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Large Basis Calculation of Positron–Hydrogen Scattering at Low Energies

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Abstract

Calculations of low energy positron–hydrogen scattering using the close coupling approach are reported at low energies. The channel space includes nine physical hydrogen and positronium states and in addition twelve hydrogen and positronium pseudo-states. For energies below the positronium formation threshold, phase shifts are reported for $J = 0$ to 6 and are believed to have an absolute accuracy of 0·0015 radian or better. Elastic scattering and positronium formation cross sections in the Ore gap for the $J = 0$ and $J = 1$ partial waves are essentially identical with previous variational calculations. Total elastic and positronium formation cross sections are reported at incident energies below the ionisation threshold. Cross sections for the excitation of the H(n=2), H(n=3) and Ps(n=2) levels are also reported over a restricted energy range, and the total reaction cross section has been computed and compared with experiment.

1. Introduction

The positron–hydrogen system along with the electron–hydrogen system form two of the fundamental three-body systems of atomic physics. From both the experimental and theoretical perspective, the positron–hydrogen system is a much more difficult proposition than the electron–hydrogen system.

The difficulties on the experimental side arise from the fact that the positrons required for a beam can only be formed as a result of nuclear decay process or in a particle accelerator (Lynn and Jacobsen 1994). The little data on positron–hydrogen scattering are the result of recent experiments and have relatively large experimental uncertainties. The positronium formation cross section has been measured by the Bielefeld–Brookhaven collaboration (Sperber *et al.* 1992; Weber *et al.* 1994). The total scattering cross section has been measured by the Detroit group (Zhou *et al.* 1994). Two separate experiments have reported ionisation cross sections (Spicher *et al.* 1990; Jones *et al.* 1993).

The theoretical difficulties arise because a genuine rearrangement process, namely positronium formation, is possible during a positron–hydrogen collision. The problems inherent in treating collision systems without a single centre of symmetry result in computations which are much more time-consuming than those occurring for electron–hydrogen scattering. As a consequence, there have been relatively few calculations of positron–hydrogen scattering that have treated positronium formation with any degree of realism. This is especially true in the

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intermediate energy range. However, at energies below the ionisation threshold, a number of different techniques have been exploited to do some accurate calculations. In kinematic regions with only a few open channels, variational techniques have frequently been used to compute the most accurate cross sections for electron–atom scattering. This is also true for positron–hydrogen scattering and there have been a number of calculations of phase shifts in the elastic scattering region below the positronium formation threshold at 6·8 eV (Schwartz 1961; Armstead 1968; Bhatia *et al.* 1971, 1974; Humberston and Wallace 1972; Humberston and Campeanu 1980; Register and Poe 1975). Of these calculations, the phase shifts of Bhatia *et al.* (1971, 1974) are generally regarded as the most accurate for the $J = 0$ and $J = 1$ partial waves.

At these energies it is also possible to ignore the positronium channels altogether and a number of authors have used the close coupling (CC) method with the positronium channels omitted from the CC expansion. When properly implemented, this approach has given results comparable in accuracy with the variational calculations. Despite its title, the convergent close coupling (CCC) method of Bray and Stelbovics (1993) appears to have yielded phase shifts that have a lesser degree of convergence than the moment T-matrix method (Winick and Reinhardt (1978) and the R-matrix method (Higgins *et al.* 1990). One characteristic of these single centre CC calculations is that they converge to the exact phase shift at a much slower rate than the equivalent calculation upon the electron–hydrogen system.

In the Ore gap (the energy region between 6·8 and 10·2 eV), positronium formation in the ground state is possible and it is necessary to include this channel explicitly in the calculation if accurate results are to be obtained. A series of high quality variational calculations for the elastic and positronium formation cross sections have been performed by Humberston and collaborators (Humberston 1982, 1984, 1986; Brown and Humberston 1985) for the $J = 0$, $J = 1$ and $J = 2$ partial waves. While the cross sections reported for the $J = 0$ and $J = 1$ waves are regarded as being close to exact, the calculations for the $J = 2$ partial wave did not achieve the same degree of precision and the $J = 2$ cross sections are expected to be accurate to only 10%. The hyperspherical close coupling method has also been applied to this problem (Archer *et al.* 1990; Igarashi and Toshima 1994; Zhou and Lin 1994). Archer *et al.* (1990) reported cross sections for the $J = 0$ partial wave that agree with those of Humberston (1984) to within $0{\cdot}01\ a_0^2$. The calculations of Zhou and Lin (1994) reported cross sections for the $J = 0$, 1, 2 and 3 partial waves but were restricted to the Ore gap. Igarashi and Toshima (1994) have reported cross sections over a more extensive energy range and also for the higher partial waves.

Most recently, techniques have been developed to evaluate the positronium formation matrix elements (Hewitt *et al.* 1990; Mitroy 1993*a*; Higgins and Burke 1993; McAlinden *et al.* 1994) as they arise in the context of the close coupling (CC) method. It is notable that while a number of different groups have now reported CC calculations, only two different techniques have been used to solve the CC equations; these are the moment space T-matrix method and the R-matrix method. Since the CC method can be used at all energies and for all partial waves with equal facility, the ability to solve the CC equations is expected to lead to a major improvement of our understanding of the dynamics

of the positron–hydrogen system. The seminal work using the T-matrix method was by Hewitt *et al.* (1990) who used a Gaussian representation of the atomic and positronium orbitals to expedite the evaluation of the rearrangement matrix elements for hydrogen and positronium orbitals with $l \leq 1$. However, they used an incorrect expression for some of the matrix elements (Hewitt 1993) and this resulted in inaccuracies in their reported cross sections. The first calculation in the R-matrix method was reported by Higgins and Burke (1991) for the coupled static model [i.e. the H(1s) and Ps(1s) levels are included in CC expansion]. Since then, more substantial calculations have been reported (Higgins and Burke 1993; McAlinden *et al.* 1994) with the calculation by McAlinden *et al.* (1994) including a total of nine hydrogen and nine positronium levels. One of the more important features of these calculations is undoubtedly the agreement achieved by the R-matrix calculations of McAlinden *et al.* (1994) and the T-matrix calculations of Mitroy and Stelbovics (1994*a*, 1994*b*). This represents the first instance of two calculations by two different groups achieving detailed agreement in the intermediate energy region for a realistic calculation.

An improved method of computing the partial wave Born matrix elements needed for the momentum space T-matrix method has been developed by Mitroy (1993*a*). A partial factorisation of positronium formation matrix element leads to an expression that is sufficiently efficient to be suitable for large scale computations. Unlike previous methods, the analysis in this case has resulted in a completely general expression for the matrix element irrespective of the angular momenta of the hydrogen and positronium states. With this expression for the matrix element, it is now possible to regard calculations having both hydrogen and positronium levels in the CC expansion as a routine rather than a heroic calculation. For instance, cross sections on a fine energy grid between 0 and 4 Ryd for the positron excitation of hydrogen and positronium formation have been computed in a model containing the H(1s, 2s, 2p) and Ps(1s, 2s, 2p) levels of hydrogen (Mitroy and Stelbovics 1994*a*, 1994*b*). At low energies, a pilot calculation (Mitroy 1993*b*), coupling six hydrogen-type states and six positronium-type states was able to reproduce all features of the best variational calculations to an overall accuracy of 10%. Subsequent to this, a more extensive calculation was performed at about two hundred and fifty different energies (Mitroy and Ratnavelu 1995) to provide a detailed description of the cross sections (including resonance structure) for incident positron energies from 0 to 1 Ryd. An even larger calculation (Mitroy *et al.* 1994), coupling twelve hydrogen-type states and eight positronium-type states was able to reproduce the best variational cross sections to within 2%.

The purpose of the present work is to present a unified treatment of positron–hydrogen scattering that predicts the elastic and positronium formation cross sections to an accuracy of 2% or better in the energy region below the ionisation threshold. The channel space includes a total of thirteen hydrogen-type states and a total of eight positronium-type states. Some of the previous variational calculations have achieved a level of accuracy of better than 1%, but these calculations are restricted to individual partial waves and confined to narrow energy ranges. The present calculations are performed over a wider energy range and there is no limitation upon the number of partial waves. Since the exact H(n=1, 2, 3) and Ps(n=1, 2) states are explicitly included in the CC expansion the model should yield cross sections which are close to exact for energies below the H(n=3) threshold.

Table 1. Specification of the hydrogen and positronium pseudo-states for the CC($\overline{13}, \overline{8}$) basis
The binding energy (in Hartrees) and coefficients of each state are under the appropriate headings

Hydrogen				
n_j	λ_j	$\overline{4s}$	$\overline{5s}$	
ϵ_i		0.285071	3.360078	
1	1.0000	-0.880380	5.035776	
1	0.5000	0.770678	0.586804	
1	2.5000	-1.334853	-1.016374	
1	0.3333	0.373400	0.229197	
2	0.3333	-1.293496	-0.793962	
3	0.3333	1.180795	0.724785	
2	1.4000	-1.505926	-7.933458	
2	1.4000	2.834330	3.209116	
		$\overline{4p}$	$\overline{5p}$	$\overline{6p}$
ϵ_i		0.022551	0.417801	2.455066
2	0.5000	-3.391823	-3.126660	2.425453
2	0.3333	-1.538524	-0.864435	0.607034
3	0.3333	2.106711	1.183676	-0.831216
2	1.6000	1.199831	3.457616	-7.185614
3	1.0000	-2.537881	-9.849359	13.835397
3	1.0000	5.232385	9.830081	-10.487478
		$\overline{4d}$		
ϵ_i		0.347227		
3	0.3333	-0.269253		
3	1.2000	1.035614		
		$\overline{4f}$		
ϵ_i		0.420		
4	1.2000	1.0		

Positronium			
n_j	λ_j	$\overline{3s}$	$\overline{4s}$
ϵ_i		0.016859	0.869757
1	0.5000	6.902090	10.522848
1	0.2500	-9.535000	-8.671815
2	0.2500	5.190136	3.871364
1	0.8000	-1.544201	-5.567323
		$\overline{3p}$	$\overline{4p}$
ϵ_i		0.004353	0.364696
2	0.2500	-2.012991	-1.503006
2	0.5000	0.272067	-2.780138
3	0.5000	1.996587	3.941771
		$\overline{3d}$	
ϵ_i		0.160000	
3	0.6000	1.000000	

2. Details of the Calculations

The primary purpose of the calculations reported in this paper is to generate benchmark cross sections for positron–hydrogen scattering in the low energy region. To generate a set of cross sections close to convergence requires a close coupling calculation using a larger basis than used in any previous calculation. To assess the degree of convergence requires comparison of a sequence of successively larger calculations. These calculations are:

CC(3, 3). This basis includes the physical H(1s), H(2s), H(2p) and Ps(1s), Ps(2s) and Ps(2p) levels. This basis entailed no new calculations since cross sections and phase shifts have been reported previously (Mitroy and Stelbovics 1994*a*).

