Effect of $H^-$ ion formation on Positronium-Hydrogen elastic scattering

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Abstract

Effect of charge-transfer recombination for positronium (Ps) scattering is studied on Ps-H system using coupled-channel formalism considering a new rearrangement channel $\mathrm{Ps} + \mathrm{H} \rightarrow e^+ + \mathrm{H}^-$ and exchange. The correlation and continuum effects introduced by this charge-transfer channel result to substantial convergence to the low energy scattering parameters. Effects on scattering length, PsH binding energy, and low-energy (0-10 eV) cross sections are evaluated and $H^-$ formation cross sections are reported from above the threshold (6.438 eV) to 100 eV.
Introduction : Charge-transfer recombinations have been found to be of fundamental importance in simulating the continuum effect in the scattering dynamics of positrons [1, 2]. Their roles are yet to be investigated for the scattering of positronium (Ps) atom - an exotic bound state of electron and positron with singlet and triplet spins. This seems to be very important since, despite a long history of theoretical studies [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26], we are yet to produce converged scattering results in the ab initio coupled-channel (CC) framework, even for the simplest Ps-H system [10].

So far, in dealing with Ps scattering, emphasis has been given to the exchange rearrangement of electrons, which is also of fundamental importance, as the static-potential for a Ps-target system vanishes due to internal charge-and-mass symmetry of Ps. However, exchange constitutes only a part of the continuum and Ps exhibits a strong polarizability of $36 a_0^3$, which is expected to make it vulnerable to continuum effects and charge transfer processes. Continuum effect can be simulated through pseudostates of Ps and target, but for Ps scattering this is expected lead to an untractable situation as the number of scattering channels grows like $N^2$, where $N$-number of intermediate states for each of Ps and target are considered. Considering the difficulty, so far, the pseudostate technique has been applied (to Ps-H and Ps-He scattering problem) employing pseudostates for only Ps. This is not expected to simulate the appropriate continuum effect as the target is kept idle to keep the calculational schemes tractable. However, from the experience in positron-atom scattering [2], we understand that allowed charge transfer processes can also enhance the continuum effect significantly and lead to the required convergence of the theoretical scheme. The effect of such charge-transfer channels is yet unexplored for Ps scattering and is the subject of this work.

Apart from the initial works [3, 4, 5, 6, 7, 8], the recent theoretical development on Ps scattering studies, has contributions from the Belfast group [3, 10, 11], the Calcutta
group \cite{12,13,14} and the São Paulo group \cite{17,18,19,20,21,22,23,24,25,26}. While the Belfast and Calcutta groups use complete \textit{ab initio} coupled-channel (CC) formalism, the São Paulo group indulges to model exchange correlation potentials (to enhance the correlation and continuum effects) in the \textit{ab initio} CC formalism. In this investigation, we concentrate on the simplest but the richest Ps-H scattering problem, where predictions of the \textit{ab initio} coupled-channel (CC) calculations are yet to converge with those of the accurate variational calculations \cite{30,28}.

In the \textit{ab initio} CC formalism, the largest continuum effect has been taken in a 22-state calculation which uses three eigen states and nineteen pseudostates of Ps keeping the target idle. This calculation yields PsH binding energy of 0.634 eV and S-wave singlet resonance energy of 4.55 eV compared to the most accurate variational estimates of 1.067 eV \cite{30} and 4.003 eV \cite{28}, respectively. The lack of convergence was expected as the virtual effects of the target are neglected. Interestingly, predictions of this CC calculation come to close agreement with the predictions of another variational calculation \cite{5} that has been performed without explicit electron-electron correlation in their trial ansatz. The precise variational calculations above \cite{30,28} includes explicit $e-e$ correlation in their trial wave functions and they also contain $H^-$ flavour. These clearly emphasize the necessity of the introduction of more electron-electron correlation and continuum effects to the present state of the art CC calculations. We understand that, for Ps-H system, electron-electron correlation and continuum effects could be enhanced through the formation of $H^-$-ion via Ps+H→$e^++H^-$ channel in the CC model.

Before finishing the introduction, we note another relevant development in this subject. For the last few years we have been engaged in addressing the Ps scattering problems by using a model exchange correlation potential in the \textit{ab initio} CC formalism. Apart from the recent theoretical development on Ps scattering by the Belfast and Calcutta groups employing complete \textit{ab initio} formalism, studies has contributions from two more
groups other than the Belfast group which has considered the Ps-pseudostate technique [3, 4, 5], mentioned above. The Calcutta group has addressed the Ps-H problem in various ways [6, 7, 8], but they have not reported the binding or resonance parameters. So, these aspects and hence the overall convergence of their low energy scattering results could not be assessed comparing with the accurate variational predictions.

