

# Close Coupling Theory of Positron–Hydrogen Scattering

*J. Mitroy*

Centre for Atomic, Molecular and Surface Physics,  
School of Mathematical and Physical Sciences,  
Murdoch University, Murdoch, W.A. 6150, Australia.  
Permanent address: Faculty of Science,  
Northern Territory University, G.P.O. Box 40146,  
Casuarina, N.T. 0811, Australia.

## *Abstract*

The equations for positron–hydrogen scattering are written as a set of coupled momentum-space Lippmann–Schwinger equations. An explicit expression for the positronium formation matrix element that is suitable for large-scale computation is derived. Elastic and positronium formation cross sections are obtained in the coupled static model as a validation of the method. Calculations at energies below the hydrogen  $n = 2$  threshold are used to study the convergence of observable quantities with increasing numbers of physical H and Ps states. At higher energies, a series of calculations including multiple hydrogen and positronium states are performed over the energy range from 1·0 to 4·0 Ryd. Cross sections for elastic scattering, excitation of the 2s and 2p hydrogen levels and positronium formation in the 1s, 2s and 2p levels are reported.

## 1. Introduction

The positron–hydrogen system, along with the electron–hydrogen system, is one of the fundamental three-body systems in atomic physics. A great deal of attention has been focused upon electron–hydrogen recently, particularly with respect to the convergence of pseudo-state expansions in the intermediate energy region (Bray and Stelbovics 1992; Scholz *et al.* 1988). However, at present our knowledge of the positron–hydrogen system is not nearly so comprehensive. Undoubtedly, one contributing reason for this is the relative paucity of data on positron–atom scattering, and in particular positron–hydrogen scattering. Another contributing factor is the difficulty in providing a proper formulation of the positronium formation process.

As a broad generalisation, calculations of positron–atom collisions can be divided into two classes. At energies below the ionisation threshold, variational techniques have been exploited to do a number of nearly exact calculations. These have been performed on a number of simple systems such as hydrogen and helium (Bhatia *et al.* 1971, 1974; Humberston 1986; Armour and Humberston 1991). However, most calculations of positron–atom scattering in the intermediate energy range have used prescriptions based upon ease of execution. Provided positronium formation is ignored, the modification of an electron–atom code to handle positron–atom scattering is trivial. The sign of the direct interaction

is reversed and the exchange interaction is omitted (e.g. Bransden *et al.* 1985; Ward *et al.* 1989). The omission of the positronium formation channels does pose questions about the overall accuracy of these approaches.

More recently, the first attempts at applying the intermediate energy  $R$ -matrix method to positron–hydrogen scattering (Higgins *et al.* 1990; Higgins and Burke 1991) and the first fully coupled calculations of positron–hydrogen scattering using a realistic channel space have been made (Hewitt *et al.* 1990, 1991). The major innovation that made the calculations of the Daresbury group possible was the representation of the atomic and positronium wave functions by Gaussians. These calculations represent improvements over previous works, where positronium formation was treated using perturbation theory (Mandal *et al.* 1975; Saha and Roy 1984; Basu and Ghosh 1988), or alternatively the close coupling equations were solved with a restricted number of channels (Bransden and Jundi 1967; Basu *et al.* 1976, 1989; Abdel-Raouf *et al.* 1984; Mukherjee and Basu 1991). More recently, the calculations of the Daresbury group have been extended to helium and lithium (Hewitt *et al.* 1992*a*, 1992*b*).

In the present work, a general theory of positron–hydrogen scattering, wherein the positronium formation channels are treated on exactly the same footing as inelastic positron channels, is presented within the close coupling formalism. The close coupling equations are written in terms of a set of coupled Lippmann–Schwinger equations. A completely general form of the positronium formation matrix, eminently suitable for large-scale computation, is derived. In this respect, the present method represents an improvement on the approach adopted by the Daresbury group. The method is employed in a series of calculations of positron–hydrogen scattering.

## 2. Details of Close Coupling Equations

The Schrödinger equation for the positron–hydrogen system is

$$\left( -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{|r_1 - r_2|} - E \right) \Psi(r_1, r_2) = 0, \quad (1)$$

where  $r_1$  and  $r_2$  are the coordinates of the electron and positron centred with respect to the proton and  $E$  is the total energy of the three-body system. An alternative way of writing the Schrödinger equation is

$$\left( -\frac{1}{4}\nabla_R^2 - \nabla_\rho^2 + \frac{1}{|\mathbf{R} - \frac{1}{2}\boldsymbol{\rho}|} - \frac{1}{|\mathbf{R} + \frac{1}{2}\boldsymbol{\rho}|} - \frac{1}{\rho} - E \right) \Psi(\boldsymbol{\rho}, \mathbf{R}) = 0, \quad (2)$$

where  $\boldsymbol{\rho}$  and  $\mathbf{R}$  are the relative and centre-of-mass coordinates for any positronium species. The relation between the two coordinate systems is

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \quad (3a)$$

or

$$\mathbf{r}_1 = \mathbf{R} + \frac{1}{2}\boldsymbol{\rho}, \quad \mathbf{r}_2 = \mathbf{R} - \frac{1}{2}\boldsymbol{\rho}. \quad (3b)$$

With these definitions the Jacobian of the transformation between the two coordinate systems gives

$$\int d^3r_1 \int d^3r_2 = \int d^3\rho \int d^3R. \quad (4)$$

In this work, the following conventions will be observed: bound states of the hydrogen atom will be designated  $\Psi$  and  $\psi$ ; bound states of the positronium atom will be denoted by  $\Phi$  and  $\phi$ . The subscripts  $\alpha$  and  $\beta$  will also be used to distinguish between the manifolds of hydrogen and positronium states.

The wavefunction is expanded in an eigenfunction expansion as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\alpha} \Psi_{\alpha}(\mathbf{r}_1) F_{\alpha}(\mathbf{r}_2) + \sum_{\beta} \Phi_{\beta}(\rho) G_{\beta}(\mathbf{R}), \quad (5)$$

where the hydrogenic  $\Psi_{\alpha}(\mathbf{r}_1)$  and positronium  $\Phi_{\beta}(\rho)$  states satisfy

$$\langle \Psi_{\alpha}(\mathbf{r}_1) | (-\frac{1}{2}\nabla_1^2 - 1/r_1 - \epsilon_{\alpha}) | \Psi_{\alpha}(\mathbf{r}_1) \rangle = 0, \quad (6a)$$

$$\langle \Phi_{\beta}(\rho) | (-\nabla_{\rho}^2 - 1/\rho - \epsilon_{\beta}) | \Phi_{\beta}(\rho) \rangle = 0. \quad (6b)$$

With these definitions the  $\Psi_{\alpha}$  and  $\Phi_{\beta}$  can represent either eigenstates or pseudo-states. The Schrödinger equation now becomes

$$(E - H) \left( \sum_{\alpha} \Psi_{\alpha}(\mathbf{r}_1) F_{\alpha}(\mathbf{r}_2) + \sum_{\beta} \Phi_{\beta}(\rho) G_{\beta}(\mathbf{R}) \right) = 0. \quad (7)$$

Multiplying on the left by  $\Psi_{\alpha'}(\mathbf{r}_1)$  and integrating with respect to  $d^3r_1$  yields the following equation:

$$\begin{aligned} (E + \frac{1}{2}\nabla_2^2 - \epsilon_{\alpha'}) F_{\alpha'}(\mathbf{r}_2) &= \sum_{\alpha} \langle \Psi_{\alpha'} | (1/r_2 - 1/r_{12}) | \Psi_{\alpha} \rangle F_{\alpha}(\mathbf{r}_2) \\ &\quad + \sum_{\beta} \langle \Psi_{\alpha'} | (H - E) | \Phi_{\beta} G_{\beta} \rangle. \end{aligned} \quad (8a)$$