CC($\overline{3}$, $\overline{3}$). This basis includes the hydrogen and positronium ground states. The pseudo H($\overline{2s}$), H($\overline{2p}$), Ps($\overline{2p}$) and Ps($\overline{2p}$) levels were chosen to be identical to those used in an R-matrix calculation (Higgins and Burke 1993) of the positron–hydrogen system. Once again, the calculations with this basis have already been done (Mitroy 1993*b*).

CC($\overline{6}$, $\overline{6}$). This basis includes the lowest three physical levels of hydrogen (1s, 2s, 2p) and well as three pseudo-levels ($\overline{3s}$, $\overline{3p}$ and $\overline{3d}$). The lowest three physical states of positronium (1s, 2s, 2p) and three pseudo-positronium levels were included ($\overline{3s}$, $\overline{4s}$ and $\overline{3p}$). Extensive calculations with this basis have been reported previously (Mitroy 1993*b*; Mitroy and Ratnavelu 1995).

CC($\overline{9}$, $\overline{9}$). This basis includes the lowest three physical levels of hydrogen (1s, 2s, 2p) and well as six pseudo-levels ($\overline{3s}$, $\overline{4s}$, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$ and $\overline{4d}$). The lowest three physical states of positronium (1s, 2s, 2p) and six pseudo-positronium levels ($\overline{3s}$, $\overline{4s}$, $\overline{3p}$, $\overline{4p}$, $\overline{3d}$ and $\overline{4d}$) were included. Calculations with this model have been reported by McAlinden *et al.* (1994).

CC($\overline{13}$, $\overline{8}$). This basis includes the lowest six physical levels of hydrogen (1s, 2s, 2p, 3s, 3p and 3d) and well as seven pseudo-levels ($\overline{4s}$, $\overline{5s}$, $\overline{4p}$, $\overline{5p}$, $\overline{6p}$, $\overline{4d}$ and $\overline{4f}$). The lowest three physical states of positronium (1s, 2s, 2p) and five pseudo-positronium levels were included ($\overline{3s}$, $\overline{4s}$, $\overline{3p}$, $\overline{4p}$ and $\overline{3d}$). This basis is almost the same as that used in an earlier calculation (Mitroy *et al.* 1994) using a CC($\overline{12}$, $\overline{8}$,) basis, the only difference being that the hydrogen $l = 1$ pseudo-state basis has been increased in size and modified. Given that the CC($\overline{12}$, $\overline{8}$) and CC($\overline{13}$, $\overline{8}$) basis sets are almost the same, the present calculations should be as regarded as representing an improved version of this earlier calculation. The present calculations were performed with an improved program on a more powerful computer, so the calculations were done at more energies, carried through to higher partial waves energies, and some of the numerical tolerances made more stringent. Under such circumstances, the results reported in this paper should be regarded as superseding those published by Mitroy *et al.* (1994). The results of the earlier CC($\overline{12}$, $\overline{8}$) calculations have not been tabulated in the present paper, since for the most part the differences between the CC($\overline{12}$, $\overline{8}$) and CC($\overline{13}$, $\overline{8}$) phase shifts and cross section are gratifyingly small, being less than 1% in almost all cases.

The generation of pseudo-states that achieve a high degree of convergence for the smallest possible close coupling expansion is something of a black art so only an overview of the manner in which the pseudo-state basis was developed will be given. The present basis was optimised by doing calculations in the elastic scattering region (at $k = 0{\cdot}5\ a_0^{-1}$) and changing the specifications of

the pseudo-states until the $J = 0$ and the $J = 1$ phase shifts achieved a local maximum. Trying to refine the basis past this stage runs into a number of complications. For instance the specification of the $\overline{3d}$ orbital that maximises the phase shift for the $J = 0$ wave (short range correlations) is not the same as the $\overline{3d}$ orbital that maximises the phase shift for the $J = 3$ wave (long range correlations). This was the chief reason for extending the $l = 1$ hydrogen basis used in the earlier CC($\overline{12}, \overline{8}$) calculation (Mitroy *et al.* 1994). The p-basis was partially optimised to give a maximum phase shift for the $J = 0$ wave, but as a result, the effective dipole polarisability of the hydrogen ground state was slightly smaller than the exact polarisability ($4 \cdot 5a_0^3$). By extending the dimensionality of the pseudo p-basis, it was possible to optimise the basis for short range correlations while maintaining the exact polarisability. The physical and pseudo-states are written as a linear combination of normalised Slater-type orbitals (STOs), i.e.

$$\psi_i(r) = \sum_j c_j (2n_j)!/(2\lambda_j)^{2n_j+1}]^{\frac{1}{2}}\, r^{n_j} \exp(-\lambda_j r)\,.$$

Only the pseudo-states for the CC($\overline{13}, \overline{8}$) basis set need to be given in Table 1 since the specification for the physical states are known.

The close coupling as applied to the present problem does have one potential drawback. The close coupling method expands the wave function in terms of a set of hydrogenic and positronium states, viz.

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_\alpha \Psi_\alpha(\boldsymbol{r}_1)\, F_\alpha(\boldsymbol{r}_2) + \sum_\beta \Phi_\beta(\boldsymbol{\rho})\, G_\beta(\boldsymbol{R})\,.$$

In this equation, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the electron and positron coordinates, $\boldsymbol{\rho}$ and $\boldsymbol{R}$ are the relative and centre-of-mass positronium coordinates, and $\Psi_\alpha(\boldsymbol{r}_1)$ and $\Phi_\beta(\boldsymbol{\rho})$ represent the hydrogenic and positronium states. In order to obtain a converged T-matrix, it necessary to let the sets of hydrogenic states, i.e. $\{\Psi_\alpha(\boldsymbol{r}_1)\}$, and positronium states, i.e. $\{\Phi_\beta(\boldsymbol{\rho})\}$, expand towards a complete set. As the separate basis sets for the hydrogen and positronium levels are increased in size, it is possible for the basis consisting of both sets of states to become overcomplete. Under these circumstances the set of Lippmann–Schwinger equations can become unstable if the basis becomes sufficiently large (Adhikari and Kowalski 1991; Bransden and Noble 1994). In numerical terms, the resulting linear equations become linearly dependent and this manifests itself in the solution vector losing numerical precision. By monitoring the conditions numbers returned upon solution of the linear equations, it is possible to determine those instances in which the computed T-matrix elements might be lacking in precision. In these instances, the calculation was usually repeated with slightly different quadrature mesh parameters. Another manner in which instabilities can reveal themselves is in the behaviour of the partial cross sections as a function of energy. Random errors in the on-shell T-matrix will result in partial cross sections that are not smooth as a function of energy. An examination of the energy dependence of the partial cross sections for $J \geq 1$ did not reveal any fluctuations at a level greater than

0·1%. Hence, there seem to be no reliability problems associated with the higher partial waves. However, fluctuations were noted in the $J = 0$ positronium cross section. The magnitude of the fluctuations appeared to have an upper limit of $0{\cdot}0002\pi a_0^2$ and were only noticeable because of the small size ($\sim 0{\cdot}005\ \pi a_0^2$) of this particular cross section.

For most of the calculations reported in this paper, 40 and 48 point Gaussian quadrature meshes were used to discretise the kernel of the integral equation. When performing calculations with large numbers of basis states, the complicated structures in the kernel make it desirable to have a reasonably dense quadrature mesh. Calculations were done at more than 200 energies below the H(n=3) threshold to map out the resonance structures associated with the H(n=2) and Ps(n=2) thresholds. Above the Ps(n=2) threshold, calculations were only performed at three energies, 0·90, 0·95 and 1·00 Ryd.

Not all the calculations associated with this work were done with the fully coupled CC($\overline{13}, \overline{8}$) model. The time taken to evaluate the positronium matrix elements increases for the higher partial waves. At the same time, the influence that the positronium channels exert on the elastic channel diminishes in importance. Accordingly the T-matrix elements were computed with the following sequence of calculations. For the lowest partial waves no approximations (apart from the purely numerical ones inherent in any calculation) were made to compromise the accuracy of the CC($\overline{13}, \overline{8}$) calculations. For an intermediate set of J-values, the matrix elements connecting the hydrogen states to the positronium states were omitted and the two manifolds were decoupled from each other in the CC($\overline{13}, \overline{8}$) calculations. For the highest partial waves, a modified effective range formula (MERT) (Mitroy and Ratnavelu 1995; O'Malley *et al.* 1962; O'Malley 1963) was used to compute the approximate T-matrix elements for the diagonal channels. The specifics of the calculation changed as the energy increased. For example, at an energy of $E = 0{\cdot}49$ Ryd, the positronium matrix elements were included up to $J = 6$; for $J = 7 \rightarrow 16$ the CC equations were solved with no coupling between hydrogenic and positronium channels; and for values of $J > 17$ MERT formulae were used. This is not expected to lead to a major error in the integrated cross section since the $J = 6$ phase shift at 0·49 Ryd with the Ps-matrix elements is 0·00336 rad and 0·00331 rad without the Ps-matrix elements. At an energy of 1·0 Ryd, the Lippmann–Schwinger equation was solved for the CC($\overline{13}, \overline{8}$) basis up to $J = 12$, the positronium matrix elements were omitted from the calculation for $J = 13$ to 32, and the MERT formulae used thereafter. The omission of the positronium matrix elements from the calculation will to lead to any significant difference in the cross section at this energy as well.