In the last few years, we are addressing Ps scattering problems by using a model regularized exchange-correlation potential (non-local) [21] in the exact coupled Lippmann-Schwinger equation [17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. In these calculations, convergence and agreement with accurate variational predictions are achieved by employing a minimum number of effective scattering channels and tuning the exchange correlation potentials by means of a parameter. The model agreed well with the measured data [21, 22, 23, 24] in Ps-He [7]. When applied to Ps-H, it reproduces the precise binding and resonances energies. Thereafter, it has also been applied to other targets (H$_2$, Ne, Ar, Li) and agreement with measured data is obtained. However, the crucial aspect of the model remains the tuning of the parameter. It appears that the exchange correlation potentials, when tuned, compensate for the correlation and continuum effects (see details in the results and discussions). Thus, we expect that the direct inclusion of correlation and continuum effects in the model CC framework, through the H$^-$ formation channel, would diminish the role of the parameter. Also, the charge transfer channel, in general, is expected to improve the results obtained in the ab-initio framework due to possible enhancement of correlation and continuum effects.

To have a preliminary assessment of these assertions, we re-investigate the Ps-H scattering including the process Ps+H → e$^+$+H$. In the present work, for a first estimation, we use a simple wave function of Chandrasekhar for the H$^-$ ion [35]. Any elaborate wave function containing the $r_{12}$ term would certainly enhance the electron-electron correlation further. We estimate the effect of this charge-transfer recombination channel in the $ab$
initio CC framework by taking exchange exactly and also by using the regularized model exchange \[21\] in the CC equations.

**Theory:** Antisymmetrizing for the constituent electrons, we expand the total wave function of the Ps-H system in terms of Ps \((\chi_{\nu})\), H \((\phi_{\mu})\), and H\(^-\) \((\psi_{\rho})\) states as

$$
\Psi^S(r_1, r_2, x) = \sum_{\nu} \sum_{\mu} \left[ F_{\nu\mu}(s_2) \chi_{\nu}(t_2) \phi_{\mu}(r_1) + (-1)^S F_{\nu\mu}(s_1) \chi_{\nu}(t_1) \phi_{\mu}(r_2) \right] + \delta_{S0} G_{\rho}(x) \psi_{\rho}(r_1, r_2),
$$

where \(r_1, r_2\) denote the electron coordinates, and \(x\) is the positron coordinate of Ps; \(s_i = (r_i + x)/2, t_i = (r_i - x); i = 1, 2\). \(S\) is the total electron spin of the system in a particular channel which can have values 0 and 1, corresponding to singlet and triplet scattering; \(\delta_{S0}\) is the Kronecker delta. \(F_{\nu\mu}\) is the continuum orbital of Ps and \(G_{\rho}\) is that of the rearranged positron with respect to the center of mass fixed in the target nucleus.

The total Hamiltonian of the system may be taken as

$$
H = -\frac{1}{4} \nabla^2_{Ps} + H_{Ps}^0 + H_{H}^0 + V(1)
$$

or

$$
H = -\frac{1}{2} \nabla^2_p + H_{H^-}^0 + V(2)
$$

where \(H_{Ps}^0\), \(H_{H}^0\), and \(H_{H^-}^0\) are the unperturbed Hamiltonian for the Ps, H, and H\(^-\), respectively; \(-\frac{1}{4} \nabla^2_{Ps}\) and \(-\frac{1}{2} \nabla^2_p\) represent the kinetic energies of the Ps and the positron, respectively. \(V(1)\) is the interaction potential in channel-1 (elastic) and \(V(2)\) is the same in the charge-transfer rearrangement channel (channel-2: \(e^+ H^-\)). For channel-1, we have direct scattering (denoted by superfix \(d\)) and exchange scattering (denoted by superfix \(e\)) and for the transfer channel, there is no notion of exchange and we have only the direct scattering. The coulomb potentials for these channels are given by:

$$
V^d(1) = \frac{1}{x} - \frac{1}{|x - r_2|} - \frac{1}{r_1} + \frac{1}{|r_1 - r_2|}
$$
\[ V^e(1) = \frac{1}{x} - \frac{1}{|x - r_1|} - \frac{1}{r_2} + \frac{1}{|r_1 - r_2|} \]  

\[ V(2) = \frac{1}{x} - \frac{1}{|x - r_2|} - \frac{1}{|x - r_1|} \]  

We use exact wave function for Ps and H, and for H\(^{-}\), we use the wave function of Chandrasekhar \[35\]. Understanding the difficulty in dealing with a coulomb wave for the outgoing positron, we treat it with a plane wave in the input Born matrix element for channel-2, as the distortion to this plane wave will partly be done through the use of dynamical Lippmann-Schwinger equation (given in the next paragraph) and coupling over intermediate states.