Similarly,

$$\begin{aligned} (E + \frac{1}{4}\nabla_R^2 - \epsilon_{\beta'}) G_{\beta'}(\mathbf{R}) &= \sum_{\beta} \langle \Phi_{\beta'} | (1/r_2 - 1/r_1) | \Phi_{\beta} \rangle G_{\beta}(\mathbf{R}) \\ &\quad + \sum_{\alpha} \langle \Phi_{\beta'} | (H - E) | \Psi_{\alpha} F_{\alpha} \rangle \end{aligned} \quad (8b)$$

can be derived by multiplying on the left by  $\Psi_{\beta'}(\rho)$  and integrating with respect to  $d^3\rho$ . The steps by which equations (8a) and (8b) are specialised to a particular entrance channel and then transferred into a set of momentum-space Lippmann–Schwinger equations are standard and do not need to be repeated here. The momentum-space Lippmann–Schwinger equations for a positron with momentum  $\mathbf{k}$  incident on a hydrogen atom in state  $\Psi_{\alpha}$  are

$$\begin{aligned}
\langle \mathbf{k}' \Psi_{\alpha'} | T | \mathbf{k} \Psi_{\alpha} \rangle &= \langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k} \Psi_{\alpha} \rangle \\
&+ \sum_{\alpha} \int d^3 k'' \frac{\langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k}'' \Psi_{\alpha''} \rangle \langle \mathbf{k}'' \Psi_{\alpha''} | T | \mathbf{k} \Psi_{\alpha} \rangle}{E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2} k''^2} \\
&\sum_{\beta''} \int d^3 k'' \frac{\langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k}'' \Phi_{\beta''} \rangle \langle \mathbf{k}'' \Phi_{\beta''} | T | \mathbf{k} \Psi_{\alpha} \rangle}{E^{(+)} - \epsilon_{\beta''} - \frac{1}{4} k''^2}, \quad (9) \\
\langle \mathbf{k}' \Phi_{\beta'} | T | \mathbf{k} \Psi_{\alpha} \rangle &= \langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Psi_{\alpha} \rangle \\
&+ \sum_{\alpha''} \int d^3 k'' \frac{\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k}'' \Psi_{\alpha''} \rangle \langle \mathbf{k}'' \Psi_{\alpha''} | T | \mathbf{k} \Psi_{\alpha} \rangle}{E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2} k''^2} \\
&+ \sum_{\beta''} \int d^3 k'' \frac{\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k}'' \Phi_{\beta''} \rangle \langle \mathbf{k}'' \Phi_{\beta''} | T | \mathbf{k} \Psi_{\alpha} \rangle}{E^{(+)} - \epsilon_{\beta''} - \frac{1}{4} k''^2}.
\end{aligned}$$

The generic term  $V$  is used to label the interaction between the different classes of channels. The  $V$ -matrix elements are

$$\begin{aligned}
\langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= (2\pi)^{-3} \int d^3 r_1 \int d^3 r_2 \Psi_{\alpha'}^*(\mathbf{r}_1) \exp(-i \mathbf{k}' \cdot \mathbf{r}_2) \\
&\times (1/r_2 - 1/r_{12}) \Psi_{\alpha}(\mathbf{r}_1) \exp(i \mathbf{k} \cdot \mathbf{r}_2), \quad (10)
\end{aligned}$$

$$\begin{aligned}
\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Phi_{\beta} \rangle &= (2\pi)^{-3} \int d^3 \rho \int d^3 R \Phi_{\beta'}^*(\rho) \exp(-i \mathbf{k}' \cdot \mathbf{R}) \\
&\times (1/r_2 - 1/r_1) \Phi_{\beta}(\rho) \exp(i \mathbf{k} \cdot \mathbf{R}) \quad (11a)
\end{aligned}$$

$$\begin{aligned}
&= (2\pi)^{-3} \int d^3 \rho \int d^3 R \Phi_{\beta'}^*(\rho) \exp(-i \mathbf{k}' \cdot \mathbf{R}) \\
&\times \left( \frac{1}{|\mathbf{R} - \frac{1}{2}\rho|} - \frac{1}{|\mathbf{R} + \frac{1}{2}\rho|} \right) \Phi_{\beta}(\rho) \exp(i \mathbf{k} \cdot \mathbf{R}), \quad (11b)
\end{aligned}$$

$$\begin{aligned}
\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= (2\pi)^{-3} \int d^3 r_1 \int d^3 r_2 \Phi_{\beta'}^*(\rho) \exp[-\frac{1}{2} i \mathbf{k}' \cdot (\mathbf{r}_1 + \mathbf{r}_2)] \\
&\times (H - E) \Psi_{\alpha}(\mathbf{r}_1) \exp(i \mathbf{k} \cdot \mathbf{r}_2). \quad (12)
\end{aligned}$$

If the states  $\Psi_{\alpha}(\mathbf{r}_1)$  and  $\Phi_{\beta'}^*(\rho)$  are hydrogen and positronium eigenstates then equation (12) can be written in one of two simplified forms:

$$\begin{aligned}
\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= (2\pi)^{-3} \int d^3 r_1 \int d^3 r_2 \Phi_{\beta'}^*(\rho) \exp[-\frac{1}{2} i \mathbf{k}' \cdot (\mathbf{r}_1 + \mathbf{r}_2)] \\
&\times (\frac{1}{2} k^2 - |\mathbf{k} - \frac{1}{2} \mathbf{k}'|^2 + \epsilon_{\alpha} + \epsilon_{\beta} + 1/r_2 - E) \Psi_{\alpha}(\mathbf{r}_1) \exp(i \mathbf{k} \cdot \mathbf{r}_2) \quad (13a)
\end{aligned}$$

or

$$\begin{aligned}
\langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= (2\pi)^{-3} \int d^3 \rho \int d^3 R \Phi_{\beta'}^*(\rho) \exp(-i \mathbf{k}' \cdot \mathbf{R}) \\
&\times (\frac{1}{4} k'^2 - \frac{1}{2} |\mathbf{k} - \mathbf{k}'|^2 + \epsilon_{\alpha} + \epsilon_{\beta} + 1/r_2 - E) \Psi_{\alpha}(\mathbf{r}_1) \exp(i \mathbf{k} \cdot \mathbf{r}_2). \quad (13b)
\end{aligned}$$

These different expressions are sometimes referred to as the post and prior forms of the matrix element. In the present context, where the interaction Hamiltonian is sandwiched between plane waves, it is irrelevant which form is adopted since the two forms yield identical matrix elements. If pseudo-states are included in the eigenfunction expansion, then the matrix elements, equations (13), have to be modified. The simplest possible reduction of the matrix element is now

$$\begin{aligned} \langle \mathbf{k}' \Phi_{\beta'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= (2\pi)^{-3} \int d^3 r_1 \int d^3 r_2 \Psi_{\beta'}^*(\rho) \exp[-\frac{1}{2}i(\mathbf{k}' \cdot (\mathbf{r}_1 + \mathbf{r}_2))] \\ &\quad \times (\frac{1}{2}k^2 + \frac{1}{2}|\mathbf{k} - \mathbf{k}'|^2 - 1/r_1 + 1/r_2 - 1/r_{12} - E) \Psi_{\alpha}(\mathbf{r}_1) \exp(i\mathbf{k} \cdot \mathbf{r}_2). \end{aligned} \quad (14)$$

For purposes of practical computation, it is convenient to write these matrix elements in a form amenable to calculations in momentum space. The direct interaction for positron scattering, equation (10), becomes

$$\langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k} \Psi_{\alpha} \rangle = \left( \delta_{\alpha' \alpha} - \int d^3 r \Psi_{\alpha'}(\mathbf{r}) \Psi_{\alpha}(\mathbf{r}) \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}] \right) / 2\pi^2 |\mathbf{k} - \mathbf{k}'|^2, \quad (15)$$

which can be written in more detail as

$$\begin{aligned} \langle \mathbf{k}' \Psi_{\alpha'} | V | \mathbf{k} \Psi_{\alpha} \rangle &= \frac{1}{2\pi^2 |\mathbf{k} - \mathbf{k}'|^2} \left[ \delta_{\alpha' \alpha} \delta_{\lambda 0} - \sum_{\lambda \mu} i^{\lambda} (-1)^{m_{\alpha'} + \mu} \right. \\ &\quad \times X_{\alpha' \alpha}^{\lambda}(|\mathbf{k} - \mathbf{k}'|) C_{-\mu}^{\lambda}(\mathbf{k} - \mathbf{k}') \hat{\ell}_{\alpha} \hat{\ell}_{\alpha'} \hat{\lambda}^2 \begin{pmatrix} \ell_{\alpha} & \lambda & \ell_{\alpha'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \ell_{\alpha} & \ell_{\alpha'} \\ \mu & m_{\alpha} & -m_{\alpha'} \end{pmatrix} \left. \right], \end{aligned} \quad (16)$$

where

$$X_{\alpha' \alpha}^{\lambda}(K) = \int_0^{\infty} dr r^2 \Psi_{\alpha'}(r) \Psi_{\alpha}(r) j_{\lambda}(Kr), \quad (17)$$

$C_{-\mu}^{\lambda}(\mathbf{k} - \mathbf{k}')$  is a spherical tensor, and  $\hat{\lambda} = (2\lambda + 1)^{\frac{1}{2}}$ .