The integrated cross sections shown in the figures required interpolations for the higher partial waves. Only the $J = 0$, 1 and 2 partial cross sections were computed on the very fine energy grid needed to characterise the resonances. The $J = 3$ and higher partial waves were computed at a total of about 60 different energies. The final integrated cross sections that are depicted in the figures were computed by merging the different sets of partial cross sections and interpolating the partial cross sections for $J \geq 3$ onto the energy mesh used for the $J = 0$, 1 and 2 partial waves. Since the cross sections for the higher partial waves were quite smooth as a function of energy, this procedure is expected to be sufficiently accurate.

Table 2. The $J = 0$ phase shifts for positron–hydrogen scattering as a function of momentum

	k (a_0^{-1})						
Method	0.1	0.2	0.3	0.4	0.5	0.6	0.7
CCC[a]	0.145	0.183	0.163	0.119	0.062	0.0034	-0.531
IERM[b]	0.142	0.180	0.159	0.111	0.055	-0.002	
IERM[c]	0.148	0.187	0.167	0.118	0.062	0.004	
CC($\overline{6}$,$\overline{6}$)[d]	0.1404	0.1767	0.1558	0.1105	0.0536	-0.0044	-0.0588
CC($\overline{13}$,$\overline{8}$)	0.1474	0.1868	0.1667	0.1191	0.0621	0.0031	-0.0518
Variational[e]	0.1483	0.1877	0.1677	0.1201	0.0624	0.0039	-0.0512
Variational[f]	0.1460	0.1849	0.1649	0.1172	0.0593	-0.00003	-0.0569
Schwinger[g]	0.1473	0.1869	0.1671	0.1202	0.0631	0.0041	-0.0514

[a]Convergent Close Coupling, Bray and Stelbovics (1993)
[b]Intermediate Energy R-Matrix (no extrapolation), Higgins *et al* (1990)
[c]Intermediate Energy R-Matrix (with extrapolation), Higgins *et al* (1990)
[d]Close coupling, Mitroy and Ratnavelu (1995)
[e]Bhatia *et al* (1971)
[f]Register and Poe *et al* (1975)
[g]Roy and Mandal (1990, 1993)

Table 3. The $J = 1$ phase shifts for positron–hydrogen scattering as a function of momentum

	k (a_0^{-1})						
Method	0.1	0.2	0.3	0.4	0.5	0.6	0.7
CCC[a]	0.0088	0.0325	0.0649	0.0986	0.128	0.151	0.171
IERM[b]	0.009	0.032	0.064	0.096	0.123	0.144	0.163
IERM[c]	0.009	0.033	0.066	0.102	0.132	0.156	0.185
CC($\overline{6}$,$\overline{6}$)[d]	0.00876	0.0321	0.0639	0.0974	0.1267	0.1496	0.1732
CC($\overline{13}$,$\overline{8}$)	0.00887	0.0327	0.0657	0.1002	0.1306	0.1542	0.1788
Variational[e]	0.0094	0.0338	0.0665	0.1016	0.1309	0.1547	0.1799
Variational[f]	0.005	0.030	0.063	0.097	0.128	0.146	0.169
Schwinger[g]	0.0088	0.0333	0.0658	0.1012	0.1318	0.1534	0.1739

[a]Convergent Close Coupling, Bray and Stelbovics (1993)
[b]Intermediate Energy R-Matrix (no extrapolation), Higgins *et al* (1990)
[c]Intermediate Energy R-Matrix (with extrapolation), Higgins *et al* (1990)
[d]Close coupling, Mitroy and Ratnavelu (1995)
[e]Bhatia *et al* (1974)
[f]Register and Poe *et al* (1975)
[g]Roy and Mandal (1990, 1993)

3. Phase Shifts in the Elastic Scattering Region

In Tables 2 and 3, phase shifts for the $J = 0$ and $J = 1$ partial waves are presented at incident energies below the Ps formation threshold, and compared with previous calculations. The purpose of this comparison is not to demonstrate that the present phase shifts are the most accurate set of phase shifts, rather it is to demonstrate that the present calculation gives phase shifts which are comparable to the best calculations and so give an indication of the accuracy of cross sections at energies above the positronium formation threshold. The numerical uncertainty of the present $J = 0$ phase shifts is of the order of $0{\cdot}0005$ rad. Most of this uncertainty is caused by a set of linear equations that are approaching linear dependence as discussed in the previous section. These problems did not arise for the $J = 1$ (and higher partial waves) and the numerical precision for these phase shifts is of the order of $0{\cdot}0001$ rad or better. Comparison of the CC($\overline{13}, \overline{8}$) and CC($\overline{6}, \overline{6}$) phase shifts reveals that the CC($\overline{13}, \overline{8}$) phase shifts are larger (as expected) indicating that the present calculation is closer to convergence. The scattering length was estimated by applying a MERT analysis (Buckman and Mitroy 1989) to the low energy s-wave phase shifts. The present scattering length of $-(2{\cdot}08 \pm 0{\cdot}02)a_0$ is close to that obtained ($-2{\cdot}103a_0$) by Bhatia *et al.* (1971).

The variational phase shifts of Bhatia *et al.* (1971, 1974) for the $J = 0$ and $J = 1$ partial waves are generally regarded as the most accurate. The maximum difference between the present calculation and the variational phase shifts of Bhatia *et al.* (1971, 1974) is less than $0{\cdot}0015$ rad for the $J = 0$ and $J = 1$ partial waves. It should be noted that the $J = 1$ phase shift of Bhatia *et al.* (1974) at $k = 0{\cdot}1a_0^{-1}$ is not the result of an explicit variational calculation. Rather it was computed using a polarisation formula for the phase shift (O'Malley *et al.* 1962; O'Malley 1963) and is not as accurate as the present phase shift.

Both sets of intermediate energy R-matrix (IERM) phase shifts (Higgins *et al.* 1990) are quoted, those resulting from their largest calculation, and those obtained by extrapolating to an infinite L^2 basis set containing an infinite number of partial waves. The moment T-matrix method of Winick and Reinhardt (1978) has a number of similarities with the IERM, and gives similar phase shifts, so these results are not tabulated. The Harris–Nesbet variational (Register and Poe 1975) and the Schwinger variational methods (Roy and Mandal 1990, 1993) have also been applied to the calculation of phase shifts for the $J = 2$ and higher partial waves.

The present phase shifts probably represent the preferred set of phase shifts for $J \geq 2$. At the lowest energies, the CC($\overline{13}, \overline{8}$) and CC($\overline{6}, \overline{6}$) phase shifts are almost identical indicating a high degree of convergence. However, as the energy increases and the positron penetrates deeper into the atomic interior, the differences between the phase shifts reveal the importance of having a larger basis to allow for short range interactions. For the $J = 2$ wave, the present phase shifts are larger than those of Register and Poe (1975), as they are for the $J = 0$ and $J = 1$ partial waves. The present series of calculations are obviously consistent with those of the IERM method, although we suspect the present phase shifts may be more precise. The agreement with the convergent close coupling phase shifts of Bray and Stelbovics (1993) is not so good at the higher momenta of $0{\cdot}6$ and $0{\cdot}7$ a_0^{-1}, with discrepancies of about 5% being present. One possible reason

for the discrepancy would be an omission by Bray and Stelbovics to investigate the convergence of the CCC method at these momenta. An examination of the phase shifts calculated by the Schwinger variational method reveals that the calculations of Roy and Mandal (1990, 1993) do not appear to have the numerical reliability of the other calculations reported in Table 4. For the $J = 3$ partial wave, they report a phase shift of 0·0133 rad at $k = 0{\cdot}5a_0^{-1}$, which is larger than the IERM and CC($\overline{13}, \overline{8}$) phase shifts of 0·0126 and 0·0125 rad respectively. At $k = 0{\cdot}6a_0^{-1}$, they report a phase shift of 0·0161 rad, which is also significantly different from the IERM and CC($\overline{13}, \overline{8}$) phase shifts of 0·0207 and 0·0198 rad. At momenta close to the positronium threshold (0·6 and $0{\cdot}7a_0^{-1}$), this particular calculation gives some phase shifts which are often 10–20% smaller than those of the present calculation. This may be due to the adoption of a restricted trial function with only four terms. In any case, the phase shifts of Roy and Mandal (1993) are unreliable for the larger angular momenta and should be treated with caution.

The last rows of Table 4 list the integral cross section for a number of different calculations. The differences between the CC($\overline{6}, \overline{6}$) and CC($\overline{13}, \overline{8}$) cross sections are about 5% to 10% for $k = 0{\cdot}1$, 0·2 and 0·3 a_0^{-1} since the integrated cross section is dominated by the s-wave cross section. This difference is reduced when the other partial waves begin to make a larger contribution to the integrated cross section. However, the most accurate cross section is the result of a composite calculation. The phase shifts of Bhatia *et al.* (1971, 1974) were used for the $J = 0$ and $J = 1$ partial waves (with the exception of the $J = 1$ phase shift at $k = 0{\cdot}1$ a_0^{-1}) and the present CC($\overline{13}, \overline{8}$) phase shifts were used for the higher partial waves. The differences of this composite cross section with the CC($\overline{13}, \overline{8}$) cross sections are at the 1% to 2% level. The overall accuracy of this composite cross section is probably at the 1% level or better.

