LETTER TO THE EDITOR

Another s-wave resonance in positron–hydrogen scattering

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Abstract. The close-coupling equations for the positron–hydrogen system restricted to s-wave scattering from the $l = 0$ levels of hydrogen and positronium are written as a set of coupled momentum space Lippmann–Schwinger equations. The matrix element for positronium formation is evaluated by integrating over the multipole projected components of the momentum space wave functions. Cross sections generated in the coupled static approximation provide a verification of the method. With a larger basis, including the 1s and 2s levels of hydrogen and the 1s and 2s levels of positronium, the broad s-wave resonance at 2.6 Ryd shifts position to 3.17 Ryd. An additional resonance is observed in the cross section at an energy of 1.10 Ryd.

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, a reason for this is the difficulty in providing a proper formulation of the positronium formation process. That the broad s-wave resonance occurring in the coupled static model was only identified recently (Hewitt et al 1991, Higgins and Burke 1991) is an indication of the scant attention paid to problems involving positronium formation.

Accordingly, a simplified model of the positron–hydrogen system, with the system constrained to s-wave scattering from the $l = 0$ levels of hydrogen and positronium, is developed. Investigations based upon the spherically symmetric electron–hydrogen system have proved valuable by providing guidance about the correctness of the pseudo-state method (Stelbovics and Winata 1990, Oza and Callaway 1983). While the spherically symmetric model of the positron–hydrogen system is necessarily similar to the spherically symmetric model of electron–hydrogen scattering, it is not possible to generate an exact solution using the method of Poet (1978) unless additional simplifications are made. The initial motivation for studying this system was to investigate positronium formation in a model simple enough to permit a high degree of convergence to be achieved while refining numerical procedures for the calculation of the positronium formation matrix element. However, the discovery of an additional s-wave resonance as the calculation size was increased indicates the model contains dynamical features which are worthy of investigation.

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The momentum space Lippmann–Schwinger equations for a positron with momentum \( k \) incident on a hydrogen atom in state \( \Psi_\alpha \) are

\[
\langle k' \Psi_{\alpha'} | T | k \Psi_\alpha \rangle = \langle k' \Psi_{\alpha'} | V | k \Psi_\alpha \rangle + \sum_{\alpha''} \int d^3k'' \left( \frac{\langle k' \Psi_{\alpha'} | V | k'' \Phi_{\beta''} \rangle \langle k'' \Phi_{\beta''} | T | k \Psi_\alpha \rangle}{(E^{(+)} - \epsilon_{\beta''} - \frac{1}{2}k'')^2} \right) \\
+ \sum_{\beta''} \int d^3k'' \left( \frac{\langle k' \Phi_{\beta'} | V | k'' \Psi_{\alpha''} \rangle \langle k'' \Psi_{\alpha''} | T | k \Psi_\alpha \rangle}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k'')^2} \right) \\
+ \sum_{\beta''} \int d^3k'' \left( \frac{\langle k' \Phi_{\beta'} | V | k'' \Psi_{\alpha''} \rangle \langle k'' \Psi_{\alpha''} | T | k \Psi_\alpha \rangle}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k'')^2} \right).
\]

(1)

The hydrogenic and positronium bound states are denoted by the functions \( \Psi_\alpha \) and \( \Phi_\beta \) respectively. The subscripts \( \alpha \) or \( \beta \) will also be used to distinguish between the manifold of hydrogen and positronium states. The following classes of interaction matrix elements occur,

\[
\langle k' \Psi_{\alpha'} | V | k \Psi_\alpha \rangle = \left[ \delta_{\alpha'\alpha} - \int d^3r \Psi_{\alpha'}(r) \Psi_\alpha(r) \exp(-i(k' - k) \cdot r) \right] 1/(2\pi^2 |k - k'|^2)
\]

(2a)

\[
\langle k' \Phi_{\beta'} | V | k \Phi_\beta \rangle = 0
\]

(2b)

\[
\langle k' \Phi_{\beta'} | V | k \Phi_\beta \rangle = (\frac{1}{2}k^2 - |k - \frac{1}{2}k'|^2 + \epsilon_\alpha + \epsilon_\beta - E)\psi_\alpha(k' - k)\phi_{\beta'}(k - \frac{1}{2}k') \\
+ (2\pi)^{-1} \int d^3q \psi_\alpha(k' - q)\phi_{\beta'}(q - \frac{1}{2}k')/|q - k|^2.
\]