The direct interaction for positronium-proton scattering is

$$\begin{aligned} \langle \mathbf{k}' \phi_{\beta'} | V | \mathbf{k} \phi_{\beta} \rangle &= \frac{1}{2\pi^2 |\mathbf{k} - \mathbf{k}'|^2} \int d^3 \rho \Phi_{\beta'}(\rho) \Phi_{\beta}(\rho) \\ &\quad \times \{ \exp[\frac{1}{2}i(\mathbf{k}' - \mathbf{k}) \cdot \rho] - \exp[-\frac{1}{2}i(\mathbf{k}' - \mathbf{k}) \cdot \rho] \}. \end{aligned} \quad (18)$$

In more detail,

$$\begin{aligned} \langle \mathbf{k}' \phi_{\beta'} | V | \mathbf{k} \phi_{\beta} \rangle &= \frac{1}{2\pi^2 |\mathbf{k} - \mathbf{k}'|^2} [1 - (-1)^{\lambda}] \sum_{\lambda \mu} i^{\lambda} (-1)^{m_{\beta'} + \mu} \\ &\quad \times Y_{\beta' \beta}^{\lambda}(|\mathbf{k} - \mathbf{k}'|) C_{-\mu}^{\lambda}(\mathbf{k} - \mathbf{k}') \hat{\ell}_{\beta} \hat{\ell}_{\beta'} \hat{\lambda}^2 \begin{pmatrix} \ell_{\beta} & \lambda & \ell_{\beta'} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \ell_{\beta} & \ell_{\beta'} \\ \mu & m_{\beta} & -m_{\beta'} \end{pmatrix}, \end{aligned} \quad (19)$$

where

$$Y_{\beta'\beta}^\lambda(K) = \int_0^\infty d\rho \rho^2 \Phi_{\beta'}(\rho) \Phi_\beta(\rho) j_\lambda(\tfrac{1}{2}K\rho). \quad (20)$$

It is clear from equation (19) that the matrix element is nonzero only when  $\lambda$  is odd, hence the positronium–proton interaction can only connect states of different parity.

The positronium formation interaction is most conveniently written in terms of products of momentum-space wavefunctions. The hydrogen and positronium momentum-space wavefunctions,  $\psi(\rho)$  and  $\phi(\rho)$ , are defined by

$$\begin{aligned} \psi_\alpha(\mathbf{p}) &= (2\pi)^{-\frac{3}{2}} \int d^3r \phi_\alpha(\mathbf{r}) \exp(-i\mathbf{p}\cdot\mathbf{r}), \\ \phi_\beta(\mathbf{p}) &= (2\pi)^{-\frac{3}{2}} \int d^3\rho \Phi_\beta(\rho) \exp(-i\mathbf{p}\cdot\rho). \end{aligned} \quad (21)$$

The inverse Fourier transforms are just

$$\begin{aligned} \Psi_\alpha(\mathbf{r}) &= (2\pi)^{-\frac{3}{2}} \int d^3p \psi_\alpha(\mathbf{p}) \exp(i\mathbf{p}\cdot\mathbf{r}), \\ \Phi_\beta(\rho) &= (2\pi)^{-\frac{3}{2}} \int d^3p \phi_\beta(\mathbf{p}) \exp(i\mathbf{p}\cdot\rho). \end{aligned} \quad (22)$$

In terms of explicit quantities, the momentum-space wavefunction for  $\psi_\alpha(\mathbf{p})$  is

$$\psi_\alpha(\mathbf{p}) = i^{\ell_\alpha} (-1)^{\ell_\alpha} Y_{\ell_\alpha m_\alpha}(\mathbf{p}) \psi_\alpha(p), \quad (23)$$

where the  $Y_{\ell m}(\mathbf{p})$  in (23) is a spherical harmonic and the spherically symmetric component of the wavefunction is defined by

$$\psi_\alpha(p) = (2/\pi)^{\frac{1}{2}} \int_0^\infty dr r^2 \Psi_\alpha(r) j_{\ell_\alpha}(pr). \quad (24)$$

Besides the momentum-space wavefunctions, the Fourier transforms of the wavefunctions divided by  $r$  (or  $\rho$ ) are required. To be specific, define

$$\begin{aligned} \psi_{r,\alpha}(\mathbf{p}) &= (2\pi)^{-\frac{3}{2}} \int d^3r [\Psi_\alpha(\mathbf{r})/r] \exp(-i\mathbf{p}\cdot\mathbf{r}), \\ \phi_{r,\beta}(\mathbf{p}) &= (2\pi)^{-\frac{3}{2}} \int d^3r [\Phi_\beta(\rho)/\rho] \exp(-i\mathbf{p}\cdot\rho). \end{aligned} \quad (25)$$

The explicit forms for  $\psi_{r,\alpha}(\mathbf{p})$  and  $\phi_{r,\beta}(\mathbf{p})$  are naturally similar to equations (19) and (20), so the radial component is

$$\psi_{r,\alpha}(p) = (2/\pi)^{\frac{1}{2}} \int_0^\infty dr r \Psi_\alpha(r) j_{\ell_\alpha}(pr). \quad (26)$$

With these definitions, the matrix element for positronium formation reduces to

$$\begin{aligned} \langle \mathbf{k}' \Phi_\beta | V | \mathbf{k} \Psi_\alpha \rangle = & (\frac{1}{2}k^2 - |\mathbf{k} - \frac{1}{2}\mathbf{k}'|^2 + \epsilon_\alpha + \epsilon_\beta - E) \psi_\alpha(\mathbf{k}' - \mathbf{k}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{k}) \\ & + (2\pi^2)^{-1} \int d^3q \psi_\alpha(\mathbf{k}' - \mathbf{q}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{q}) / |\mathbf{q} - \mathbf{k}|^2 \end{aligned} \quad (27)$$

in the case of (13a). The more general expression equation (14) becomes

$$\begin{aligned} \langle \mathbf{k}' \Phi_\beta | V | \mathbf{k} \Psi_\alpha \rangle = & (\frac{1}{2}|\mathbf{k} - \mathbf{k}'|^2 - E) \psi_\alpha(\mathbf{k}' - \mathbf{k}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{k}) \\ & - \psi_{r,\alpha}(\mathbf{k}' - \mathbf{k}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{k}) - \psi_\alpha(\mathbf{k}' - \mathbf{k}) \phi_{r,\beta}^*(\frac{1}{2}\mathbf{k}' - \mathbf{k}) \\ & + (2\pi^2)^{-1} \int d^3q \psi_\alpha(\mathbf{k}' - \mathbf{q}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{q}) / |\mathbf{q} - \mathbf{k}|^2. \end{aligned} \quad (28)$$

In both equations (27) and (28), the most compact form of the interaction matrix element involves a three-dimensional integral. The difficulties in doing the partial-wave reduction have led to a number of attempts to circumvent the problem. At present, two different approaches to the computation of the rearrangement matrix elements have seen some use. The traditional approach makes use of Feynman integrals to reformulate the integrand as a one-dimensional integral (Massey and Mohr 1954; Cheshire 1964; Darewych 1987; Sil *et al.* 1979). This approach is the easiest to adopt for calculations involving simple wavefunctions, e.g. the coupled static model involving the H(1s) and Ps(1s) states (Basu *et al.* 1976). For states with  $n \geq 2$ , parametric differentiation is used, and resulting expressions become increasingly complicated. Further complications arise when  $\ell_\alpha$  and  $\ell_\beta$  are both greater than zero. Parametric differentiation of the spherical harmonics leads to expressions which become increasingly ferocious as  $\ell_\alpha$  and  $\ell_\beta$  increase, and the method has only been applied to calculations with relatively restricted close coupling expansions (Basu *et al.* 1989). An innovative technique by Hewitt *et al.* (1990) relies on the convenient translational properties of Gaussian-type orbitals. By expanding the hydrogen and positronium wave functions as a linear combinations of Gaussians, the evaluation of the three-dimensional integral is greatly simplified. This technique also relies upon parametric differentiation of spherical harmonics to develop formulae to handle cases with nonzero angular momentum factors.