Projecting over final states of Ps (\(\chi_\nu\)), H (\(\phi_\mu\)), and H\(^-\)(\(\psi_\rho\)), the LS equation for particular electronic spin state ‘S’, (which can have values 0 and 1, in general but for \(e^+H^-\) channel, it is ought to be 0 only as H\(^-\) can exist only in singlet state), can be recast as \[36\]:

\[
\begin{align*}
 f^S_{\nu',\mu',\mu}(k_f, k_1) &= B^S_{\nu',\mu',\mu}(k_f, k_1) \\
 &- \frac{1}{2\pi^2} \sum_{\nu''} \sum_{\mu''} \int dk_1'' \frac{B^S_{\nu',\mu',\mu''}(k_f, k_1'') f^S_{\nu',\mu',\mu''}(k_1'', k_i)}{k_{\nu',\mu''}^2 - k_{1''}^2 + i0} \\
 &- \delta_{\nu''0} \frac{1}{2\pi^2} \sum_{\rho''} \int dk_2'' \frac{B^S_{\nu',\mu',\rho''}(k_f, k_2'') f^S_{\nu',\mu',\rho''}(k_2'', k_i)}{k_{\rho'',\mu''}^2 - k_{2''}^2 + i0} \\
 &- \frac{1}{2\pi^2} \sum_{\nu''} \sum_{\mu''} \int dk_1'' \frac{B^S_{\rho',\mu',\rho''}(k_f, k_2'') f^S_{\rho',\mu',\rho''}(k_2'', k_i)}{k_{\rho',\mu''}^2 - k_{2''}^2 + i0} \\
 f^S_{\rho',\mu',\mu}(k_f, k_i) &= B^S_{\rho',\mu',\mu}(k_f, k_i) \\
 &- \frac{1}{2\pi^2} \sum_{\rho''} \int dk_2'' \frac{B^S_{\rho',\mu',\rho''}(k_f, k_2'') f^S_{\rho',\mu',\rho''}(k_2'', k_i)}{k_{\rho'',\mu''}^2 - k_{2''}^2 + i0} \\
 &- \frac{1}{2\pi^2} \sum_{\nu''} \sum_{\mu''} \int dk_1'' \frac{B^S_{\nu',\mu',\rho''}(k_f, k_2'') f^S_{\nu',\mu',\rho''}(k_2'', k_i)}{k_{\nu',\mu''}^2 - k_{2''}^2 + i0}
\end{align*}
\]  

where, \(k_{\nu',\mu''} = \frac{2m_1}{\hbar^2}(E - \epsilon_{\nu'} - \Upsilon_{\mu''})\); and \(k_{\rho'',\mu''} = \frac{2m_2}{\hbar^2}(E - \nu_{\rho''})\); \(k_{\nu',\mu''}\) and \(k_{\rho'',\mu''}\) are the on-shell momenta; \(m_1\) and \(m_2\) are the masses of \(e^+\) and Ps, respectively. \(E\) represents the total energy of the system; \(\epsilon_{\nu'}, \Upsilon_{\mu''}\), and \(\nu_{\rho''}\) represent the binding energies of Ps, H, and H\(^-\) ion, respectively. It is interesting to note that, for the charge-transfer channel, the
summation over $\rho''$ is restricted by itself as without a magnetic field, $H^-$ can exist only in its ground singlet state ($S = 0$) \[17\]. We study the effect of this channel over the elastic scattering channel (channel-1) and thus we restrict the summation over $\nu''$ and $\mu''$ to the ground states of Ps and H, respectively. The input potentials to the coupled equations, in general, are given by

\[
B^{0,1}_{\nu',\mu',\nu\mu}(k_f, k_i) = B^d_{\nu',\mu',\nu\mu}(k_f, k_i) + (-1)^{0,1}B^e_{\nu',\mu',\nu\mu}(k_f, k_i)
\]

\[
B^0_{\rho,\nu\mu}(k_f, k_i) = B^d_{\rho,\nu\mu}(k_f, k_i)
\]

(9)

Where, $B^d$ and $B^e$ are the direct Born and exchange Born-Oppenheimer (BO) amplitudes.