4. Elastic Scattering above the Positronium Threshold

At energies above 0·5 Ryd, the positronium channel opens and inelastic as well as elastic scattering events are possible. Elastic cross sections from the positronium threshold to the ionisation threshold are listed in Table 5. A plot of the $J = 0$, 1 and 2 partial cross sections for elastic scattering from threshold to the ionisation threshold is shown in Fig. 1.

We do not report the R-matrix calculation of the CC($\overline{3}, \overline{3}$) model (Higgins and Burke 1993) in Table 5. Their cross sections were substantially different from those obtained with an identical channel space using the momentum space approach method (Mitroy 1993*b*). Higgins and Burke (1993) match the wave functions in the inner region directly to spherical Bessel functions without taking into account long range couplings in the external region. While the dipole polarisability for hydrogen ground state is small ($4{\cdot}5$ a_0^3), that of the positronium ground state is eight times larger. Under these circumstances, the omission of dipole coupling between the different positronium channels at large distances is most likely the cause of the discrepancy.

One notable feature of Table 5 is the agreement achieved between the CC($\overline{13}, \overline{8}$) calculation and the variational calculations of Humberston and collaborators.

Table 4. Phase shifts for positron–hydrogen scattering for the $J = 2$ to 6 partial waves as a function of incident momentum
The integrated elastic cross sections (in πa_0^2) are given in the last rows

Method	k (a_0^{-1}) 0.1	0.2	0.3	0.4	0.5	0.6	0.7
			J = 2				
CCC[a]	0.0014	0.0055	0.0127	0.0239	0.0389	0.0582	0.0839
IERM[b]		0.005	0.013	0.024	0.039	0.058	
IERM[c]		0.005	0.013	0.025	0.041	0.062	
CC($\overline{6}$,$\overline{6}$)[d]	0.00135	0.00546	0.0127	0.0237	0.0386	0.0580	0.0856
CC($\overline{13}$,$\overline{8}$)	0.00136	0.00551	0.0129	0.0242	0.0397	0.0598	0.0885
Variational[e]	0.0013	0.0054	0.0125	0.0235	0.0389	0.0593	0.0863
Schwinger[f]	0.00131	0.00543	0.01260	0.02348	0.03817	0.05925	0.0870
			J = 3				
CCC[a]	0.0004	0.0018	0.0040	0.0075	0.0121	0.0191	0.0287
IERM[b]		0.0018	0.0040	0.0075	0.0124	0.0200	
IERM[c]		0.0018	0.0040	0.0075	0.0126	0.0207	
CC($\overline{6}$,$\overline{6}$)[d]	0.452^{-3}	0.00179	0.00405	0.00746	0.0124	0.0193	0.0299

CC($\overline{13},\overline{8}$)	0.452^{-3}	0.00180	0.00409	0.00754	0.0126	0.0198	0.0307
Schwinger[f]	0.454^{-3}	0.00178	0.00404	0.00710	0.0133	0.0161	0.0218
			J = 4				
CC($\overline{6},\overline{6}$)[d]	0.205^{-3}	0.816^{-3}	0.00183	0.00328	0.00528	0.00796	0.0118
CC($\overline{13},\overline{8}$)	0.205^{-3}	0.819^{-3}	0.00183	0.00329	0.00530	0.00807	0.0121
Schwinger[f]	0.204^{-3}	0.813^{-3}	0.00188	0.00323	0.00507	0.00746	0.00994
			J = 5				
CC($\overline{13},\overline{8}$)	0.109^{-3}	0.443^{-3}	0.986^{-3}	0.00175	0.00277	0.00410	0.00587
Schwinger[f]	0.109^{-3}	0.436^{-3}	0.987^{-3}	0.00177	0.00273	0.00396	0.00535
			J = 6				
CC($\overline{13},\overline{8}$)	0.633^{-3}	0.266^{-3}	0.593^{-3}	0.00105	0.00165	0.00241	0.00336
Schwinger[f]	0.650^{-4}	0.259^{-3}	0.589^{-3}	0.00105	0.00167	0.00234	0.00326
			$\sigma_{elastic}$				
CC($\overline{6},\overline{6}$)[d]	7.988	3.464	1.690	1.094	0.953	0.966	1.120
CC($\overline{13},\overline{8}$)	8.736	3.787	1.844	1.192	1.026	1.026	1.186
Composite	8.83	3.84	1.872	1.217	1.030	1.031	1.194

[a]Convergent Close Coupling, Bray and Stelbovics (1993)
[b]Intermediate Energy R-Matrix (no extrapolation), Higgins *et al* (1990)
[c]Intermediate Energy R-Matrix (with extrapolation), Higgins *et al* (1990)
[d]Close Coupling, Mitroy and Ratnavelu (1995)
[e]Register and Poe *et al* (1975)
[f]Roy and Mandal (1990, 1993)

Table 5. Elastic cross sections (in units of πa_0^2) for the $J = 0$, 1, 2 and 3 partial waves at six different energies below the ionisation threshold
The summed cross sections are also given

	Energy (Ryd)					
Model	0.5041	0.5625	0.64	0.7225	0.8000	1.0000
			J = 0			
CC(3,3)[a]	0.374	0.397	0.419	0.434	0.441	0.434
CC($\bar{3}$,$\bar{3}$)[b]	0.0511	0.0711	0.0946	0.1157		
CC($\bar{6}$,$\bar{6}$)[c]	0.0324	0.0504	0.0730	0.0937	0.110	0.136
CC($\bar{9}$,$\bar{9}$)[d]			0.071			
CC($\bar{13}$,$\bar{8}$)	0.0258	0.0430	0.0657	0.0849	0.101	0.128
Hypersperical[e]	0.033	0.050	0.076	0.100		
Hypersperical[f]	0.0325	0.0548	0.0838	0.111		0.172
Hypersperical[g]	0.0234	0.0415	0.0637	0.0863		
Variational[h]	0.026	0.043	0.065	0.085		
			J = 1			
CC(3,3)[a]	0.189	0.170	0.134	0.107	0.0864	0.0496
CC($\bar{3}$,$\bar{3}$)[b]	0.627	0.570	0.490	0.428		
CC($\bar{6}$,$\bar{6}$)[c]	0.756	0.684	0.589	0.517	0.451	0.310
CC($\bar{9}$,$\bar{9}$)[d]			0.624			
CC($\bar{13}$,$\bar{8}$)	0.802	0.726	0.626	0.551	0.481	0.331
Hypersperical[f]	0.748	0.650	0.532	0.449		0.237
Hypersperical[g]	0.810	0.720	0.608	0.528		
Variational[h]	0.789	0.724	0.622	0.547		

			J = 2			
CC(3,3)[a]	0.118	0.158	0.178	0.176	0.171	0.144
CC($\bar{3}$,$\bar{3}$)[b]	0.265	0.349	0.382	0.374		
CC($\bar{6}$,$\bar{6}$)[c]	0.319	0.418	0.455	0.448	0.435	0.370
CC($\bar{9}$,$\bar{9}$)[d]			0.482			
CC($\overline{13}$,$\bar{8}$)	0.341	0.446	0.484	0.477	0.463	0.392
Hyperspherical[f]	0.304	0.376	0.389	0.366		0.280
Hyperspherical[g]	0.330	0.401	0.420	0.391		
Variational[h]	0.323	0.403	0.423	0.413		
			J = 3			
CC(3,3)[a]	0.0221	0.0303	0.0439	0.0544	0.0597	0.0641
CC($\bar{3}$,$\bar{3}$)[b]	0.0469	0.0634	0.0901	0.110		
CC($\bar{6}$,$\bar{6}$)[c]	0.0544	0.0737	0.105	0.127	0.138	0.144
CC($\overline{13}$,$\bar{8}$)	0.0575	0.0781	0.111	0.135	0.147	0.154
Hyperspherical[f]	0.0471	0.0541	0.0675	0.0761		0.0841
Hyperspherical[g]	0.0676	0.0739	0.0853	0.0950		
			Total			
CC(3,3)[a]	0.710	0.763	0.786	0.787	0.778	0.717
CC($\bar{3}$,$\bar{3}$)[b]	1.004	1.071	1.081	1.059		
CC($\bar{6}$,$\bar{6}$)[c]	1.177	1.246	1.248	1.221	1.177	1.019
CC($\overline{13}$,$\bar{8}$)	1.242	1.313	1.316	1.285	1.239	1.068
Hyperspherical[f]	1.16	1.15	1.08	1.01		0.803

[a]Mitroy and Stelbovics (1994b)
[b]Mitroy (1993b).
[c]Mitroy and Ratnavelu (1995).
[d]McAlinden *et al* (1994).
[e]Hyperspherical CC, Archer *et al* (1990).
[f]Hyperspherical CC, Igarashi and Toshima (1994).
[g]Hyperspherical CC, Zhou and Lin (1994).
[h]Variational, Humberston (1984), Brown and Humberston (1985).