In the present work, equation (28) will be adopted since it is preferable to work with expressions of the widest generality. The integrand will be separated into two parts, an angular term corresponding to the two spherical harmonics, and a term arising from the product of the radial parts of the two momentum-space wavefunctions, i.e.

$$\begin{aligned} I = & \int d^3q \psi_\alpha(\mathbf{k}' - \mathbf{q}) \phi_\beta^*(\frac{1}{2}\mathbf{k}' - \mathbf{q}) / |\mathbf{q} - \mathbf{k}|^2 \\ = & \int d^3q P_\alpha(|\mathbf{k}' - \mathbf{q}|) P_\beta^*(|\frac{1}{2}\mathbf{k}' - \mathbf{q}|) Y_{\ell_\alpha m_\alpha}(\mathbf{k}' - \mathbf{q}) Y_{\ell_\beta m_\beta}^*(\frac{1}{2}\mathbf{k}' - \mathbf{q}) / |\mathbf{q} - \mathbf{k}|^2. \end{aligned} \quad (29)$$

Since the radial part is only a function of the magnitude of  $q, k'$ , and the angle  $\cos\theta = \mathbf{q} \cdot \mathbf{k}'$ , a Legendre expansion of the product of  $P_\alpha(|\mathbf{k}' - \mathbf{q}|) P_\beta^*(|\frac{1}{2}\mathbf{k}' - \mathbf{q}|)$  is

practical. Once the Legendre expansion is performed, the partial-wave reduction of the matrix element leads to a completely general expression which is eminently manageable.

### 3. Partial-wave Reduction of Interaction Matrix Elements

For a calculation to be feasible, the matrix elements must be reduced to partial-wave form. The matrix elements are reduced by the formula

$$V_{\alpha' L' \alpha L}^{(J)}(k', k) = \sum_{m_{\alpha'} m_{\alpha} M M'} \int d\hat{k} \int d\hat{k}' Y_{L' M'}^*(\hat{k}') \langle L' M' \ell_{\alpha'} m_{\alpha'} | J M_J \rangle \\ \times \langle k' \alpha' | V | \alpha k \rangle \langle L M \ell_{\alpha} M_{\alpha} | J M \rangle Y_{LM}(\hat{k}), \quad (30)$$

where  $\langle L M \ell_{\alpha} M_{\alpha} | J M \rangle$  is a Clesbch–Gordan coefficient. In writing down equation (30) all considerations of spin coupling have been ignored, since the absence of an exchange interaction leads to the singlet and triplet partial-wave  $T$ -matrix elements being identical. Performing the reductions, the following expressions are realised:

$$V_{\alpha' L' \alpha L}^{(J)}(k', k) = \sum_{\lambda \lambda' \tau} i^{\lambda} (-1)^{\tau + \lambda' + \lambda + J} \hat{\lambda}^3 \hat{\lambda}'^2 \hat{\ell}_{\alpha} \hat{\ell}_{\alpha'} \hat{L} \hat{L}' \\ \times \left( \frac{(2\lambda)!}{(2\tau)!(2\lambda - 2\tau)!} \right)^{\frac{1}{2}} k^{\lambda - \tau} k'^{\tau} X_{\alpha' \alpha}^{\lambda' \lambda}(k', k) \quad (31)$$

$$\times \begin{pmatrix} L' & \lambda' & \lambda - \tau \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_{\alpha'} & \lambda & \ell_{\alpha} \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{array}{ccc} \lambda & L' & L \\ \lambda' & \lambda - \tau & \tau \end{array} \right\} \left\{ \begin{array}{ccc} \ell_{\alpha'} & L' & J \\ L & \ell_{\alpha} & \lambda \end{array} \right\}.$$

The  $X_{\alpha' \alpha}^{\lambda' \lambda}(k', k)$  is an angular integral defined by

$$X_{\alpha' \alpha}^{\lambda' \lambda}(k', k) = 2\pi \int_{-1}^1 du P_{\lambda'}(u) [\delta_{\lambda 0} \delta_{\alpha \alpha'} - X_{\alpha' \alpha}^{\lambda}(K)] / 2\pi^2 K^{(\lambda+2)}, \quad (32)$$

where  $P_{\lambda'}(u)$  is a Legendre polynomial,  $K = |\mathbf{k} - \mathbf{k}'|$ ,  $u = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}'}$ , and  $X_{\alpha' \alpha}^{\lambda}$  is given in equation (17).

The interaction between the different positronium channels is nonzero only when the levels have different parities. When this occurs, the matrix element is very similar to the interaction between the different hydrogen channels,

$$V_{\beta' L' \beta L}^{(J)}(k', k) = \sum_{\lambda \lambda' \tau} i^{\lambda} (-1)^{\tau + \lambda + \lambda' + J} \hat{\lambda}^3 \hat{\lambda}'^2 \hat{\ell}_{\beta} \hat{\ell}_{\beta'} \hat{L} \hat{L}' \\ \times \left( \frac{(2\lambda)!}{(2\tau)!(2\lambda - 2\tau)!} \right)^{\frac{1}{2}} k^{\lambda - \tau} k'^{\tau} Y_{\beta' \beta}^{\lambda' \lambda}(k', k) [1 - (-1)^{\lambda}] \quad (33)$$

$$\times \begin{pmatrix} L' & \lambda' & \lambda - \tau \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda & \tau & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_{\beta'} & \lambda & \ell_{\beta} \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{array}{ccc} \lambda & L' & L \\ \lambda' & \lambda - \tau & \tau \end{array} \right\} \left\{ \begin{array}{ccc} \ell_{\beta'} & \ell_{\beta} & J \\ L & L' & \lambda \end{array} \right\},$$

where

$$Y_{\beta'\beta}^{\lambda'\lambda}(k', k) = 2\pi \int_{-1}^1 du P_{\lambda'}(u) Y_{\beta'\beta}^{\lambda'\lambda}(K)/2\pi^2 K^{(\lambda+2)}, \quad (34)$$

and where the definitions of  $K$  and  $u$  are the same as those used for equation (32). The numerical evaluation of the integrals of equations (32) and (34) to yield  $X_{\alpha'\alpha}^{\lambda'\lambda}(k', k)$  and  $Y_{\beta'\beta}^{\lambda'\lambda}(k', k)$  is done using a composite Gauss-Legendre quadrature mesh. This technique is highly reliable and has received extensive use in numerous calculations of electron-atom scattering.

The matrix element for positronium formation is considerably more complicated, involving as it does an additional integration. The specific form of this matrix element that is most amenable to large-scale computation seems to be

$$\begin{aligned} V_{\beta L' \alpha L}^{(J)}(k', k) &= \sum_{\lambda \tau_\alpha \tau_\beta c j k} i^{\ell_\alpha + \ell_\beta} (-1)^{L+J+c+\ell_\alpha} \hat{\lambda}^2 \hat{\lambda}'^2 \hat{\ell}_\alpha \hat{\ell}_\beta \hat{L} \hat{L}' \\ &\times \left( \frac{(2\ell_\alpha)(2\ell_\beta)!}{(2\tau_\alpha)!(2\tau_\beta)!(2\ell_\alpha - 2\tau_\alpha)!(2\ell_\beta - 2\tau_\beta)!} \right)^{\frac{1}{2}} \left( \frac{1}{2} \right)^{\ell_\beta - \tau_\beta} k'^{\ell_\alpha + \ell_\beta - \tau_\alpha - \tau_\beta} \\ &\times \begin{pmatrix} j & \lambda & L' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} k & \lambda & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_\alpha - \tau_\alpha & j & \lambda_\beta - \tau_\beta \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau_\alpha & k & \tau_\beta \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} L & c & L' \\ j & \lambda & k \end{Bmatrix} \\ &\times \begin{Bmatrix} \ell_\beta & L' & J \\ L & \ell_\alpha & c \end{Bmatrix} \begin{Bmatrix} k & c & j \\ \tau_\alpha & \ell_\alpha & \ell_\alpha - \tau_\alpha \\ \tau_\beta & \ell_\beta & \ell_\beta - \tau_\beta \end{Bmatrix} [Z_{1,\beta\alpha}^{\lambda,\tau}(k', k) + Z_{2,\beta\alpha}^{\lambda,\tau L}(k', k)], \quad (35) \end{aligned}$$

where  $\tau = \tau_\alpha + \tau_\beta$ . This matrix element involves two separate integrals. The first integral is over the angle between  $\mathbf{k}$  and  $\mathbf{k}'$ , *viz.*

$$\begin{aligned} Z_{1,\beta\alpha}^{\lambda\tau}(k', k) &= \frac{1}{2} k^\tau \int_{-1}^1 du [( \frac{1}{2} k^2 + \frac{1}{2} K_1^2 - E ) \psi_\alpha(K_1) \phi_\beta(K_2) \\ &\quad - \psi_{r,\alpha}(K_1) \phi_\beta(K_2) - \psi_\alpha(K_1) \phi_{r,\beta}(K_2)] P_\lambda(u), \quad (36) \end{aligned}$$

with  $K_1 = |\mathbf{k} - \mathbf{k}'|$  and  $K_2 = |\mathbf{k} - \frac{1}{2}\mathbf{k}'|$ . No problems are encountered in the numerical evaluation of (36) since the integrations are similar to those encountered previously, e.g. (32) and (34). The second term in (35) is

$$Z_{2,\beta\alpha}^{\lambda\tau L}(k', k) = \frac{1}{8\pi^3} \int_0^\infty dq q^{2+\tau} H_{\beta\alpha}^\lambda(k', q) V_L(q, k), \quad (37)$$

where  $V_L(k, q)$  is just the partial-wave component of the momentum-space form of the Coulomb potential, i.e.