The exact form for $B^d_{\nu',\mu',\nu\mu}$, is available in the literature \[9, 21\] but here we follow the sign convention for the Ps-wave function as used in \[18\]. For $B^e$, we consider both the exact form (Appendix I) as well as the regularized form \[21\] with appropriate sign convention \[18\]. We use $\hbar = c = m_2 = 1$, where $m_2$ is the mass of electron or positron and $m_1 = 2$, the mass of Ps.

The elastic cross section and $H^-$ formation cross section is given by:

\[
\sigma_{el} = \frac{1}{4}|f^0_{1s1s,1s1s}|^2 + \frac{3}{4}|f^1_{1s1s,1s1s}|^2
\]

\[
\sigma_{H^-} = \frac{|k_f|}{|k_i|} \frac{1}{4}|f^0_{1s^2,1s1s}|^2
\]

(10)

(11)

Recently, a concern has been raised by Adhikari and Mandal (AM) \[38\] regarding the validity of the calculation of the BO exchange term of Sinha et al \[13\] and provided a different results for this BO exchange term. We were also concern with AM regarding the feature of a minimum in the elastic cross section with BO exchange near 35 eV. However, present results for $B^e_{1s1s,1s1s}$ exchange agree exactly with those of Sinha et al \[13\] and when this BO amplitude is used in the coupled equations, along with the required off-shell matrix element, it reproduces the static-exchange phase shifts of Campbell et al \[10\], Sinha et al \[13\], and Hara and Fraser \[4\] quite precisely (discussed in the results
and discussion). So, it implies that the BO exchange amplitudes in these calculations are
same and the minimum in the cross section is a feature of the BO exchange term and not
due to any error in its evaluation. AM evaluates the BO exchange term relying mostly
on numerical calculations where the integrand contains spherical Bessel functions and
they have reported to use 400 Gauss-quadrature points in the evaluation of the integrals.
Whereas, using Fourier transform and Chasire integrals, we reduce the nine-dimensional
integrals (Appendix I) to simple two-dimensional integrals which is found to converge with
mere eight Gauss-quadrature points for each integration variable and hence any numerical
problem is ruled out in this methodology compared to that provided by AM [38].

In Appendix I, we provide the analytical form of the \textit{ab initio} BO exchange matrix
element \(B_{1s1s,1s1s}^e\) and the charge-transfer matrix element \(B_{1s1s,1s1s}^d\) is detailed in Appendix
II. In a separate study, we employ the regularized model exchange for \(B_{1s1s,1s1s}^e\), which is
taken from ref.[18] (it differs only in sign convention from ref.[21]).

\textbf{Numerical Procedures} : In the present investigation, we consider static-exchange
(SE) and SE plus charge-transfer reactions of Ps-H to \(e^+\)-H\(^-\). The three-dimensional
LS equations, for a particular electronic-spin state \((S)\) are decomposed to coupled one-
dimensional partial wave equations, which are then solved by the method of matrix in-
version. We find that at low energies, 44-48 Gauss quadrature points (24 points for
\(k''_1 = 0 - 2k_{\nu''\mu''}\) interval and 20-24 points for \(k'' = 2k_{\nu''\mu''} - \infty\) interval and similarly for
\(k''_2\) are needed for the discretization of the Kernel of the LS equation, to achieve numerical
convergence up to 4-decimal places.

\textbf{Results and Discussions} : We begin the discussions of our results with the singlet
channel cross sections. The effect of the Ps+H\(\rightarrow\) \(e^+\)H\(^-\) channel would be revealed in
this singlet channel, as H\(^-\) belongs to a spin singlet state only. Also, the binding and
resonance of PsH occur in this channel. In figure-1, we plot the S-wave singlet cross section
from 0-10 eV to exhibit the influence of this channel (channel-2) over the static-exchange
prediction (using both exact and model exchange). In both the cases, we find that this channel reduces the singlet scattering cross section significantly, at low energies. This implies that this channel effectively makes the attractive potential more strong and we can expect a smaller scattering length and a greater binding energy. Using an effective-range expansion of the form
\[ k \cot \delta = -1/a + r_0 k^2/2 + D k^4, \]
and finding solution of the equation
\[ k \cot \delta - i k = 0 \]
for the bound state, where \( k \) is the momentum of Ps, \( \delta \) is the S-wave singlet phase shift, \( r_0 \) is the corresponding effective range, and \( D \) is the coefficient for the \( k^4 \) term, we obtain the binding energy and scattering length which are tabulated in table 1.