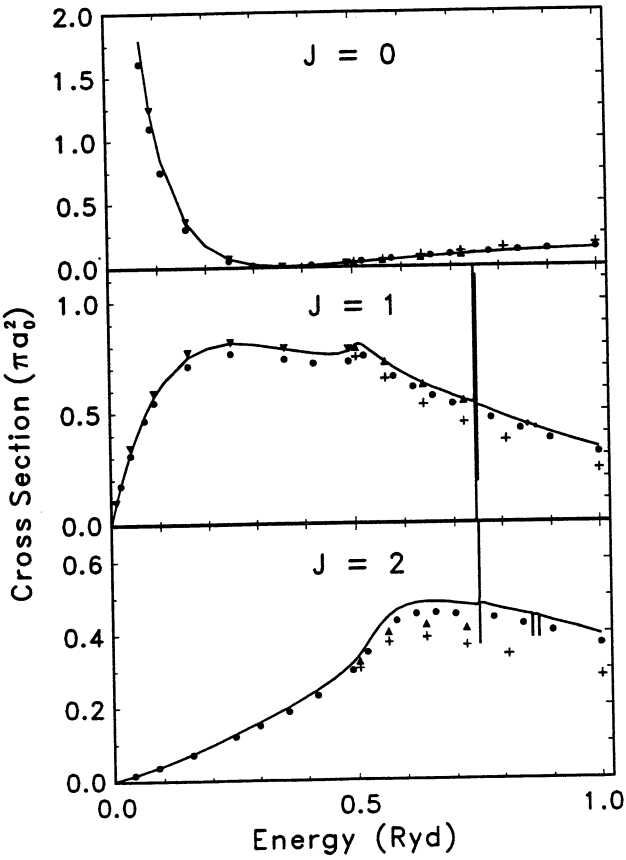

Fig. 1. The $J = 0$, 1 and 2 partial cross sections (in πa_0^2) for elastic scattering (curves). Partial cross sections from the CC($\overline{6}, \overline{6}$) model (dots), Bhatia *et al.* (1971, 1974) (inverted triangles), Humberston and co-workers (triangles) and Igarashi and Toshima (1994) (pluses) are also shown.

For the $J = 0$ wave, the decrease in the elastic cross section as the basis is enlarged from the CC($\overline{6}, \overline{6}$) to the CC($\overline{13}, \overline{8}$) basis is sufficient to achieve excellent agreement with the cross sections of Humberston (1984). The apparently good agreement between the CC($\overline{6}, \overline{6}$) model and the hyperspherical CC calculation of Archer *et al.* (1990) was purely coincidental.

The situation is repeated for the $J = 1$ wave. As the size of the CC basis was increased, the partial cross sections increased until they were very close to the variational cross sections of Brown and Humberston (1985). From the plot shown in Fig. 1, the agreement between the CC($\overline{13}, \overline{8}$) and variational cross section sets could hardly be better. The maximum difference between the two cross sections for the $J = 1$ wave is only $0{\cdot}013\ \pi a_0^2$.

The quality of agreement achieved for the $J = 2$ wave is not quite so good. There are differences of $0{\cdot}06\pi a_0^2$ between the CC($\overline{13}, \overline{8}$) and variational cross

sections. The present CC($\overline{13}, \overline{8}$) cross section is probably the preferred cross section. Evidence for the superiority of the CC($\overline{13}, \overline{8}$) calculation is provided by the agreement with the R-matrix calculation in the CC($\overline{9}, \overline{9}$) model (McAlinden *et al.* 1994). Although only one energy point ($E = 0{\cdot}64$ Ryd) has been reported, the two cross sections ($0{\cdot}482$ and $0{\cdot}484\ \pi a_0^2$) are almost identical. Furthermore, at an energy of $0{\cdot}5041$ Ryd the CC($\overline{13}, \overline{8}$) cross section is $0{\cdot}341\ \pi a_0^2$ and the variational cross section is $0{\cdot}323\ \pi a_0^2$. Since a larger cross section implies a larger phase shift, this indicates that the variational flexibility of the CC($\overline{13}, \overline{8}$) basis is greater than the trial wave function adopted by Brown and Humberston. Furthermore, as the calculation size is increased from CC($\overline{3}, \overline{3}$) to CC($\overline{6}, \overline{6}$) and then to CC($\overline{13}, \overline{8}$), the elastic cross sections also tended to increase. Given that the CC($\overline{13}, \overline{8}$) cross sections are already larger than the variational cross sections, and that the numerical reliability of the present calculations has been validated, it must be surmised that the present calculation represents an improvement upon the variational calculation. It should be noted that Brown and Humberston (1985) have attached a notional error bound of 10% to their $J = 2$ cross section, and the maximum difference between the two cross sections sets is about 13%.

Cross sections for the $J = 3$ and higher partial waves show a systematic trend to increase as the size of the channel space is enlarged. The difference between the CC($\overline{6}, \overline{6}$) and CC($\overline{13}, \overline{8}$) cross sections gives an indication of the degree of the convergence of the largest calculation. Since there have been no accurate variational calculations for these partial waves, the present CC($\overline{13}, \overline{8}$) cross sections represent the state of the art.

The hyperspherical close coupling cross sections of Igarashi and Toshima (1994) are in reasonable agreement with the CC($\overline{13}, \overline{8}$) cross sections for the lower partial waves. The quality of the agreement deteriorates for the higher partial waves. A brief examination of Table II of Igarashi and Toshima (1994) shows that the partial cross sections behave quite erratically for the larger angular momenta. This is to be expected since the computational difficulties associated with the hyperspherical method increase as the angular momentum increases. On the other hand, the calculations of Zhou and Lin (1994) appear to suffer from a different problem at large angular momentum. They use a hyperspherical radius of $29{\cdot}3\ a_0$, which is much smaller than adopted by Archer *et al.* (1990) and Igarashi and Toshima (1994). Under these circumstances it is not clear that a proper treatment can be made of the long-range dipole couplings that occur in positron–atom scattering. The omission of these couplings is expected to particularly important for the high partial waves since the centrifugal barrier will keep the positron away from the hydrogen atom and the long-range interactions assume a greater relative importance.

Since it is not altogether clear whether the variational cross sections of Humberston and collaborators are to be preferred over the CC($\overline{13}, \overline{8}$) cross sections, it was not appropriate to compute a composite cross section by combining partial cross sections from the two different calculations. The present CC($\overline{13}, \overline{8}$) cross section should be adopted as the preferred cross section and the differences with the variational cross sections for the $J = 0$ and $J = 1$ partial can be used to give an indication of the uncertainty.

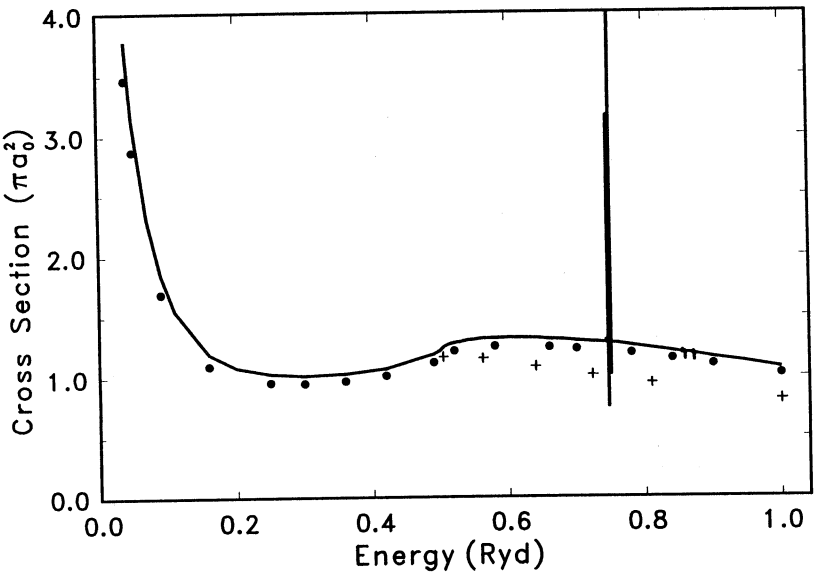

Fig. 2. Elastic cross sections (in πa_0^2) for positron–hydrogen scattering at energies below the ionisation threshold. Besides the present CC($\overline{13},\overline{8}$) calculation (curve), cross sections for the CC($\overline{6},\overline{6}$) model (dots) and from Igarashi and Toshima (1994) (pluses) are also shown.

The integrated elastic cross section for energies up to the ionisation threshold is depicted in Fig. 2. The overall accuracy of the integrated cross section is probably about 2% or better. It is likely that the residual errors in the calculation will result in the computed cross section being slightly smaller than the actual cross section.

Resonances associated with the H(n=2) and Ps(n=2) thresholds reveal themselves as structures just below these two thresholds. The widths of these resonances are very narrow, and the structures in the elastic cross section would be difficult to observe in an experiment. A major improvement in the technology of positron beam physics will be required before these resonances can be detected experimentally.

5. Positronium Formation

Partial and total cross sections for ground state positronium formation for energies up to the ionisation threshold are presented in Table 6. The $J = 0$, 1 and 2 partial cross sections for positronium formation are shown in detail in Fig. 3.

One of the pleasing features of Table 6 is the tendency for the series of successively larger close coupling calculations to show signs of convergence as the model space is enlarged. The differences between the CC($\overline{6},\overline{6}$), R-matrix CC($\overline{9},\overline{9}$) and CC($\overline{13},\overline{8}$) cross sections are small for all the partial waves. However, at some energies, the R-matrix CC($\overline{9},\overline{9}$) cross sections are 10% or 20% different from the present results. Given the overall level of consistency between the CC($\overline{13},\overline{8}$) cross sections and the variational cross sections it would appear that occasional numerical instability is present in the R-matrix calculation.