$$V_L(k, q) = 2\pi \int_0^\infty du |\mathbf{q} - \mathbf{k}|^2 P_L(u); \quad u = \hat{\mathbf{q}} \cdot \hat{\mathbf{k}} \quad (38a)$$

$$= \frac{2\pi}{qk} Q_\lambda(\frac{1}{2}(q/k + k/q)). \quad (38b)$$

In expression (38b),  $Q_\lambda(\frac{1}{2}(q/k + k/q))$  is a Legendre function of the second kind. The  $H_{\beta\alpha}^\lambda(k', q)$  are just projections of the product of the spherically symmetric part of the momentum-space wavefunctions, e.g.

$$H_{\beta\alpha}^\lambda(k', q) = 2\pi \int_{-1}^1 du \phi_\beta(|\frac{1}{2}\mathbf{k}' - \mathbf{q}|) \psi_\alpha(|\mathbf{k}' - \mathbf{q}|) P_\lambda(u), \quad (39)$$

$u = \hat{\mathbf{q}} \cdot \hat{\mathbf{k}'}$  in this case. A great deal of care has to be taken to ensure that the numerical computations involved in the evaluation of (37) are done reliably and efficiently. Of crucial importance to the efficient integration of (37) is the fact that the functions  $H_{\beta\alpha}^\lambda(q, k')$  are only a function of  $k'$ , *but not k*. Therefore, the functions  $H_{\beta\alpha}^\lambda(k', q)$  can be computed and stored for all possible combinations of  $\lambda$ ,  $\beta$ ,  $\alpha$  and  $k'$  before the final integration over  $q$  is performed. This leads to a substantial decrease in the time needed to compute the matrix elements for all combinations of  $k$  and  $k'$ . There is an additional difficulty associated with (37), namely the presence of the Coulomb singularity. The argument of the Legendre function of the second kind goes to 1 as  $q$  goes to  $k$  and so a logarithmic singularity occurs at  $q = k$ . This singularity is handled by a subtraction technique. The basic integral that has to be done is of the type,

$$I_L(k', k) = \int_0^\infty dq H(k', q) Q_L(\frac{1}{2}(q/k + k/q)). \quad (40)$$

This is rewritten as

$$\begin{aligned} I_L(k', k) &= \int_0^\infty dq [H(k', q) - F(q)] Q_L(\frac{1}{2}(q/k + k/q)) \\ &\quad + \int_0^\infty dq F(q) Q_L(\frac{1}{2}(q/k + k/q)). \end{aligned} \quad (41)$$

By normalising  $F(q)$  so that

$$F(k) = H(k', k), \quad (42)$$

the logarithmic singularity in the first term in (41) can be removed. The utility of this method depends on choosing a suitable form for  $F(q)$  that permits the analytic evaluation of the second term of (41). The specific details of the procedure used in the present work are quite involved so this discussion is postponed to the Appendix.

Since all of the integrals involved in the formation of the kernel [e.g. equations (32), (34), (36) and (39)] involve the Fourier transforms of wavefunctions or products of wavefunctions, some comments on the evaluation of the Fourier transforms are appropriate. In the present work, the exact hydrogenic and positronium states are written as linear combinations of Slater-type orbitals (STOs) in the variables  $r_1$  and  $\rho$  respectively. This permits the analytic evaluation of the functions in (17), (20), (24) and (26) using equation (6.621) of Gradsteyn and Ryhzik (1980). To expedite later calculations, these functions are tabulated and converted to cubic splines. However, it should be noted

that the representation of the target wavefunctions in terms of STOs is not an essential feature of the current approach. It would be just as straightforward to represent the target wavefunctions by a numerical tabulation on an  $r$ -space grid and perform the Fourier transforms using numerical quadrature.

One modification is made to the kernel matrix elements to facilitate numerical computation. In general, the kernel elements are either pure real or pure complex quantities. Dividing each individual matrix element by  $i^{L-L'}$  leads to purely real kernel elements. When this is done, the partial-wave form of the Lippmann–Schwinger equation is

$$\begin{aligned} T_{\alpha'L'\alpha L}^{(J)}(k', k) &= V_{\alpha'L'\alpha L}^{(J)}(k', k) \\ &+ \sum_{\alpha''} \int d^3k'' \frac{V_{\alpha'L'\alpha''L''}^{(J)}(k', k'') T_{\alpha''L''\alpha L}^{(J)}(k'', k)}{E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2} \\ &+ \sum_{\beta''} \int d^3k'' \frac{V_{\alpha'L'\beta''L''}^{(J)}(k', k'') T_{\beta''L''\alpha L}^{(J)}(k'', k)}{E^{(+)} - \epsilon_{\beta''} - \frac{1}{4}k''^2}, \end{aligned} \quad (43)$$

$$\begin{aligned} T_{\beta'L'\alpha L}^{(J)}(k', k) &= V_{\beta'L'\alpha L}^{(J)}(k', k) \\ &+ \sum_{\alpha''} \int d^3k'' \frac{V_{\beta'L'\alpha''L''}^{(J)}(k', k'') T_{\alpha''L''\alpha L}^{(J)}(k'', k)}{E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2} \\ &+ \sum_{\beta''} \int d^3k'' \frac{V_{\beta'L'\beta''L''}^{(J)}(k', k'') T_{\beta''L''\alpha L}^{(J)}(k'', k)}{E^{(+)} - \epsilon_{\beta''} - \frac{1}{4}k''^2}. \end{aligned} \quad (44)$$

Apart from the fact that energy denominators arising from intermediate positronium states ( $\beta''$ ) have a  $\frac{1}{4}k^2$  factor instead of the usual  $\frac{1}{2}k^2$  factor, these equations are identical to those occurring in electron–atom scattering. Hence, techniques introduced to solve these equations for electron–atom scattering (McCarthy and Stelbovics 1983) can be adopted with minimal modification.

#### 4. Calculations

The calculations presented in this paper have been performed for two complementary purposes. First, the results of calculations more extensive than any previous calculations are reported. Second, as a validation of the formal and computational details of the present method, calculations using a restricted channel space have been made and the cross sections from these calculations are in agreement with those from earlier calculations.

*CC(1, 1).* This calculation includes the H(1s) and Ps(1s) levels. This model is often called the coupled static approximation. This calculation was used to validate the numerical procedures.

*CC(3, 0) and CC(6, 0).* One aim of this paper was to investigate the influence that inclusion of positronium formation channels would have on the positron impact excitation of hydrogen levels. Accordingly, calculations of positron–hydrogen scattering that omit the positronium channels have also been carried out. The calculations include the lowest three (1s, 2s, 2p) and six (1s, 2s, 3s, 3p, 3d) levels of hydrogen respectively.

*CC(3, 1).* This basis includes the H(1s), H(2s), H(2p) and Ps(1s) levels. This calculation was primarily done as a validation check of the present method. There have been a number of previous calculations (Wakid and LaBahn 1972; Basu *et al.* 1989; Hewitt *et al.* 1991) using this basis.

*CC(3, 3).* This basis includes the H(1s), H(2s) and H(2p) and Ps(1s), Ps(2s) and Ps(2p) levels.

*CC(6, 3).* This basis includes the lowest six levels of hydrogen (1s, 2s, 2p, 3s, 3p, 3d), and the three lowest states of positronium (1s, 2s, 2p). The motivation for this calculation is that the energy and spatial extent of the Ps( $n=2$ ) levels are closer to the H( $n=3$ ) levels than the H( $n=2$ ) levels. Therefore, the inclusion of the H( $n=3$ ) levels in the channel expansion is probably necessary for some sort of convergence to be achieved in the cross sections for the Ps( $n=2$ ) levels.

For most of the calculations reported in this paper, a 24-point Gaussian quadrature mesh was used to discretise the kernel of the integral equation. A 32-point quadrature mesh was used for the CC(6, 3) calculation because the kernel contains more complicated structures than the kernels of the smaller calculations.