(2c)

In equations (2), \( \psi(p) \) and \( \phi(p) \) are the hydrogen and positronium momentum space wavefunctions defined by

\[
\psi_\alpha(p) = (2\pi)^{-3/2} \int d^3r \psi_\alpha(r) \exp(-ip \cdot r)
\]

and

\[
\phi_\alpha(p) = (2\pi)^{-3/2} \int d^3r \phi_\alpha(r) \exp(-ip \cdot r).
\]

Provided only s states are involved, the radial component of the momentum space function can be written

\[
\psi_\alpha(p) = (2/\pi)^{1/2} \int_0^\infty dr \ r^2 \psi_\alpha(r) j_0(pr)
\]

(4)

with a similar result holding for \( \phi(p) \). In equation (4) \( j_0(pr) \) is a spherical Bessel function. In deriving equations (2c) it was assumed that the hydrogenic states and positronium states are eigenstates. When pseudo-states are included it is necessary to generalise the expression for the first term of the kernel, namely

\[
\langle k' \Phi_{\beta'} | V | k \Psi_\alpha \rangle = (\frac{1}{2}k^2 + \frac{1}{2}|k - k'|^2 - E)\psi_\alpha(k' - k)\phi_{\beta'}(k - \frac{1}{2}k') - \psi_\alpha(k' - k)\phi_{\beta'}(k - \frac{1}{2}k') \\
- \psi_\alpha(k' - k)\phi_{\beta'}^*(k - \frac{1}{2}k') + (2\pi)^{-1} \int d^3q \psi_\alpha(k' - q)\phi_{\beta'}^*(q - \frac{1}{2}k')/|q - k|^2.
\]

(5)
Equation (5) is adopted for the present work. Although no pseudo-states are used, it is preferable to work with the expression of widest generality. In the above expressions, the Fourier transforms of the wavefunctions divided by \( r \) are required, i.e.

\[
\psi_{r,a}(p) = (2\pi)^{-3/2} \int d^3r \psi_{a}(r)/r \exp(-ip \cdot r)
\]

and

\[
\phi_{r,b}(p) = (2\pi)^{-3/2} \int d^3r \phi_{b}(r)/r \exp(-ip \cdot r).
\]

The radial components can be written

\[
\psi_{r,a}(p) = (2/\pi)^{1/2} \int_0^\infty dr r \psi_{a}(r) j_0(pr)
\]

with a similar expression holding for \( \phi_{r,b}(p) \).

When the partial wave analysis is performed the s-wave Lippmann–Schwinger reduces to

\[
T_{\alpha'\alpha}(k', k) = V_{\alpha'\alpha}(k', k) + \sum_{\alpha''} \int d^3k'' \frac{V_{\alpha''\alpha}(k', k''') T_{\alpha''\alpha}(k'', k)}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2)} + \sum_{\beta'} \int d^3k'' \frac{V_{\beta'\alpha}(k', k''') T_{\beta'\alpha}(k'', k)}{(E^{(+)} - \epsilon_{\beta'} - \frac{1}{2}k''^2)}
\]

\[
T_{\beta'\alpha}(k', k) = V_{\beta'\alpha}(k', k) + \sum_{\alpha''} \int d^3k'' \frac{V_{\beta''\alpha}(k', k''') T_{\alpha''\alpha}(k'', k)}{(E^{(+)} - \epsilon_{\alpha''} - \frac{1}{2}k''^2)} + \sum_{\beta''} \int d^3k'' \frac{V_{\beta''\alpha}(k', k''') T_{\beta''\alpha}(k'', k)}{(E^{(+)} - \epsilon_{\beta''} - \frac{1}{2}k''^2)}.
\]

The techniques involved in solving integral equations of this type have been detailed elsewhere (McCarthy and Stelbovics 1983). Partial wave matrix elements for the different classes of interaction are straightforward to derive. The interactions connecting the different hydrogenic levels is

\[
V_{\alpha'\alpha}(k', k) = 2\pi \int_0^\infty du F_{\alpha'\alpha}(K) P_0(u) \quad u = \hat{k} \cdot \hat{k}'
\]

where \( P_0(u) \) is a Legendre polynomial. The form factor is

\[
F_{\alpha'\alpha}(K) = \frac{1}{2\pi^2 K^2} \left[ \delta_{\alpha'\alpha} - \int_0^\infty dr r^2 \psi_{\alpha}(r) \psi_{\alpha}(r) j_0(Kr) \right]
\]

and \( K = |\mathbf{k} - \mathbf{k}'| \). There is no interaction between the different positronium states, i.e. \( V_{\beta'\beta}(k', k) = 0 \).