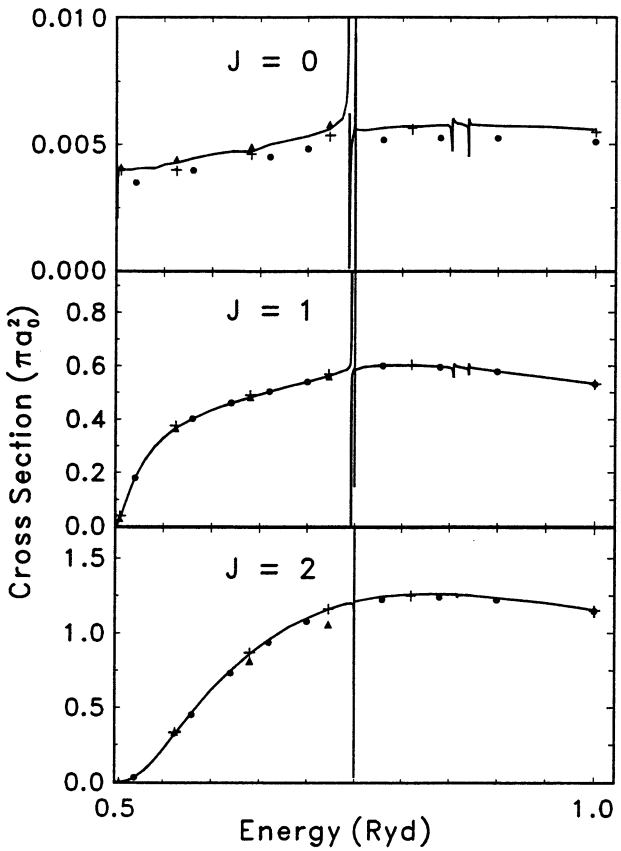

Fig. 3. The $J = 0$, 1 and 2 partial cross sections (in πa_0^2) for the e^++H(1s) $\rightarrow$ Ps(1s)+p positronium formation reaction. The cross sections of the CC($\overline{6}, \overline{6}$) model (dots), Humberston and collaborators (triangles) and Igarashi and Toshima (1994) (pluses) are also shown.

The discrepancies between the close coupling cross sections and variational cross sections for the $J = 0$ and $J = 1$ partial waves diminish as the size of the calculation increases. For the $J = 0$ partial wave, the maximum difference between the CC($\overline{13}, \overline{8}$) cross section and the variational cross section of Humberston (1984) is only $0{\cdot}0002\ \pi a_0^2$. For the $J = 1$ partial wave, the maximum difference between the two cross section sets occurs at 0·7225 Ryd and is only $0{\cdot}002\ \pi a_0^2$. Looking at Fig. 3, it is seen that the agreement of the $J = 0$ and $J = 1$ partial cross sections with those of Humberston and collaborators could hardly be any better. The small irregularities present in energy dependence of the $J = 0$ partial cross section are the result of poorly conditioned linear equations that arise because the combined basis of hydrogen and positronium target states is becoming increasingly linearly dependent.

The present CC($\overline{13}, \overline{8}$) model gives the most accurate cross sections yet computed for the $J = 2$ and higher partial waves. The sequence of successively larger close coupling calculations, CC($\overline{6}, \overline{6}$), CC($\overline{9}, \overline{9}$) and CC($\overline{13}, \overline{8}$), show a tendency to converge to cross sections that are 5–10% different from those given by Brown

Table 6. Ground state positronium formation cross sections (in units of πa_0^2) for the $J = 0$, 1, 2, 3 partial waves at six different energies below the ionisation threshold

The summed cross sections are also given

	Energy (Ryd)					
Model	0.5041	0.5625	0.64	0.7225	0.800	1.0000
			J = 0			
CC(3,3)[a]	0.181^{-3}	0.142^{-4}	0.426^{-4}	0.881^{-4}	0.779^{-4}	0.212^{-4}
CC($\overline{3}$,$\overline{3}$)[b]	0.283^{-2}	0.317^{-2}	0.329^{-2}	0.354^{-2}		
CC($\overline{6}$,$\overline{6}$)[c]	0.349^{-2}	0.382^{-2}	0.439^{-2}	0.506^{-2}	0.522^{-2}	0.509^{-2}
CC($\overline{9}$,$\overline{9}$)[d]	0.33^{-2}	0.30^{-2}	0.41^{-2}	0.47^{-2}		
CC($\overline{13}$,$\overline{8}$)	0.405^{-2}	0.427^{-2}	0.472^{-2}	0.560^{-2}	0.572^{-2}	0.559^{-2}
Hyperspherical[e]	0.34^{-2}	0.38^{-2}	0.43^{-2}	0.49^{-2}		
Hyperspherical[f]	0.404^{-2}	0.398^{-2}	0.462^{-2}	0.535^{-2}		0.548^{-2}
Hyperspherical[g]	0.407^{-2}	0.421^{-2}	0.473^{-2}	0.553^{-2}		
Variational[h]	0.41^{-2}	0.44^{-2}	0.49^{-2}	0.58^{-2}		
			J = 1			
CC(3,3)[a]	0.172^{-1}	0.294	0.405	0.460	0.482	0.409
CC($\overline{3}$,$\overline{3}$)[b]	0.244^{-1}	0.349	0.474	0.548		
CC($\overline{6}$,$\overline{6}$)[c]	0.262^{-1}	0.366	0.484	0.562	0.601	0.531
CC($\overline{9}$,$\overline{9}$)[d]	0.46^{-1}	0.376	0.485	0.573		
CC($\overline{13}$,$\overline{8}$)	0.266^{-1}	0.366	0.483	0.563	0.603	0.534
Hyperspherical[f]	0.366^{-1}	0.376	0.490	0.570		0.532
Hyperspherical[g]	0.23^{-1}	0.370	0.480	0.552		
Variational[h]	0.27^{-1}	0.365	0.482	0.561		

			J = 2			
CC(3,3)[a]	0.435^{-3}	0.199	0.575	0.809	0.893	0.851
CC($\bar{3}$,$\bar{3}$)[b]	0.628^{-3}	0.290	0.794	1.085		
CC($\bar{6}$,$\bar{6}$)[c]	0.664^{-3}	0.312	0.841	1.139	1.235	1.147
CC($\bar{9}$,$\bar{9}$)[d]	0.85^{-3}	0.373	0.871	1.170		
CC($\overline{13}$,$\bar{8}$)	0.682^{-3}	0.320	0.859	1.158	1.256	1.153
Hyperspherical[f]	0.934^{-3}	0.334	0.866	1.16		1.15
Hyperspherical[g]	0.345^{-3}	0.254	0.770	1.031		
Variational[h]	0.62^{-3}	0.335	0.812	1.057		
			J = 3			
CC(3,3)[a]	0.333^{-5}	0.0248	0.185	0.415	0.563	0.710
CC($\bar{3}$,$\bar{3}$)[b]	0.42^{-5}	0.0332	0.251	0.556		
CC($\bar{6}$,$\bar{6}$)[c]	0.43^{-5}	0.0348	0.264	0.583	0.774	0.942
CC($\overline{13}$,$\bar{8}$)	0.44^{-5}	0.0356	0.270	0.596	0.788	0.953
Hyperspherical[f]	0.573^{-5}	0.0382	0.276	0.592		0.946
Hyperspherical[g]	0.363^{-4}	0.0133	0.188	0.484		
			Total			
CC(3,3)[a]	0.0179	0.520	1.198	1.812	2.20	2.55
CC($\bar{3}$,$\bar{3}$)[b]	0.0279	0.677	1.563	2.35		
CC($\bar{6}$,$\bar{6}$)[c]	0.0304	0.719	1.635	2.46	2.952	3.368
CC($\overline{13}$,$\bar{8}$)	0.0313	0.728	1.660	2.49	3.00	3.40
Hyperspherical[f]	0.0416	0.755	1.68	2.50		3.36

[a]Mitroy and Stelbovics (1994b).
[b]Mitroy (1993b).
[c]Mitroy and Ratnavelu (1995).
[d]McAlinden *et al* (1994).
[e]Hyperspherical CC, Archer *et al* (1990).
[f]Hyperspherical CC, Igarashi and Toshima (1994).
[g]Hyperspherical CC, Zhou and Lin (1994).
[h]Variational, Humberston (1984), Brown and Humberston (1985).

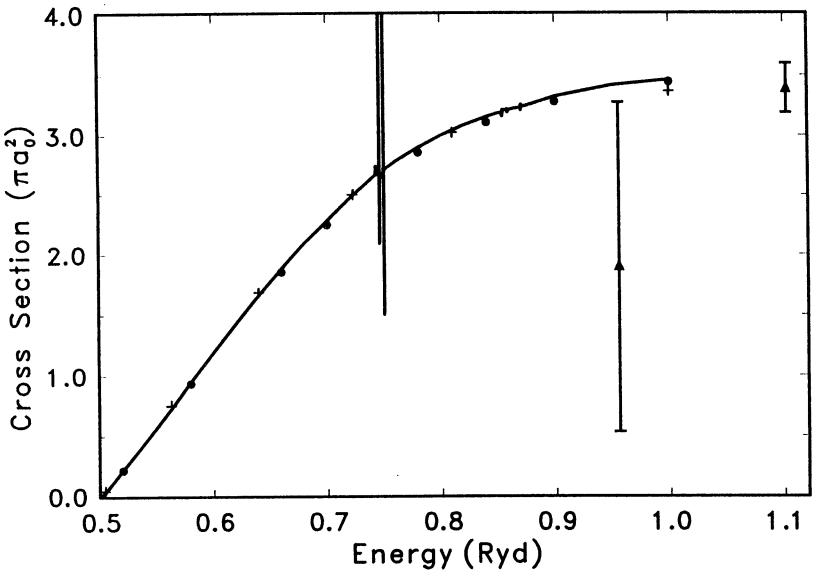

Fig. 4. Cross sections (in πa_0^2) for positronium formation [obtained by summing the Ps(1s), Ps(2s) and Ps(2p) cross sections]. The present CC($\overline{13}, \overline{8}$) cross section (curve) is depicted with the CC($\overline{6}, \overline{6}$) cross section (dots) and the cross section of Igarashi and Toshima (1994) (pluses) [includes only Ps(1s) formation]. There are two data points (triangles) from the Bielefeld—Brookhaven experiment (Sperber *et al.* 1992; Weber *et al.* 1994).

and Humberston (1985) for the $J = 2$ partial wave. As mentioned previously, Brown and Humberston (1985) have stated that the probable error in their $J = 2$ partial cross section is about 10% which is compatible with the differences with the CC($\overline{13}, \overline{8}$) cross section. Given that the differences between the CC($\overline{6}, \overline{6}$) and CC($\overline{13}, \overline{8}$) cross sections are about 2%, it seems likely that the overall error in the present calculation will be of similar size.