**Table 1.** Elastic and positronium formation cross sections (in units of  $\pi a_0^2$ ) for the  $J = 0, 1$  and 2 partial waves at a number of energies (in Rydbergs) above the positronium formation threshold for the coupled static approximation

HB: Higgins and Burke (1991). BBG: Basu, Banerji and Ghosh (1976). HNB: Hewitt, Noble and Bransden (1991)

Energy	0.64	1.0	1.471	2.0	3.0	4.0
Elastic $J = 0$						
Present	0.6689	0.6140	0.5199	0.4317	0.3132	0.2426
HB	0.6633	0.6122	0.5213	0.4316	0.3159	
BBG		0.6152	0.5216			0.2428
$J = 1$						
Present	0.0231	0.0165	0.0411	0.0895	0.1420	0.1261
HB	0.0236	0.0174	0.0420	0.0907	0.1435	
BBG		0.0169	0.0435			0.1266
$J = 2$						
Present	0.0850	0.0874	0.0673	0.0578	0.0490	0.0434
HB	0.0833	0.0881	0.0691	0.0586	0.0500	
BBG		0.0882	0.0689			0.0436
Positronium $J = 0$						
Present	$2 \cdot 31^{-4}$	$1 \cdot 50^{-3}$	$2 \cdot 12^{-3}$	$1 \cdot 02^{-3}$	$1 \cdot 02^{-2}$	$3 \cdot 51^{-3}$
HB	$1 \cdot 8^{-4}$	$1 \cdot 34^{-3}$	$1 \cdot 94^{-3}$	$9 \cdot 1^{-4}$	$1 \cdot 04^{-2}$	
BBG		$1 \cdot 53^{-3}$	$2 \cdot 22^{-3}$			$3 \cdot 12^{-3}$
HNB		$1 \cdot 43^{-3}$		$9 \cdot 0^{-4}$	$1 \cdot 11^{-2}$	
$J = 1$						
Present	0.2880	0.4279	0.4617	0.4533	0.1960	0.0633
HB	0.2960	0.4386	0.4721	0.4586	0.1991	
BBG		0.4323	0.4721			0.0580
HNB		0.4286		0.4549	0.1990	
$J = 2$						
Present	0.420	0.9742	0.8862	0.6333	0.2526	0.0986
HB		0.9865	0.8974	0.6370	0.2556	
BBG		0.9864	0.8976			0.0934
HNB		0.9748		0.6343	0.2547	

The first check made of the integrity of the present method involved the replication of the cross section computed in the first Born approximation (Saha and Roy 1984; Nahar 1989). Cross sections for positronium formation to the Ps(1s), Ps(2s), Ps(2p), Ps(3p) and Ps(3d) levels have been successfully reproduced at a variety of energies. Cross sections for electron capture from positronium to the H(1s) and H(2s) levels (Darewych 1987) have also been reproduced.

Another check of the numerical integrity of the program is made by evaluating the  $Z_2(k', k)$  factor of (37) by two completely different techniques and comparing the results. For scattering calculations restricted to  $\ell = 0$  hydrogenic and positronium levels, it is straightforward to evaluate  $Z_2(k', k)$  taking recourse to techniques originally due to Feynman (Cheshire 1964). There were no significant differences between calculated phase shifts and cross sections using two different methods of computing this term when constructing the kernel of the integral equation.

Since the results of the coupled static CC(1,1) model have been reported on a number of occasions (Basu *et al.* 1976; Higgins and Burke 1991; Hewitt *et al.* 1991), these results provide a good benchmark for testing the present method. Cross sections for the  $J = 0, 1$ , and 2 partial waves for elastic scattering and positronium formation are reported in Table 1. There are small differences, generally of the order of 1%, between the present cross sections and those reported by previous calculations. The largest differences occur when the Ps(1s) cross section is very small and much more sensitive to numerical details. While it would be desirable to eliminate these minor discrepancies, the quality of the agreement indicates that the present method is certainly capable of performing reliable calculations.

**Table 2.** S-wave phase shifts (in radians) for positron–hydrogen scattering as a function of incident momentum (in  $a_0^{-1}$ ) at energies below the threshold for positronium formation

$k$	CC(1,1)	CC(1,1) <sup>A,B</sup>	CC(3,1)	CC(3,1) <sup>A</sup>	CC(3,3)	CC(6,3)	Converged variational <sup>C</sup>
0.1	-0.0190	-0.0191 <sup>A</sup>	0.0328	0.0324	0.0521	0.0656	0.1483
0.2	-0.0472	-0.0472 <sup>A</sup>	0.0212	0.0204	0.0449	0.0634	0.1877
0.3	-0.0874	-0.0872 <sup>A</sup>	-0.0164	-0.0189	0.00531	0.0276	0.1677
0.4	-0.1365	-0.1365 <sup>A</sup>	-0.0672	-0.0696	-0.0475	-0.0273	0.1201
		-0.135 <sup>B</sup>					
0.5	-0.1891	-0.1894 <sup>A</sup>	-0.1231	-0.1259	-0.1042	-0.0857	0.0624
		-0.188 <sup>B</sup>					
0.6	-0.2413	-0.2415 <sup>A</sup>	-0.1796	-0.1831	-0.1607	-0.1442	0.0039
		-0.242 <sup>B</sup>					
0.7	-0.2897	-0.2901 <sup>A</sup>	-0.2324	-0.2362	-0.2137	-0.1990	-0.0512
		-0.292 <sup>B</sup>					

<sup>A</sup> Wakid and LaBahn (1972). <sup>B</sup> Basu *et al.* (1976). <sup>C</sup> Bhatia *et al.* (1971).

In Table 2 phase shifts for the  $J = 0$  partial waves are presented for incident energies below the Ps formation threshold. The agreement between the present CC(1,1) phase shifts and those previously calculated by Wakid and LaBahn (1972) and Basu *et al.* (1976) for the  $J = 0$  partial wave is as good as can be expected.

A comparison between the present CC(3,1) phase shifts and the variational calculation of Wakid and LaBahn (1972) provides another benchmark. The overall agreement between the two calculations is good, with the largest discrepancy being only 0.004 rad. However, the differences between the two calculations show a systematic trend in that the present phase shifts are always larger (by 1% to 2%) than the variational phase shifts. The differences can probably be ascribed to the use of a trial wavefunction by Wakid and LaBahn that was not sufficiently flexible. A similar conclusion also holds for the CC(3,3) calculation. Although the values are not tabulated in Table 2, Wakid and LaBahn also reported phase shifts for the CC(3,3) basis. Once again, there is an overall consistency between the two calculations with the present phase shifts being 3–5% larger at most energies. The difference between the large CC(6,3) calculation and the converged variational result of Bhatia *et al.* (1971) is not surprising. It is known from previous calculations of  $e^\pm$ -hydrogen scattering (Burke *et al.* 1969; Burke and Mitchell 1973; Fon *et al.* 1978; Fon and Gallahar 1972) that the convergence of the close coupling expansion with increasing numbers of basis states is very slow, unless pseudo-states are added to the basis.

**Table 3.** P-wave phase shifts (in radians) for positron–hydrogen scattering as a function of incident momentum (in  $a_0^{-1}$ ) at energies below the threshold for positronium formation

$k$	CC(1,1)	CC(3,1)	CC(3,3)	CC(6,3)	Converged variational <sup>A</sup>
0.1	0.000763	0.00533	0.00627	0.00669	0.0094
0.2	0.00472	0.0182	0.0222	0.0236	0.0338
0.3	0.0134	0.0342	0.0402	0.0439	0.0665
0.4	0.0223	0.0496	0.0558	0.0620	0.1016
0.5	0.0287	0.0615	0.0679	0.0755	0.1309
0.6	0.0314	0.0690	0.0759	0.0841	0.1547
0.7	0.0339	0.0770	0.0856	0.0942	0.1799

<sup>A</sup> Bhatia *et al.* (1974).

Phase shifts for the  $J = 1$  partial wave at incident energies below the Ps formation threshold are listed in Table 3. Unfortunately, there are no reported phase shifts that can be compared with the present models. The overall trend is quite similar to that occurring for the S-wave. As the size of the channel space is increased, the phase shifts increase monotonically towards the variational calculation (Bhatia *et al.* 1971). However, once again the omission of any pseudo-states from the basis leads to the overall level of convergence being relatively poor.

Partial cross sections for ground-state positronium formation at energies above the positronium formation threshold, but below the first excitation threshold for hydrogen, are presented in Table 4. The present cross sections are in excellent agreement with the cross sections of Basu *et al.* (1989) for the  $J = 1$  and  $J = 2$  partial waves. The only major disagreement occurs for the  $J = 0$  partial wave at  $k = 0.71 a_0^{-1}$ . Calculations with different quadrature meshes have been performed to try and reproduce the value of Basu *et al.* but only minor changes to the cross section occur. The cross section reported by Basu *et al.* is probably incorrect. The convergence of the cross sections computed with the larger CC(3,3) and CC(6,3) basis sets to the accurate variational cross sections of Brown and Humberston

(1985) is very slow. The  $J = 1$  and  $J = 2$  partial cross sections are generally about 25% too small. The unusually small  $J = 0$  partial cross section exhibits no discernible signs of convergence.