**Table 1:** Scattering length (S.L.) and binding energies (B.E.) in the singlet channel of Ps-H, from static-exchange (SE), static-exchange plus charge-transfer rearrangement (2CH) employing exact exchange. Model exchange results without any parameterization (\( C = 1 \)) are represented by (ME). a) present predictions; b) prediction of Campbell et al [10]

|        | SE          | 2CH         | SE(ME)      | 2CH(ME)     | 22-state |
|--------|-------------|-------------|-------------|-------------|----------|
| S.L.   |    a) 7.273 | 6.90        | 8.427       | 5.544       |          |
|        |    b) 7.25  |             |             |             | 5.20     |
| B.E.   | a)-0.253    | -0.291      | -0.139      | -0.394      |          |
|        | b)-0.263    |             |             |             | -0.634   |

As expected, we find the scattering length (S.L.) is reduced and the binding energy (B.E.) is increased with the influence of the H\(^-\) formation channel. The effect is much pronounced in the case of model exchange calculation, thus signifying a lesser role for the parameter in the model potential. The scattering length prediction in the 2CH(ME) is quite close to the 22-state prediction. Keeping in mind the simple form of H\(^-\) wave function used in this calculation, and the proven role of the direct \( r_{12} \) term in the variational prediction [28], we get the impression that the impact of this channel in the \( ab \)
initio model could be improved significantly by using a more sophisticated wave function for H\(^-\) which contains the \(\mathbf{r}_{12}\) term. The small difference in the scattering length (S.L.) and binding energy (B.E.) of SE calculations of set (a) and set (b) is due to the fact that in (b) we have used an effective range expansion to extrapolate the phase shifts to the negative energy region while in set (a) those parameters are directly solved. The positive energy scattering phase shifts for (a) and (b) agree exactly. We tabulate the phase shifts for different models in table 2 for future reference.

**Table 2**: Variation of singlet and triplet scattering phase shifts for different models with energy \((E = 6.8k^2 \text{ eV})\): SE-static exchange; 2CH-static exchange plus \(e^+H^-\) channel; (ME)-represents the calculations with model exchange but without any parameterization \((C = 1)\).

| \(k\) | singlet | triplet |
|------|---------|---------|
|      | SE      | 2CH     | SE(ME) | 2CH(ME) | SE      | SE(ME) |
| 0.1  | 2.455   | 2.485   | 2.387  | 2.610   | -0.247  | -0.145  |
| 0.2  | 1.927   | 1.966   | 1.910  | 2.176   | -0.489  | -0.283  |
| 0.3  | 1.539   | 1.577   | 1.604  | 1.848   | -0.721  | -0.410  |
| 0.4  | 1.239   | 1.275   | 1.381  | 1.596   | -0.940  | -0.521  |
| 0.5  | 0.997   | 1.032   | 1.207  | 1.396   | -1.143  | -0.613  |
| 0.6  | 0.797   | 0.831   | 1.065  | 1.232   | -1.330  | -0.683  |
| 0.7  | 0.631   | 0.664   | 0.946  | 1.094   | -1.499  | -0.731  |
| 0.8  | 0.491   | 0.523   | 0.845  | 0.977   | -1.653  | -0.757  |
| 0.9  | 0.373   | 0.406   | 0.758  | 0.876   | -1.790  | -0.763  |
| 1.0  | 0.274   | 0.307   | 0.683  | 0.786   | -1.913  | -0.781  |

First we discuss about SE phase shifts where recently a dispute has been raised [38]. Table 2 shows that the present phase shifts for the SE calculation for the singlet and triplet scattering agree exactly with the existing SE predictions of Hara and Fraser [4] and Sinha et al [13]. Campbell et al [10] provided SE phase shifts for other \(k\)-values (Ps energy, \(E = 6.8k^2\)).
$k^2 = 0.1639, 0.2478, \text{ and } 0.5588 \text{ (a.u.)}$ the singlet phase shifts of Campbell et al are given by (table 1 of ref. [10]) 1.23, 1.00, 0.56, respectively and our predicted values are 1.228, 1.002, and 0.5614, respectively (all cross sections are in units of $\pi a_0^2$). So all these SE predictions, which use BO exchange amplitude as the input, agree among themselves. This suggests that the minimum in the BO cross section is a true feature of the model and the results of Adhikari and Mondal (AM) [38] cannot agree with Campbell et al [10]. Since, at $k^2 = 0.5588$, the BO cross sections of AM [38] is about $23.5\pi a_0^2$, which is approximately 22% higher than the BO cross sections ($19.3\pi a_0^2$) of Sinha et al and present calculation. So, it is certain that any static exchange prediction made using the BO exchange amplitude of AM as input to the CC equations, will disagree with all existing SE results including those of Campbell et al [10]. While trying to get an answer to the minimum in the elastic BO cross section, we find that for forward scattering the exchange potential changes its sign at about 26-27 eV, which is causing the minimum in the cross section. We now come to the main business of the assessment of the influence of the H$^-$ formation channel over the SE predictions.