Comparison with the hyperspherical close coupling calculations of Igarashi and Toshima (1994) gives additional confidence in the overall accuracy of the present cross section set. The hyperspherical calculation appears to give partial cross sections that are numerically more reliable for positronium formation than for elastic scattering. The overall quality of the agreement between two cross section sets is good for all the partial waves listed in Table 6. From Fig. 3, it can be seen that the hyperspherical cross sections for the $J = 1$ and $J = 2$ partial waves are almost identical to the present cross sections. The other hyperspherical CC calculation (Zhou and Lin 1994) shows discrepancies with the present cross sections and the cross sections of Igarashi and Toshima (1994) for the higher partial waves. The most likely cause for the discrepancy is the small size of the hyper-radius adopted by Zhou and Lin (1994).

Integrated cross sections for positronium formation in its ground state are tabulated in the last rows of Table 6. The cross section depicted in Fig. 4 includes contributions from Ps formation in the Ps(2s) and Ps(2p) states above the Ps(n=2) threshold. It is noticeable that an overall degree of consistency

exists between the C($\overline{6},\overline{6}$), CC($\overline{13},\overline{8}$) and hyperspherical calculation (Igarashi and Toshima 1994). The spread between the three sets of cross sections is less than $0{\cdot}04\,\pi a_0^2$. On the basis of the information given in Table 6 and depicted in Figs 3 and 4, it would seem reasonable to ascribe an uncertainty of about 2% to the positronium cross section as given by the CC($\overline{13},\overline{8}$) calculation.

6. Excitation of the H(n=2), H(n=3) and Ps(n=3) Levels

Cross sections for excitation of the $n = 2$ and $n = 3$ levels of hydrogen and cross sections for electron transfer to the $n = 2$ levels of positronium are given in Table 7. While these cross sections are probably the most accurate that have so far been computed for these transitions, there has been no systematic attempt to determine the degree to which these cross sections have converged with respect to the purely numerical aspects of the calculation since the main focus of this article is upon the elastic and ground state positronium formation cross sections. As the T-matrices for these other transitions are automatically generated when the Lippmann–Schwinger equation is solved and there is very little information available for these transitions, the cross sections are reported in this paper. The agreement between the CC($\overline{6},\overline{6}$) and CC($\overline{13},\overline{8}$) cross sections for excitation of the H(2s) and H(2p) levels would indicate that these cross sections at least should be reasonably accurate. This is apparent from Fig. 5 where the integrated cross sections for the H(2s) and H(2p) levels are compared with the CC($\overline{6},\overline{6}$) cross sections at a few select energies. The CC($\overline{6},\overline{6}$) cross sections are very close to the present cross section for all the points shown in Fig. 5.

This agreement does not hold for the excitation cross sections to the Ps(2s) and Ps(2p) levels. Given that the Ps(n=2) and H(n=3) states have almost the same excitation energies and roughly the same spatial extent, it is not surprising that the CC($\overline{13},\overline{8}$) model gives cross sections which are very different from the CC($\overline{6},\overline{6}$) model cross sections.

The energy region between the Ps(n=2) and H(n=3) thresholds is likely to have some very complicated structures. This is certainly the case for the hyperspherical CC cross sections of Archer *et al.* (1990). There has been no attempt to investigate this particular energy region in any detail since it would be necessary to increase the size of the Gaussian mesh used to discretise the integral equation.

The total reaction cross section is shown in Fig. 6 and compared with experimental data from the Detroit group (Zhou *et al.* 1994). This cross section is dominated by the elastic cross section and the ground state Ps-formation cross section. At the highest energy, the Ps(1s) cross sections constitutes 65% of the reaction cross section with the elastic cross section accounting for 20%. Even if the remaining contributions to the reaction cross section have larger relative uncertainties, these uncertainties will not greatly increase the uncertainty in the reaction cross section. A very conservative estimate of the accuracy of the non-resonant part of the total reaction cross section would be that present cross section was accurate to better than 5% with the uncertainty being smallest at low energies and largest at energies close to the ionisation threshold. The interpretation of the comparison with experiment is subject to a number of complications. First, there is some uncertainty regarding the efficiency of dissociation of H_2 molecules into H atoms. Two sets of experimental data are given, one

Table 7. Cross sections (in units of πa_0^2) for excitation of the H(n=2), H(n=3) and Ps(n=2) states at selected energies below the ionisation threshold

	Final State						
	H(2s)	H(2p)	Ps(2s)	Ps(2p)	H(3s)	H(3p)	H(3d)
				E = 0.80 Ryd			
CC(3,3)[a]	0.0531	0.0461					
CC($\bar{6}$,$\bar{6}$)[b]	0.0820	0.0702					
CC($\overline{13}$,$\bar{8}$)	0.0846	0.0746					
				E = 0.85 Ryd			
CC(3,3)[a]	0.103	0.0942					
CC($\bar{6}$,$\bar{6}$)[b]	0.159	0.147					
CC($\overline{13}$,$\bar{8}$)	0.165	0.156					
				E = 0.90 Ryd			
CC(3,3)[a]	0.137	0.153	0.00643	0.00847			
CC($\bar{6}$,$\bar{6}$)[b]	0.210	0.232	0.00942	0.0125			
CC($\overline{13}$,$\bar{8}$)	0.215	0.242	0.00861	0.0112	0.00157	0.00372	0.00255

			E = 0.95 Ryd				
CC(3,3)[a]	0.164	0.212	0.0142	0.0180			
CC($\bar{6}$,$\bar{6}$)[b]	0.251	0.318	0.0188	0.0272			
CC($\bar{\bar{1}}\bar{3}$,$\bar{8}$)	0.259	0.327	0.0137	0.0224	0.00701	0.00886	0.00474
			E = 1.00 Ryd				
CC(3,3)[a]	0.184	0.279	0.0232	0.0298			
CC($\bar{6}$,$\bar{6}$)[b]	0.284	0.407	0.0309	0.0433			
CC($\bar{\bar{1}}\bar{3}$,$\bar{8}$)	0.284	0.420	0.0266	0.0328	0.0161	0.0187	0.00787

[a]Mitroy and Stelbovics (1994b).
[b]Mitroy and Ratnavelu (1995).

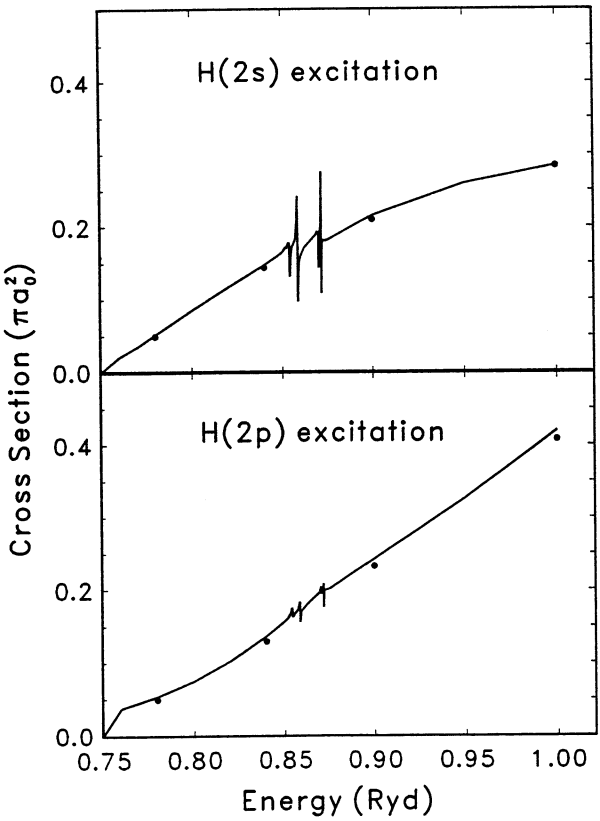

Fig. 5. Cross sections (in πa_0^2) for positron impact excitation of the H(2s) and H(2p) states (—). Also shown are the H(2s) and H(2p) cross sections from the CC($\overline{6},\overline{6}$) model (•).

set assuming molecular hydrogen is dissociated into atomic hydrogen with 100% efficiency, and the other set assuming the dissociation is 55% efficient. Second, the experiment is an attenuation experiment and is unable to discriminate against small angle elastic scattering. Knowledge of the entrance aperture of the positron detector (Zhou *et al.* 1994) enabled a corrected reaction cross section to be computed by subtracting the contribution from small angle elastic scattering from the present cross section. It is seen from Fig. 6 that this results in the reaction cross section decreasing by amounts from 0·45 to 0·65 a_0^2. At the two lowest energies (5·0 and 6·5 eV), the corrected cross sections lie outside the error tolerances of the experimental data. This is not cause for concern since a number of different calculations get essentially the same phase shifts in this energy region. Given that the positron–hydrogen reaction cross section experiment is extremely difficult to measure, the discrepancy is probably of experimental origin.