The differences between the present calculations and those of the Daresbury group using the CC(3,3) model are too large to be attributed to numerical effects. The present calculation or the Hewitt *et al.* calculation must have a more fundamental error, such as the phase in a matrix element. Since the present formalism was tested by a number of independent checks, which does not seem to have been done by Hewitt *et al.*, it is the latter which is most likely in error.

**Table 4.** Positronium formation cross sections (in units of  $\pi a_0^2$ ) for the  $J = 0, 1$  and  $2$  partial waves and the total cross section at four different momenta (in  $a_0^{-1}$ ) in the Ore gap

Model	$J = 0$	$J = 1$	$J = 2$	Total
$k = 0.71$				
CC(3,1)	$0.253^{-2}$	$0.115^{-1}$	$0.289^{-3}$	$0.144^{-1}$
CC(3,1) <sup>B</sup>	$0.608^{-2}$	$0.121^{-1}$	$0.286^{-3}$	$0.157^{-2}$
CC(3,3)	$0.181^{-3}$	$0.172^{-1}$	$0.435^{-3}$	$0.179^{-1}$
CC(6,3)	$0.220^{-3}$	$0.199^{-1}$	$0.521^{-3}$	$0.206^{-1}$
Var <sup>C</sup>	$0.41^{-2}$	$0.27^{-1}$	$0.62^{-3}$	
$k = 0.75$				
CC(3,1)	$0.407^{-2}$	$0.276$	$0.145$	$0.4462$
CC(3,1) <sup>A</sup>	$0.405^{-2}$	$0.277$	$0.144$	
CC(3,1) <sup>B</sup>	$0.418^{-2}$	$0.278$	$0.144$	
CC(3,3)	$0.150^{-4}$	$0.294$	$0.199$	$0.5194$
CC(3,3) <sup>A</sup>	$0.49^{-2}$	$1.47$	$0.570$	
CC(6,3)	$0.129^{-3}$	$0.301$	$0.228$	$0.557$
Var <sup>C</sup>	$0.44^{-2}$	$0.365$	$0.335$	
$k = 0.80$				
CC(3,1)	$0.277^{-3}$	$0.412$	$0.465$	$1.0544$
CC(3,1) <sup>A</sup>	$0.270^{-3}$	$0.412$	$0.459$	
CC(3,1) <sup>B</sup>	$0.244^{-3}$	$0.411$	$0.465$	
CC(3,3)	$0.538^{-4}$	$0.406$	$0.576$	$1.2012$
CC(3,3) <sup>A</sup>	$0.64^{-2}$	$0.259$	$0.933$	
CC(6,3)	$0.224^{-7}$	$0.418$	$0.618$	$1.2654$
Var <sup>C</sup>	$0.49^{-2}$	$0.482$	$0.812$	
$k = 0.85$				
CC(3,1)	$0.143^{-3}$	$0.470$	$0.687$	$1.6128$
CC(3,1) <sup>A</sup>	$0.137^{-3}$	$0.443$	$0.706$	
CC(3,1) <sup>B</sup>	$0.157^{-3}$	$0.470$	$0.684$	
CC(3,3)	$0.886^{-4}$	$0.460$	$0.809$	$1.8124$
CC(3,3) <sup>A</sup>	$0.12^{-2}$	$1.44$	$0.771$	
CC(6,3)	$0.363^{-4}$	$0.479$	$0.842$	$1.8888$
Var <sup>C</sup>	$0.58^{-2}$	$0.561$	$1.057$	

<sup>A</sup> Hewitt *et al.* (1991).

<sup>B</sup> Basu *et al.* (1989).

<sup>C</sup> Variational, Brown and Humberston (1984, 1985).

For all the calculations reported in Tables 5 and 6, rearrangement terms were included in the kernel for all partial waves up to and including  $J = 12$ . The maximum number of partial waves for which complete solutions of the integral equations were found (excluding rearrangement terms) varied from 16 at 1.0 Ryd

to 24 at 4·0 Ryd. The higher partial waves needed to ensure convergence of the partial-wave sum were included using the unitarised Born approximation.

The influence of the rearrangement channels upon the elastic and excitation cross sections can be gauged from Table 5. Comparison of the CC(3,0) elastic cross sections with the CC(3,1) and CC(3,3) cross sections reveals that inclusion of the rearrangement channels leads to the elastic cross section increasing by about 25%. The enhancement of the elastic cross section is also apparent when

**Table 5.** Total cross sections (in units of  $\pi a_0^2$ ) for elastic scattering and excitation of hydrogen levels at selected energies (in Rydbergs)

Model	1·0	1·2	1·5	2·0	3·0	4·0
H(1s) → H(1s)						
CC(1,1)	0·7603	0·7201	0·6674	0·6135	0·5317	0·4318
CC(3,0)	0·5957	0·5605	0·5142	0·4595	0·3822	0·3304
CC(3,1)	0·7246	0·6758	0·6120	0·5419	0·4634	0·3894
CC(3,3)	0·7174	0·6850	0·6206	0·5311	0·4670	0·4026
CC(6,0)	0·5831	0·5511	0·5037	0·4502	0·3775	0·3249
CC(6,3)	0·7282	0·6428	0·6224	0·5228	0·4613	0·3749
H(1s) → H(2s)						
CC(3,0)	0·1309	0·1778	0·2004	0·1995	0·1526	0·1267
CC(3,1)	0·1676	0·2299	0·2768	0·2339	0·0998	0·0869
CC(3,3)	0·1768	0·1562	0·1971	0·2544	0·1021	0·0812
CC(6,0)	0·1827	0·2316	0·2211	0·2019	0·1607	0·1200
CC(6,3)	0·1932	0·2164	0·1345	0·2266	0·1173	0·0800
H(1s) → H(2p)						
CC(3,0)	0·2816	0·4912	0·7624	0·9819	1·0378	1·0022
CC(3,1)	0·2816	0·4762	0·6026	0·5843	0·7524	0·8573
CC(3,3)	0·2857	0·4334	0·6622	0·6254	0·7243	0·8297
CC(6,0)	0·3392	0·5753	0·8004	0·9812	0·9998	0·9688
CC(6,3)	0·3048	0·5203	0·7204	0·6732	0·7210	0·8272

**Table 6.** Total cross sections (in units of  $\pi a_0^2$ ) for positronium formation in the Ps(1s), Ps(2s) and Ps(2p) levels at selected energies (in Rydbergs)

Model	1·0	1·2	1·5	2·0	3·0	4·0
H(1s) → Ps(1s)						
FBA	4·7810	4·2275	3·2516	2·0062	0·8053	0·3627
CC(1,1)	2·5902	2·8814	2·8717	2·3597	1·1207	0·4895
CC(3,1)	2·3529	2·4203	2·3475	2·1337	1·1047	0·4693
CC(3,3)	2·5554	2·8421	2·2960	1·9269	0·9815	0·4257
CC(6,3)	2·5943	2·4988	2·2083	1·8143	1·0276	0·4291
H(1s) → Ps(2s)						
FBA	0·0741	0·1695	0·2299	0·2076	0·1071	0·0522
CC(3,3)	0·0196	0·0706	0·1042	0·1296	0·2261	0·1241
CC(6,3)	0·0136	0·0530	0·0949	0·0946	0·2020	0·1264
H(1s) → Ps(2p)						
FBA	0·2554	0·2710	0·2169	0·1376	0·0541	0·0222
CC(3,3)	0·0309	0·1696	0·1646	0·2003	0·0761	0·0189
CC(6,3)	0·0256	0·1248	0·1750	0·1699	0·0757	0·0209

the CC(6,0) and CC(6,3) cross sections are compared. The major part of the increase occurs when the Ps(1s) state is added to the calculation; the further inclusion of the Ps(2s) and Ps(2p) levels leads to a smaller increase.

The situation for the 2s and 2p excitation cross sections is more complicated. These cross sections have an uneven energy dependence when the positronium states are added to the calculation. This is probably due to the presence of unresolved resonances. A broad resonance is present in the  $J = 0$  partial wave for the CC(1,1) model at an incident energy of 2·6 Ryd (Higgins and Burke 1991; Hewitt *et al.* 1991). A further resonance occurs when the Ps(2s) state is added to the basis (Mitroy 1993). Irrespective of the existence of these resonances, the inclusion of the positronium levels leads to the 2s and 2p excitation cross sections changing by amounts of the order of 20%.