In table 2, we compare the phase shifts of SE and 2CH calculations. For 2CH we do not tabulate the triplet phase shifts since they do not change by the influence of channel-2 (as H$^-$ exists only in singlet state). From table 2, we see that singlet phase shifts increase significantly with the inclusion of the H$^-$ formation channel. This signifies an increase in the attractive potential, which was expected and needed in the CC theory to improve the convergence and hence improve the PsH binding energy. It is interesting to note that the effect of this channel continues significantly around $k = 1.0$.

In figure 2, we plot the elastic cross sections for SE, SE(ME), 2CH, and 2CH(ME) models. In this figure we also plot the recent variational prediction [39] on the zero energy cross section. Elastic cross sections for both the \textit{ab initio} and model calculations are reduced by the influence of the charge transfer channel. At low energies, the 2CH(ME) model gives much lower cross section than the 2CH model and the former is quite close to the recent variational prediction [39]. We have earlier find that this model can lead to more converged results if the model exchange
potential is tuned by means of a parameter \( C \). While trying to analyze the physics behind such agreement with measurements and accurate variational predictions, we find that effectively, while making approximate mapping of a basis set \( (\psi_\mu(r_2)) \) belonging to a different Fock-space to its original Fock-space \( (\psi_\mu(r_1)) \), basically we are indulging to approximations like:

\[
\int \psi_\mu(r_2) \frac{1}{|r_1 - r_2|} dr_2 = \frac{1}{Ck^2_\mu} \psi_\mu(r_1) \tag{12}
\]

\[
\int \phi_\nu(x - r_2) \frac{1}{|r_1 - r_2|} dr_2 = \frac{1}{Ck^2_\nu} \phi_\nu(x - r_1) \tag{13}
\]

where \( k^2_\mu \) and \( k^2_\nu \) are the average values of the square of the momenta of the respective electrons when they were bound in the hydrogen \( (\psi_\mu(r_2)) \) or in the positronium atom \( (\phi_\nu(x - r_1)) \) and \( C \) is a parameter which is fixed to unity but could be varied to tune results. Clearly, the above relations are introducing some amount of \( e_1 - e_2 \) correlation and the continuum effects of the target (eqn.()) and the projectile (eqn.()), respectively. Also, these effects would be modified when the value of \( Ck^2_\mu \) or \( Ck^2_\nu \) are changed. Interestingly, the model provides best results \([17, 22, 18]\) when \( Ck^2_\mu \) and \( Ck^2_\nu \) become close to the ionization energies for the respective electrons. Although the mixing of such model exchange with \textit{ab initio} charge-transfer process yielded very good response, we are doubtful about the overcompleteness of the Hilbert space if such mixing is continued with a larger basis for Ps. However, from the results of the 2CH model and from our experience in such rearrangement for positron-atom scattering [], we understand that for the full \textit{ab initio} model (2CH) the possibility of overcompleteness is remote unless a very large basis is used. The information we gain here in terms of the convergence of the 2CH prediction appears consistent and encouraging due to the fact that virtual excitations of Ps are absent here. The charge-transfer reaction becomes exothermic for \( n \geq 5 \) and higher discrete excited states and continuum of Ps and hence the effect of such a channel is likely to be significant with higher Ps eigen states and pseudostates. Consideration of this channel along with the Ps-excited states would also reveal its effect on resonances, which manifest in the theory with the inclusion of Ps excited states.

Another interesting feature of such study is that it provides the \( \text{H}^- \) formation cross section.
which is of importance in Astrophysics. Here we provide the $\text{H}^-$ formation cross sections from Ps(1s)-H(1s) scattering in figure-2. Solid curve is obtained with the regularized exchange \cite{21, 18} while the dotted curve is obtained with *ab initio* exchange. It is observed that from 60 eV onwards the two sets of results are same signifying the fact that the regularized model exchange asymptotically coalesce with the exact one. From the two curves we also see that, in the low and intermediate energies, the cross sections calculated with the regularized exchange CC model (2CH(ME)) are higher than those calculated with *ab initio* exchange (2CH). This was quite expected as the regularized exchange potential, as discussed above, was found to simulate the continuum effect substantially and yield converged results for the PsH binding and resonances \cite{17, 22}. The contribution from virtual Ps excitations, no doubt will increase the $\text{H}^-$ formation cross section and this trend has been revealed in the 2CH(ME) calculation.

