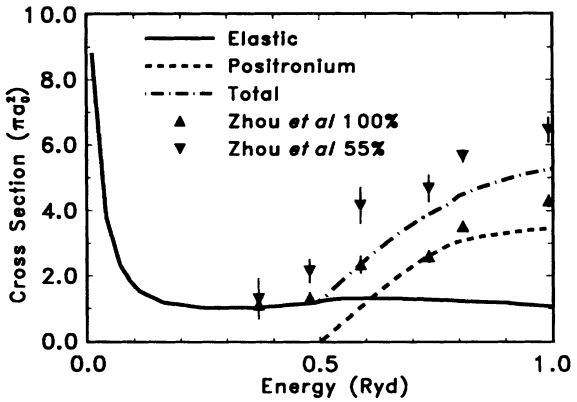

FIG. 1. Cross sections (in πa_0^2) for elastic scattering, the summed cross section to the Ps(1s), Ps(2s), and Ps(2p) states, and the total cross section for positron-hydrogen scattering. The total cross sections of the Detroit group, Zhou *et al.* [20], are also depicted.

calculations. The dominant contributions to the total cross section come from ground-state positronium formation and elastic scattering. While the positronium-formation cross section shown in Fig. 1 includes Ps formation in the Ps(2s) and Ps(2p) levels, these states contribute only 2%–3% to the total Ps formation at the energy of 1.0 Ry.

The only experiments germane to the present calculations are the measurements of the positronium-formation cross section by the Bielefeld-Brookhaven Collaboration [18,19] and the total-cross-section measurements of the Detroit group [20]. The Bielefeld-Brookhaven Collaboration observes a maximum in the positronium cross section of $(3.39 \pm 0.20)\pi a_0^2$ at 15 eV. Given that their experimental energy resolution was 2.8 eV, this cross section is consistent with the present calculation. Two sets of total-cross-section data were presented by the Detroit group, one set assuming 100% dissociation of the H_2 target and another set assuming 55% dissociation of the H_2 target. Both of these cross sections are shown in Fig. 1. Our cross sections are consistent with the experiment although the error tolerances are large.

To conclude, we have presented high-accuracy elastic, positronium-formation, and total cross sections for energies below the ionization threshold. For the $J = 0$ and $J = 1$ partial waves, phase shifts below the Ps threshold and cross sections in the Ore gap agree with previous variational calculations [1,2,10] and demonstrate the accuracy of the present calculations. Extending the calculations to the higher partial waves, we have computed cross sections for elastic scattering and positronium formation up to the ionization threshold. We estimate the theoretical uncertainty associated with the quoted total cross sections for elastic scattering and positronium formation to be less than 5% in this energy range and regard the present cross sections as the benchmark for future theoretical and experimental work.

We would like to thank the Detroit and Bielefeld-Brookhaven groups for making their data available to us in tabular form.

*Electronic address: j_mitroy@bligh.ntu.edu.au
†Electronic address: berge@atsibm.murdoch.edu.au
‡Electronic address: stelbovi@atsibm.murdoch.edu.au

[1] A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, Phys. Rev. A **3**, 1328 (1971).
[2] A. K. Bhatia, A. Temkin, and H. Eiserike, Phys. Rev. A **9**, 219 (1974).
[3] R. L. Armstead, Phys. Rev. **171**, 91 (1968).
[4] C. Schwartz, Phys. Rev. **124**, 1468 (1961).
[5] D. Register and R. T. Poe, Phys. Lett. **51A**, 431 (1975).
[6] U. Roy and P. Mandal, J. Phys. B **23**, L55 (1990); U. Roy and P. Mandal, Phys. Rev. A **48**, 2952 (1993).
[7] J. W. Humberston and J. B. Wallace, J. Phys. B **5**, 1138 (1972).
[8] J. R. Winick and W. P. Reinhardt, Phys. Rev. A **18**, 910 (1978).
[9] K. Higgins, P. G. Burke, and H. R. J. Walters, J. Phys. B **23**, 1345 (1990).
[10] J. W. Humberston, Can. J. Phys. **60**, 591 (1982); J. Phys. B **17**, 2353 (1984); C. J. Brown and J. W. Humberston, J. Phys. B **18**, L401 (1985).
[11] B. J. Archer, G. A. Parker, and R. T. Pack, Phys. Rev. A **41**, 1303 (1990).
[12] J. Mitroy, J. Phys. B **26**, 4861 (1993).
[13] J. Mitroy, Aust. J. Phys. **46**, 751 (1993).
[14] K. Higgins and P. G. Burke, J. Phys. B **24**, L343 (1991).
[15] J. Mitroy and A. T. Stelbovics, J. Phys. B **27**, L59 (1994).
[16] J. Mitroy and A. T. Stelbovics, J. Phys. B **27**, 3257 (1994).
[17] K. Higgins and P. G. Burke, J. Phys. B **26**, 4269 (1993).
[18] W. Sperber, D. Becker, K. G. Lynn, W. Raith, A. Schwab, G. Sinapius, G. Spicher, and M. Weber, Phys. Rev. Lett. **68**, 3690 (1992).
[19] M. Weber, A. Hofmann, W. Raith, W. Sperber, F. Jacobsen, and K. G. Lynn, Hyperfine Interact. (to be published).
[20] S. Zhou, W. E. Kauppila, C. K. Kwan, and T. S. Stein, Phys. Rev. Lett. **72**, 1443 (1994).