Cross sections for positronium formation are listed in Table 6. Comparison of the first Born approximation (FBA) with the close coupling calculations indicates the FBA is not accurate for energies less than 4·0 Ryd. This is especially true for Ps formation in the 2s and 2p excited states. The uneven energy dependence of the cross sections makes it difficult to draw any definite conclusions about the convergence of the cross sections with respect to increasing numbers of channels. A systematic series of calculations using a very fine energy mesh needs to be performed.

## 5. Conclusions

In this work the general theory of positron–hydrogen scattering is presented as a set of coupled Lippmann–Schwinger equations in momentum space. The major improvement over the seminal calculations of Hewitt *et al.* (1990) is an explicit and completely general form for the positronium matrix element. The use of a Gaussian representation for the atomic orbitals will introduce inaccuracies into the wavefunctions, and moreover is not particularly suited to describing highly excited orbitals. These drawbacks are absent in the current approach which is not limited to a particular representation for the wavefunction. However, no definite conclusions on the respective merits of the two approaches can be made since the computations of Hewitt *et al.* are marred by an error of unknown origin.

At low energies, extensive calculations have been made and demonstrate the overall reliability of the method. However, larger basis sets (including pseudo-states) have to be employed if the present method is to approach the accuracy of the best variational calculations. At intermediate energies, the present calculations, including the six lowest hydrogen and three lowest positronium states are the most extensive yet reported.

The present calculations represent the largest that could be carried out on the available computational facilities (an IBM RISC-6000) in a reasonable length of time. For the calculations using CC(6,3) channel space, the initial calculation of the  $H_{\beta\alpha}^{\lambda}(k', p)$  table took about 80 minutes, while the computation of the kernel for each partial wave (mostly taken in the computation of the rearrangement terms) takes 30 minutes for  $J = 2$  and 80 minutes for  $J = 12$ . Since the present calculations were done with a patched-up electron–atom scattering program, there are many aspects of the program that could be improved and it would certainly be possible to do larger calculations.

In principle, the extension of the present method to the case of positron–atom scattering is straightforward. However, there are two complications that

make positron–atom scattering much more complicated than positron–hydrogen scattering. First, the residual ion can exist in a number of different states. Hence, the coupled channel expansion should include the set of residual ion states as well as the set of positronium states. Second, the electron in positronium and the electrons in the residual ion core can have an interaction of the exchange type. The most compact representation of the positronium–ion exchange matrix element interaction involves a six-dimensional integral (Massey and Mohr 1954) and so could be extremely difficult to evaluate.

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## Appendix: Avoiding the Coulomb Singularity

In this appendix the details of the procedures to remove the singularity from the integrand in equation (37) are presented. This singularity is handled by a subtraction technique. In its most reduced form the basic integral that has to be done can be written as

$$I(L, k) = \int_0^\infty dq H(q) Q_L\left(\frac{1}{2}(q/k + k/q)\right). \quad (\text{A1})$$

This can be rewritten as

$$I(L, k) = I_1(L, k) + I_2(L, k), \quad (\text{A2})$$

where the first term, namely

$$I_1(L, k) = \int_0^\infty dq [H(q) - F(q)] Q_L\left(\frac{1}{2}(q/k + k/q)\right), \quad (\text{A3})$$

is easily evaluated by numerical quadrature since the subtracting function  $F(q)$  is scaled so that  $F(k) = H(k)$ , which eliminates the singularity from (A3). The second term, namely

$$I_2(L, k) = \int_0^\infty dq F(q) Q_L\left(\frac{1}{2}(q/k + k/q)\right) \quad (\text{A4})$$

will be evaluated analytically. A subtracting function can be derived using the identity

$$\frac{1}{2\pi^2} \int d^3q \frac{\psi(\mathbf{q})}{|\mathbf{q} - \mathbf{p}|^2} = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3r \frac{\Psi(\mathbf{r})}{r} \exp(-i\mathbf{p} \cdot \mathbf{r}), \quad (\text{A5})$$

where

$$\psi(\mathbf{q}) = (2\pi)^{-\frac{3}{2}} \int d^3r \Psi(\mathbf{r}) \exp(-i\mathbf{q} \cdot \mathbf{r}). \quad (\text{A6})$$

Performing the angular integrations yields

$$\frac{1}{\pi p} \int_0^\infty dq q\psi(q) Q_L\left(\frac{1}{2}(q/p + p/q)\right) = (2/\pi)^{\frac{1}{2}} \int_0^\infty dr r\Psi(r) j_L(pr). \quad (\text{A7})$$

The identity (A7) is not restricted to functions which are solutions of the radial Schrödinger equation: it is also satisfied by a square-integrable function such as a Slater-type orbital. The choice

$$\psi(r) = r^L \exp(-\alpha r) \quad (\text{A8})$$

leads to the result

$$\int_0^\infty dq \frac{q^{L+1}}{(\alpha^2 + q^2)^{L+1}} Q_L\left(\frac{1}{2}(q/p + p/q)\right) = \frac{\pi}{\alpha} \frac{p^{L+1}}{(2L+2)(\alpha^2 + p^2)^{L+1}}. \quad (\text{A9})$$

In practice, the use of (A3) and (A4) in conjunction with (A9) proved disappointing. In a number of instances,  $I(L, k)$  proved to be much smaller than either of the two terms that contribute to it, i.e.

$$I(L, K) = |I_1(L, k) + I_2(L, k)| \ll I_1(L, k).$$

When this occurs, the large cancellations between  $I_1(L, k)$  and  $I_2(L, k)$  lead to a significant degradation in the precision of  $I(L, k)$  and to an overall loss of accuracy.

Because of this problem, an alternative strategy was used in the evaluation of  $I(L, k)$ . Rather than having a subtracting function spanning the entire  $[0, \infty]$  interval, the subtracting function was confined to a finite range. This is possible since the integrations are performed using a composite Gaussian quadrature mesh. The subtraction procedure was only applied to the particular element of the composite mesh in which the singularity occurred. The explicit form of the subtraction used for the calculation presented in this work was

$$I(L, k) = J_1(L, k) + J_2(L, k) + J_3(L, k), \quad (\text{A10})$$

where

$$\begin{aligned} J_1(L, k) &= \int_0^{q_1} dq H(q) Q_L\left(\frac{1}{2}(q/k + k/q)\right) \\ &\quad + \int_{q_2}^\infty dq H(q) Q_L\left(\frac{1}{2}(q/k + k/q)\right), \end{aligned} \quad (\text{A11})$$

which is evaluated using numerical quadrature since the singularity at  $k$  is not contained in the  $[0, q_1]$  and  $[q_2, \infty]$  intervals. The second term, namely

$$\begin{aligned} J_2(L, k) &= \int_{q_1}^{q_2} dq H(q) Q_L\left(\frac{1}{2}(q/k + k/q)\right) \\ &\quad - H(k) Q_0\left(\frac{1}{2}(q/k + K/q)\right) \end{aligned} \quad (\text{A12})$$

can also be evaluated numerically. It is possible to use  $Q_0\left(\frac{1}{2}(q/k + k/q)\right)$  as the subtracting function for all values of  $L$  because  $(Q_L(x) - Q_0(x))$  goes to a constant as  $x \rightarrow 1$ . The final term,

$$J_3(L, k) = H(k) \int_{q_1}^{q_2} dq Q_0\left(\frac{1}{2}(q/k + k/q)\right), \quad (\text{A13})$$

is evaluated analytically. The reason  $Q_0\left(\frac{1}{2}(q/k + k/q)\right)$ , and not  $Q_L\left(\frac{1}{2}(k/q + q/k)\right)$ , is used for the subtraction is that an analytic expression for the indefinite integral involving  $Q_0\left(\frac{1}{2}(k/q + q/k)\right)$  exists. This is not true for  $Q_L\left(\frac{1}{2}(k/q + q/k)\right)$  with a

general value of  $L$ . No difficulties are encountered in integrating (A13) and the result is

$$\begin{aligned}
 J_3(L, k) = & (q_2/k)H(k)[(q_2/k+1)\log_e(1+q_2/k) \\
 & - 2\log_e(2) - (q_2/k-1)\log_e(q_2/k-1)] \\
 & + (q_1/k)H(k)[(q_1/k-1)\log_e(1-q_1/k) \\
 & + 2\log_e(2) - (q_1/k+1)\log_e(1+q_1/k)]. \tag{A14}
 \end{aligned}$$

The procedure outlined in equations (A10) to (A14) cannot be applied if the singularity occurs in the last element of the composite quadrature mesh used for the numerical integrations, as the integral (A13) diverges when  $q_2 \rightarrow \infty$ . In these cases the subtraction is performed using the procedure outlined in (A1) to (A9).

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