**Conclusion:** In summary, we make a first time study of the effect of charge transfer recombination for Ps scattering from hydrogen. Considering the rearrangement of PsH to $e^+\text{H}^-$ we get the information that such rearrangement can introduce the continuum effect more effectively than considering only exchange. The attractive potential introduced by this channel improves the scattering length and binding energy predictions significantly. The influence of the channel is also found to help converging the low energy cross sections (see figure 1). Similar effect of charge-transfer recombination was found in the cases of positron-atom scattering \cite{1, 2} and in the present case of Ps-atom scattering it could be more interesting as the threshold for the transfer process Ps(1s)+H(1s)→ $e^+\text{H}^-$ decreases with higher Ps states and the reaction becomes exothermic for $n \geq 5$ discrete excited states and continuum of Ps. So, it is expected that the channel would contribute substantially through virtual Ps excitations and lead to further convergence for the low energy Ps scattering parameters. As a by product we get $\text{H}^-$ formation cross sections which has astrophysical importance.

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Appendix I

The Born-Oppenheimer exchange matrix element for the elastic transition is given by:

\[ B_{1s1s,1s1s}(k_f, k_i) = -\frac{m_1}{2\pi} \int \int e^{-i\frac{1}{2}(r_2+x)} \chi_{1s}(r_2-x) \phi_{1s}(r_1) V_{int} \times e^{i\frac{1}{2}k_i(r_1+x)} \chi_{1s}(r_1-x) \phi_{1s}(r_2) dx dr_1 dr_2. \] (14)

where \( k_i, k_f \) are the initial and final momentum of the Ps atom with respect to the center of mass. We use \( \hbar = c = m_2 = 1 \), \( m_2 \) is the mass of the electron or positron; the Ps mass \( m_1 = 2 \).

Splitting with the four terms of \( V_{int}^{(1)} \) of eqn(4), we write \( B_{1s1s,1s1s} = B_1 + B_2 + B_3 + B_4 \), where subscripts denote the terms on the r.h.s. of eqn(4), in sequence. We use Fourier transform, delta-function integration, and Chasire integrals to reduce each nine dimensional integrals to two dimensions. We follow same procedure for \( B_1, B_2, B_3, B_4 \). We detail for \( B_4 \), which contains \( 1/|r_1 - r_2| \) term of \( V_{int}^{(1)} \). Using \( \chi_{1s}(r) = \frac{1}{\sqrt{8\pi}} e^{-\beta r} \) and \( \phi_{1s}(r) = \frac{1}{\sqrt{\pi}} e^{-\alpha r} \), with \( \beta = 0.5 \) and \( \alpha = 1.0 \), we perform integration over \( dx \) first, then over \( dr_1 \), and finally over \( dr_2 \) to get,

\[ B_4 = 4\beta^2\alpha \int_0^1 du u(1-u) \int_0^1 dv v \left( \frac{1}{\mu_1} \frac{\partial}{\partial \mu_1} \right)^2 \left( \frac{1}{\mu_2} \frac{\partial}{\partial \mu_2} \right)^2 \frac{1}{\mu_2} \left( |\Lambda|^2 + \mu_{2\alpha}^2 \right) \] (15)

where

\[ \mu_1^2 = \beta^2 + u(1-u)(0.5(k_i - k_f))^2 \] (16)
\[ \mu_2^2 = \nu\alpha^2 + (1-v)\mu_1^2 + v(1-v)|Q|^2 \] (17)
\[ Q = (1-0.5u)k_i - 0.5(1-u)k_f \] (18)
\[ \Lambda = (0.5u + v - 0.5uv)k_i - 0.5(1+u+v-uv)k_f \] (19)
\[ \mu_{2\alpha} = \mu_2 + \alpha \] (20)

For the rest of \( B_1, B_2 \) and \( B_3 \), we perform integration over \( dr_1 \) first, then over \( dx \), and finally over \( dr_2 \) and arrive at similar final forms as above, with changed definition for \( \mu_2, Q, \Lambda \) etc. Integration over each of \( du \) and \( dv \) is converged with mere eight Gauss-quadrature points.
Appendix II