Finally, it is best to split the interaction matrix element for positronium formation into two parts,

\[
V_{\beta\alpha}(k', k) = V_{\beta\alpha}^1(k', k) + V_{\beta\alpha}^2(k', k).
\]
The partial wave form of $V_{\beta\alpha}^{1}(k', k)$ equivalent to equation (5) is presented below since it is the form used for numerical computations. It is

\[
V_{\beta\alpha}^{1}(k', k) = \frac{1}{2} \int_{-1}^{1} du [(\frac{1}{2} k^2 + \frac{1}{2} k'^2 - E)\psi_{\alpha}(K_1)\phi_{\beta}(K_2) - \psi_{\alpha}(K_1)\phi_{\beta}(K_2)] P_0(u) 
\]

(12)

with $K_1 = |k - k'|$ and $K_2 = |k - \frac{1}{2} k'|$.

Analysis of the second term yields

\[
V_{\beta\alpha}^{2}(k', k) = \sum_{\lambda} \frac{(2\lambda + 1)}{16\pi^2 k} \int_{0}^{\infty} dq \frac{q}{2} \psi_{\alpha}^{\lambda}(q, k') \phi_{\beta}^{\lambda}(q, \frac{1}{2} k') Q_0 \left( \frac{1}{2} \left( \frac{q}{k} + \frac{k}{q} \right) \right) 
\]

(13)

where $Q_0(\frac{1}{2}(q/k + k/q))$ is a Legendre function of the second kind. The $\psi_{\alpha}^{\lambda}(q, k')$ and $\phi_{\beta}^{\lambda}(q, \frac{1}{2} k')$ are just projections of the momentum space wavefunctions, with

\[
\psi_{\alpha}^{\lambda}(q, k') = 2\pi \int_{-1}^{1} du \psi_{\alpha}(|k' - q|) P_{\lambda}(u) \quad u = \hat{q} \cdot \hat{k}'
\]

(14)

and

\[
\phi_{\beta}^{\lambda}(q, \frac{1}{2} k') = 2\pi \int_{-1}^{1} du \phi_{\beta}(|q - \frac{1}{2} k'|) P_{\lambda}(u) \quad u = \hat{q} \cdot \hat{k}'.
\]

The functions $\psi_{\alpha}^{\lambda}(q, k')$ and $\phi_{\beta}^{\lambda}(q, \frac{1}{2} k')$ are only functions of $k'$ and not $k$ and can be computed before evaluating the integrand in equation (13). Taking advantage of this feature leads to a substantial decrease in the calculation time.

Equation (13) does have one troublesome feature, there is an integrable singularity at $q = k$ associated with the Legendre function of the second kind. This singularity is handled by a subtraction technique. The evaluation of equation (13) requires an infinite sum over $\lambda$. In practice, the contributions to the matrix element decrease as $\lambda$ increases and the sum can be truncated. For the present calculations the sum has been truncated at $\lambda = 12$.

Results are presented for two different model calculations.

(i) CC(1,1). This calculation includes the H(1s) and Ps(1s) levels. This is often referred to as the coupled static approximation. This calculation was primarily done to validate the numerical procedures.

(ii) CC(2,2). This calculation includes the H(1s), H(2s) and Ps(1s), Ps(2s) levels.

The following checks have been made of the numerical integrity of the calculations. First, the CC(1,1) results can be compared with previously published results. Second, cross sections for the H(1s)→Ps(2s), and Ps(1s)→H(2s) transitions can be computed in the first Born approximation and compared with previous calculations (Saha and Roy 1984, Darewych 1987, Nahar 1989). There are no significant differences with previous calculations. Finally, the matrix element $V_{\beta\alpha}^{2}(k', k)$ can also be evaluated by making recourse to techniques originally due to Feynman (Cheshire 1964). There were no significant differences between calculated phase shifts and cross sections when two different methods are used to evaluate $V_{\beta\alpha}^{2}(k', k)$.