7. Resonance Positions and Widths

It was about thirty years ago that Mittleman (1966) showed that the degeneracy of the H(2s) and H(2p) levels leads to an infinite series of resonances

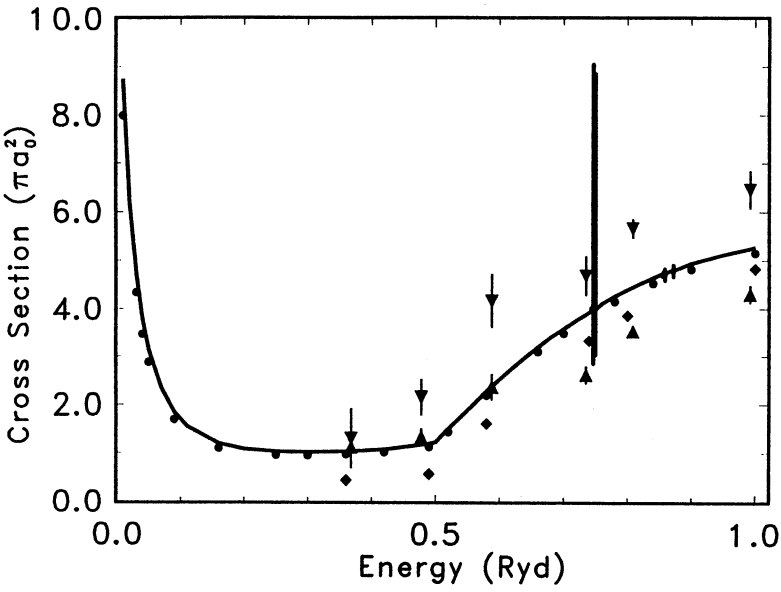

Fig. 6. Total reaction cross sections (in πa_0^2) for positron–hydrogen scattering (curve). The experimental data of the Detroit group are assumed to be either 100% dissociation (triangles) or 55% dissociation (inverted triangles). The present cross sections corrected for small angle elastic scattering are shown at a discrete number of points (diamonds). Total reaction cross sections from the CC($\overline{6},\overline{6}$) model (dots) are also plotted.

for positron–hydrogen scattering at energies below the H(n=2) channels. Since then a number of resonances associated with the H(n=2), H(n=3) and Ps(n=2) thresholds have been identified (Doolen 1978; Pelikan and Klar 1983; Ho and Greene 1987; Ho 1990, 1992; Archer *et al.* 1990; Mitroy and Stelbovics 1994*b*; Mitroy and Ratnavelu 1995). The most comprehensive investigation was that of Mitroy and Ratnavelu (1995), however, this calculation did not have the precision of some of the previous calculations (Doolen 1978; Ho and Greene 1987; Ho 1990, 1992) and the resonance positions of the CC($\overline{6},\overline{6}$) model were quite different from the accurate variational results. This was due to the omission of the exact H(n=3) levels from the basis. The Ps(n=2) and H(n=3) levels have roughly the same binding energies and same range in coordinate space so the interaction between these two sets of levels is expected to be strong.

The present resonance positions and widths were computed using a technique due to Meetz (1962). The details of this method in the context of electron–atom and positron–hydrogen scattering are described elsewhere (Stelbovics and Bransden 1989; Mitroy and Stelbovics 1994). The use of the more extensive CC($\overline{13},\overline{8}$) basis has resulted in resonance positions and widths (Table 8) in improved agreement with the previous variational results. The position and width ($0{\cdot}74296$ and $1{\cdot}56^{-4}$ Ryd) of the lowest $J = 0$ resonance is in much better agreement with the high precision calculation of Ho (1992) ($0{\cdot}74269$ and $1{\cdot}33^{-4}$ Ryd). No significance should be attached to the fact that the present position is almost identical with

Table 8. Positions and widths (in Ryd) for resonances of the e^+–H system

Resonances occur for the $J = 0$, 1, 2 partial waves. The resonance parameters reported in other calculations are written in a (ϵ_r,Γ) notation. The calculations by a number of groups do not assume an infinitely heavy proton and their resonance energies have been adjusted to be compatible with the present energy scale

	CC($\overline{13}$,$\overline{8}$)		CC($\overline{6}$,$\overline{6}$)[g]		Other Calculations
J	ϵ_r	Γ	ϵ_r	Γ	
0	0.74294	1.56^{-4}	0.74370	1.80^{-4}	(0.74414,5.1^{-5})[a], (0.74294)[b], (0.74298)[d], (0.74275,1.33^{-4})[h]
0	0.74964	7.9^{-6}	0.74967	9.3^{-6}	(0.74983, < 2.0^{-5})[h]
0	0.85206	5.9^{-4}	0.85658	7.0^{-4}	(0.85773,5.5^{-4})[a], (0.8501)[b], (0.84972,6.70^{-4})[c], (0.84968,6.68^{-4})[f]
0	0.86960	2.2^{-4}	0.87039	2.3^{-4}	(0.87066,1.76^{-4})[a], (0.8687)[b], (0.86834,3.26^{-4})[c], (0.8684,1.74^{-4})[f]
1	0.74609	1.58^{-5}	0.74670	1.27^{-5}	(0.74696,3.8^{-5})[a], (0.74589,1.62^{-5})[e]
1	0.74987	4.5^{-7}	0.74989	4.1^{-7}	
1	0.85421	5.1^{-4}	0.85868	5.1^{-4}	(0.85982,4.1^{-3})[a], (0.85182,5.94^{-4})[e]
1	0.87041	1.92^{-4}	0.87112	1.58^{-4}	(0.87137,1.26^{-3})[a], (0.86927,3.34^{-4})[e]
2	0.74990	2.1^{-6}	0.74994	7.8^{-7}	(0.74992,1.10^{-6})[a]
2	0.85850	3.1^{-4}	0.86285	2.5^{-4}	(0.86387,1.73^{-4})[a]
2	0.87187	8.4^{-5}	0.87235	6.6^{-5}	(0.87265,4.5^{-5})[a]

[a]CC(3,3) model, Mitroy and Stelbovics (1994b).
[b]Hyperspherical CC, Archer *et al* (1990).
[c]Ho and Greene (1987).
[d]Pelikan and Klar (1983).
[e]Ho (1990).
[f]Doolen, (1978).
[g]Mitroy and Ratnavelu (1995).
[h]Ho (1992).

those of Pelikan and Klar (1987) and Archer *et al.* (1990) (0·74294 and 0·74298 Ryd respectively) since it is unlikely either of those calculations had achieved convergence. Similarly the position and width of the lowest $J = 1$ resonance (0·74609 and $1{\cdot}58^{-5}$ Ryd) is in much better agreement with the calculation of Ho (1990) (0·74589 and $1{\cdot}62^{-5}$ Ryd). Although final convergence has not been achieved, it is gratifying that the trend shows the position and width converging to the high precision estimates as the calculation size increases.

For the resonances associated with the Ps(n=2) threshold there are larger differences between the present resonance energies and those of previous complex coordinate calculations (up to 0·0025 Ryd) notwithstanding the fact that the CC($\overline{13}$, 8) model is a clear improvement over the CC($\overline{6}, \overline{6}$) model. In lieu of a larger calculation any explanation of this difference is at best speculative, but one possible cause for the relatively poor convergence of the resonance positions is the omission of the physical H(n=4) and Ps(n=3) levels from the channel space.

The only previous calculations for the $J = 2$ resonances have been performed using smaller channel spaces within the context of the present method. Given the comments of the previous paragraph, we would expect the positions of the resonances associated with the Ps(n=2) threshold to be too high by about 0·001 to 0·002 Ryd. The widths should be accurate to better than ±20%.

8. Conclusions

Calculations in the elastic scattering region indicate that the present calculations are capable of reproducing the $J = 0$ and $J = 1$ phase shifts of the best variational calculation (Bhatia *et al.* 1971, 1974) to within 0·0015 rad. For $J = 2$ and the higher partial waves, the present phase shifts represent the most precise set of phase shifts that have so far been computed. The aim of the calculations in this energy region was not to surpass the accuracy of the variational calculations, rather it was to give an indication of the accuracy of the present model calculation for situations for which highly precise variational calculations have not been performed. Nevertheless if a benchmark set of cross sections are required for this energy region, it is recommended that the phase shifts of Bhatia *et al.* (1971, 1974) be used for the $J = 0$ and $J = 1$ waves (with the exception of the $J = 1$ phase at $k = 0{\cdot}1a_0^{-1}$), and the present phase shifts be used for the higher partial waves.

The cross sections for positronium formation in the Ore gap have duplicated those of the previous variational calculations (Humberston 1982, 1984; Brown and Humberston 1985) for the $J = 0$ and $J = 1$ partial waves. For the $J = 2$ and higher partial waves, the present cross sections represent the best that have so far been computed and should be regarded as providing a benchmark for future calculations. By extending the calculations of high precision cross sections to the higher partial waves, we have been able to determine a set of positronium cross sections that have an overall precision of better than 2%. At energies above the Ps($n = 2$) threshold the Ps(2s) and Ps(2p) cross sections were added to the total Ps-formation cross section for comparison with the experimental data of the Bielefeld–Brookhaven collaboration (Sperber *et al.* 1992; Weber *et al.* 1994). At the highest energy, the computed Ps-formation cross section of $3{\cdot}46\ \pi a_0^2$ is consistent with the maximum in the observed cross section of $3{\cdot}39{\pm}0{\cdot}20\ \pi a_0^2$ at

15 eV when the experimental energy resolution of 2·8 eV is taken into account (Weber *et al.* 1994).

The present calculation was to some extent the best calculation that could be done with the present method and supersedes the CC($\overline{12}, \overline{8}$) cross sections reported by Mitroy *et al.* (1994). Since the present calculations did exhibit numerical instabilities associated with an overcomplete basis, it is not clear whether it would be worth while to increase the size of the calculation. The gain in accuracy from having an enlarged channel space could be offset by the increased difficulties in solving the resulting set of linear equations. However, given that the overall accuracy of our resulting integrated cross sections was of the order of a couple of per cent it is now desirable to try and describe the behaviour of the positron–hydrogen system at energies above the ionisation threshold. As this will entail different procedures to select the CC channel space, the existence of the present low energy cross sections will provide a valuable benchmark. It is anticipated that the results of attempts to calculate the ionisation cross section will be reported in near the future.

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