The charge transfer matrix element for the $\text{Ps}+\text{H} \rightarrow e^++\text{H}^-$ channel is given by:

$$B^d_{1s^2,ls1s}(k_f,k_i) = -\frac{m_1}{2\pi} \int \int e^{-\mathbf{k}_f \cdot \mathbf{x}} \psi_H^-(\mathbf{r}_1, \mathbf{r}_2) V^{(2)}_{\text{int}} e^{i\frac{\mathbf{k}_f}{2} \cdot (\mathbf{r}_1 - \mathbf{x})} \chi_{ls}(\mathbf{r}_1 - \mathbf{x}) \phi_{ls}(\mathbf{r}_2) d\mathbf{x} d\mathbf{r}_1 d\mathbf{r}_2 \tag{21}$$

where $k_f$ now represents the momentum of the ejected positron with respect to the center of mass rest on the proton; $m_1 = 1$; $\psi_H^-(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{N} \left( e^{-ar_1} e^{-br_2} + e^{-ar_2} e^{-br_1} \right)$, the $\text{H}^-$ wave function with binding energy $E = -0.51330$ and $a = 1.03925$, $b = 0.28309$ and the normalization constant has been worked out to be $N = 31.80348105$. As in Appendix I, we split the integral as $B^d_{1s^2,ls1s} = B_1 + B_2 + B_3$, with the three terms of $V^{(2)}_{\text{int}}$ of eqn(5), where subscripts denote the terms on the r.h.s. of eqn(5), in sequence. Using the symmetry of the $\text{H}^-$ wave function we write $B_j = B_j(a,b) + B_j(b,a); j = 1, 2, 3$. We use Fourier transform, delta-function integration and Chasire integrals and evaluate $B_2$ exactly.

$$B_2(a,b) = -\frac{64\sqrt{2}\pi^2 a}{(\alpha + b)^3(|q_{1/2}|^2 + \beta^2)^2 + (|q|^2 + a^2)^2} \tag{22}$$

where $q_{1/2} = \frac{1}{2} k_i - k_f$ and $q = k_i - k_f$. Integration over $d\mathbf{r}_2$ in $B_1$ is simple and in $B_3(a,b)$, it gives

$$I = \int e^{-(\alpha+b)r_2} \frac{d\mathbf{r}_2}{|\mathbf{x} - \mathbf{r}_2|} = \frac{8\pi}{(\alpha + b)^3 x} - \frac{8\pi e^{-(\alpha+b)x}}{(\alpha + b)^3 x} - \frac{4\pi e^{-(\alpha+b)x}}{(\alpha + b)^2} \tag{23}$$

With this form of $I$, we write $B_3(a,b) = B_3^1(a,b) + B_3^2(a,b) + B_3^3(a,b)$. Now $B_3^3(a,b)$ cancels out with $B_1(a,b)$ and similarly for $B_3^2(b,a)$ and $B_1(b,a)$. We evaluate $B_3^2(a,b)$ and obtain $B_3^2(a,b)$ from it with a derivative w.r.to $(\alpha + b)$. The final form of $B_3^2(a,b)$ is

$$B_3^2(a,b) = \frac{32\sqrt{2}\pi^2 \beta}{(\alpha + b)^3} \int_0^1 du \left( \frac{1}{\mu} \frac{\partial}{\partial \mu} \right) \frac{1}{\mu} \frac{\mu + a}{(|Q|^2 + (\mu + a)^2)^2} \tag{24}$$

where

$$\mu^2 = u\beta^2 + (1 - u)(\alpha + b)^2 + u(1 - u)|q_{1/2}|^2 \tag{25}$$

$$Q = (1 - 0.5u)k_i - (1 - u)k_f \tag{26}$$
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Figure Captions:

Fig. 1: Variation of S-wave singlet cross sections (in units of $\pi a_0^2$) for Ps-H scattering employing static-exchange (SE), SE plus charge-transfer rearrangement to $e^+H^-$ (2CH). (ME) represents calculations using model exchange [21]:

Fig. 2: Variation of elastic cross sections (in units of $\pi a_0^2$) for Ps-H scattering employing static-exchange (SE), SE plus charge-transfer rearrangement to $e^+H^-$ (2CH). (ME) represents calculations using model exchange [21]:

Fig. 3: $H^-$ formation cross sections from Ps(1s)-H(1s) scattering (in units of $\pi a_0^2$). 2CH corresponds to results from the two-channel calculation with \textit{ab initio} exchange while 2CH(ME) is the same using regularized model exchange.
Figure 1

S-wave singlet cross sections (in units of $\pi a_0^2$) vs. Incident Ps Energy (eV)

- -- SE
- --- 2CH
- - - - SE(ME)
- --- 2CH(ME)
Figure 2

Elastic cross sections (in units of $\pi a_0^2$) vs. Incident Ps Energy (eV)

- SE(ME)
- 2CH(ME)
- SE
- 2CH
- Variational [37]
Figure 3

\begin{figure}
\centering
\includegraphics[width=\textwidth]{Figure3.png}
\caption{H\textsuperscript{−} formation cross sections (in units of \(\pi a_0^2\)) for 2CH(ME) and 2CH.}
\end{figure}