In table 1, the $J = 0$ partial cross sections for Ps formation threshold are presented. The agreement of the present CC(1,1) calculations with the previous CC(1,1) calculations of Higgins and Burke (1991) and Abdel-Raouf et al (1984) is reasonable when the small size of cross section is considered. The CC(2,2) calculation gives cross sections which are
larger and in closer agreement with the accurate calculations of Humberston (1982, 1984) and Archer et al (1990). The CC(2,2) model shows no sign of the extremely rapid rise in the cross section occurring in these calculations.

In Table 2, the \( J = 0 \) partial cross sections for elastic scattering, excitation of the H(2s) level, and formation of the Ps(1s) and Ps(2s) states are presented. The agreement of the present CC(1,1) results with previous calculations using this model is acceptable. There are some differences between some of the Ps(1s) cross sections, but this cross section is very small and is more sensitive to the details of the calculation.

<table>
<thead>
<tr>
<th>Energy (Ryd)</th>
<th>( \text{cc}(1,1) ) (present)</th>
<th>( \text{cc}(2,2) )</th>
<th>( \text{cc}(1,1) ) (other)</th>
<th>Other</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.71</td>
<td>0.18(^{-5})</td>
<td>0.58(^{-3})</td>
<td>0.41(^{-2c})</td>
<td>0.34(^{-2d})</td>
</tr>
<tr>
<td>0.75</td>
<td>0.54(^{-4})</td>
<td>0.256(^{-2})</td>
<td>0.4(^{-4a})</td>
<td>0.44(^{-2c})</td>
</tr>
<tr>
<td>0.80</td>
<td>0.21(^{-3})</td>
<td>0.389(^{-2})</td>
<td>0.18(^{-3a})</td>
<td>0.49(^{-2c})</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.18(^{-3b})</td>
<td>0.43(^{-2d})</td>
</tr>
<tr>
<td>0.85</td>
<td>0.50(^{-3})</td>
<td>0.404(^{-2})</td>
<td>0.41(^{-3a})</td>
<td>0.58(^{-2c})</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.41(^{-3b})</td>
<td>0.49(^{-2d})</td>
</tr>
</tbody>
</table>

\(^b\) Higgins and Burke (1991) (interpolated where necessary).

<table>
<thead>
<tr>
<th>Model</th>
<th>( J = 0 )</th>
<th>( J = 1 )</th>
<th>( J = 2 )</th>
<th>( J = 3 )</th>
<th>( J = 4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}(1s) \rightarrow \text{H}(1s) )</td>
<td>( \text{cc}(1,1) )</td>
<td>0.6125</td>
<td>0.5734</td>
<td>0.5141</td>
<td>0.4317</td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(1,1)(^a) )</td>
<td>0.6122</td>
<td>0.4316</td>
<td>0.3159</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(1,1)(^b) )</td>
<td>0.6152</td>
<td>0.4316</td>
<td>0.3159</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(2,2) )</td>
<td>0.4613</td>
<td>0.4719</td>
<td>0.4441</td>
<td>0.3857</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>( J = 0 )</th>
<th>( J = 1 )</th>
<th>( J = 2 )</th>
<th>( J = 3 )</th>
<th>( J = 4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}(1s) \rightarrow \text{H}(2s) )</td>
<td>( \text{cc}(2,2) )</td>
<td>2.67(^{-3})</td>
<td>1.01(^{-2})</td>
<td>5.50(^{-3})</td>
<td>1.03(^{-2})</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>( J = 0 )</th>
<th>( J = 1 )</th>
<th>( J = 2 )</th>
<th>( J = 3 )</th>
<th>( J = 4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}(1s) \rightarrow \text{Ps}(1s) )</td>
<td>( \text{cc}(1,1) )</td>
<td>1.51(^{-3})</td>
<td>1.97(^{-3})</td>
<td>2.11(^{-3})</td>
<td>1.02(^{-2})</td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(1,1)(^a) )</td>
<td>1.34(^{-3})</td>
<td>9.1(^{-4})</td>
<td>1.04(^{-2})</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(1,1)(^b) )</td>
<td>1.53(^{-3})</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \text{cc}(2,2) )</td>
<td>1.64(^{-3})</td>
<td>2.15(^{-4})</td>
<td>6.43(^{-4})</td>
<td>6.12(^{-4})</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>( J = 0 )</th>
<th>( J = 1 )</th>
<th>( J = 2 )</th>
<th>( J = 3 )</th>
<th>( J = 4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}(1s) \rightarrow \text{Ps}(2s) )</td>
<td>( \text{cc}(2,2) )</td>
<td>9.91(^{-4})</td>
<td>3.06(^{-2})</td>
<td>1.73(^{-2})</td>
<td>3.68(^{-3})</td>
</tr>
</tbody>
</table>

\(^a\) Higgins and Burke (1991).
\(^b\) Basu et al (1976).

There are substantial differences between the elastic and Ps(1s) cross sections for the CC(1,1) and CC(2,2). Calculations using a finer energy mesh than that reported in Table 2,
Figure 1. The \( J = 0 \) partial cross sections (units of \( \pi a_0^2 \)) for elastic scattering (full curve) and the excitation of the 2s level \((\times 10, \text{broken curve})\) of hydrogen. The curves represent smoothed spline fits to data calculated at a discrete number of points.

Figure 2. The \( J = 0 \) partial cross sections (units of \( \pi a_0^2 \)) for excitation to the Ps(1s) \((\times 10, \text{full curve})\) and the Ps(2s) \((\text{broken curve})\) levels. The curves represent smoothed spline fits to data calculated at a discrete number of points.

and depicted in figures 1 and 2, show the position of the resonance peak of the 2.62 Ryd resonance in the Ps(1s) cross section has shifted to a higher energy. An estimate of the position can be obtained by fitting to a Fano profile, this yields a resonance position of about 3.17 Ryd and a width of 0.24 Ryd.

The plots of the cross sections show evidence of an additional resonance at a lower energy. All of the cross sections have a sharp structure near 1.1 Ryd. A striking feature is the large value \((0.1 \pi a_0^2)\) of the Ps(2s) cross section at its maximum. Using a fitting procedure based on the Fano profile yields 1.10 Ryd for the position and 0.05 Ryd for the
width. Since there is no evidence of a resonance in a calculation involving the H(1s), H(2s) and Ps(1s) states, it is concluded that the 1.10 Ryd resonance results from the interaction of the Ps(2s) state with the other states. The additional resonance is consistent with the larger basis calculations reported by Hewitt et al. (1991). They report a $J = 0$ partial cross section which was uneven at energies below 20 eV, but it was not clear whether the irregularities are due to resonances or other factors.

The present calculation has shown that the s-wave model for positron–hydrogen scattering, unlike that for electron–hydrogen scattering, possesses a considerable degree of structure. While Higgins and Burke (1991) suggested that the higher energy resonance is the result of the effective potential in the positronium channel, the exact mechanism still needs to be specified. The present calculations reinforce the suggestion (Hewitt et al. 1991) that the previously identified 2.62 Ryd resonance is not a feature that is specific to the coupled static calculation. Indeed, an additional resonance appeared when Ps(2s) level was added to the channel space. The origins of this class of resonances is worth further investigation in a systematic study of the spherically symmetric positronium–hydrogen model as it is not known whether additional resonances will appear as additional Ps channels are added to the calculation.

This model is also ideal as a prototype to refine numerical procedures used in the evaluation of the positronium formation matrix element. While there are algebraic complications involved in the generalization of equation (13), the details of the numerical integration will be identical to those of the present restricted calculation. Consequently, the extension of the present method for the evaluation of the positronium matrix element is feasible.

The author would like to thank Dr A T Stelbovics for suggesting the first application of this method be upon the spherically symmetric model of positron–hydrogen scattering. The hospitality of the Centre for Atomic, Molecular and Surface Physics, located jointly at Murdoch University and the University of Western Australia, is acknowledged.

References

Abdel-Raouf M A, Darewych J W, McEachran R P and Stauffer A D Phys. Lett. 100A 353