Detailed calculations on low-energy positron-hydrogen-molecule and helium-antihydrogen scattering

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Abstract. In this paper, we consider two scattering processes: low-energy positron-hydrogen-molecule and helium-antihydrogen scattering. In the positron-hydrogen-molecule scattering calculations, we use the Kohn variational method to calculate $Z_{\text{eff}}$, the number of target electrons available to the positron for annihilation. In the helium-antihydrogen scattering calculations, we use the Rayleigh-Ritz variational method to calculate a wave function for the leptons as a function of the distance between the helium and the antihydrogen. This is used, together with the associated nuclear wave function and the wave function for $\alpha \bar{p} + Ps^-$, to calculate the cross section for the rearrangement reaction $\text{He} + \bar{H} \rightarrow \alpha \bar{p} + Ps^-$, using the $T$-matrix and a form of the distorted wave approximation. For both processes, positron-electron correlation is taken into account accurately using Hylleraas-type functions.
1. Introduction

The two scattering processes to be considered are positron-hydrogen-molecule and helium-antihydrogen scattering, both at low energies. These systems both contain two nuclei and the same leptons, namely a positron and two electrons. The calculations are carried out with the nuclei in a fixed position. Thus in the two scattering processes, we treat the motion of the same three light particles. As a consequence, the calculations on the two processes have many features in common.

We will begin by considering positron-hydrogen-molecule scattering. Attention will be focussed on the calculation of $Z_{\text{eff}}(k)$, the effective number of electrons in the H$_2$ target that are available to the incident positron for annihilation. $k$ is the wave number of the positron. The positron annihilation rate, $\lambda$, is given by

$$\lambda = \pi r_0^2 c D Z_{\text{eff}}(k),$$

(1)

where $r_0$ is the classical radius of the electron and $D$ is the density of H$_2$ molecules in the vicinity of the positron.

Another area of great current interest is the preparation of cold antihydrogen ($\bar{H}$) and the study of its properties by the ALPHA and ATRAP collaborations at CERN [1, 2]. It is of interest to determine the interaction of antihydrogen with simple atoms and molecules. In view of this, we have carried out calculations of very low-energy H$\bar{H}$ scattering [3] and, more recently, of He$\bar{H}$ scattering [4]. In this paper, we describe calculations that we have carried out of cross sections for the rearrangement reaction

$$\text{He} + \bar{H} \rightarrow \alpha \bar{p} + \text{Ps}^-, \quad (2)$$

at very low energies.

Unless otherwise states, the units used in these calculations are hartree atomic units.

2. Positron-hydrogen-molecule scattering

2.1. Calculations using the complex Kohn method

The coordinate system used in our calculations on e$^+$H$_2$ scattering is illustrated in Fig 1. The protons are fixed at $A$ and $B$, which have coordinates $(0, 0, -R)$ and $(0, 0, R)$, respectively, where $R$ is the internuclear distance. The prolateral spheroidal coordinates $(\lambda, \mu, \phi)$ used in the calculations are of the form

$$\lambda = \frac{r_A + r_B}{R} \quad \text{and} \quad \mu = \frac{r_A - r_B}{R},$$

$\phi$ is the usual azimuthal angle of spherical polar coordinates. Unless stated otherwise, the internuclear distance $R$ was fixed at 1.4$a_0$, the equilibrium value for the H$_2$ molecule.

The Kohn trial function was taken to be of the form

$$\Psi_{\text{trial}} = \psi_p \phi_{\text{target}} + \sum_{i=0}^{n} g_i \chi_i.$$  (3)

The open channel function $\psi_p$ was taken to have the form

$$S + a e T$$

where

$$T = S + iC$$        (4)
$S = N \frac{\sin[c(\lambda_1 - 1)]}{\lambda_1 - 1}$  \hspace{1cm} (5)

$C = N \frac{\cos[c(\lambda_1 - 1)]}{\lambda_1 - 1} \left(1 - \exp[-\gamma(\lambda_1 - 1)]\right)$  \hspace{1cm} (6)

where $\lambda_1$ is the ellipsoidal prolate spheroidal coordinate for the positron, $\gamma = \frac{1}{2} k R$, $N$ is a normalisation constant and $\phi_{\text{target}}$ is the H$_2$ target wave function. This is the simplest form for the function, $\psi_p$. It represents the $s$-wave component of the part of the overall scattering wave function that is of $\sum^{+}_{\sigma}$ symmetry. $\{\lambda_i\}^n_{i=0}$ are short-range correlation functions and $a_i$ and $\{g_i\}$ are linear parameters to be determined by the complex Kohn method.

The short-range correlation functions are of the form

$\chi_0 = C \exp[-\gamma(\lambda_1 - 1)] \phi_{\text{target}}$  \hspace{1cm} (7)

$\chi_i = S_{23} N \alpha \lambda_1^2 \lambda_2^2 \lambda_3^2 \mu_1^2 \mu_2^2 \mu_3^2 C(s_i, t_i) \exp[-\alpha \lambda_1 - \beta (\lambda_2 + \lambda_3)] \Omega$  \hspace{1cm} (i $\neq 0$, (8)

where particle 1 is the positron and particles 2 and 3 the electrons, $S_{23}$ is the electron symmetriser, $\alpha$ and $\beta$ are positive, non-linear parameters and $N$ is a normalisation constant. $a_i, b_i, c_i, d_i, e_i, f_i$ are non-negative integers. The forms used for $C(s_i, t_i)$ are given in Table 1. If the method of models [5] is used

$\Omega = \phi_{\text{target}}$.

Otherwise $\Omega$ is taken to be equal to one.

Earlier calculations by the generalised Kohn method used the method of models [6]. In this method, the target Hamiltonian, $\hat{H}_t$, is taken to be

$\hat{H}_t \phi_{\text{target}} = E_t \phi_{\text{target}}$  \hspace{1cm} (10)

where $E_t$ is the expectation value of the energy of $\phi_{\text{target}}$. No knowledge of $V_{\text{mod}}$ is required when carrying out Kohn calculations. Also we do not have to consider the $\frac{1}{R^2}$ electron repulsion term in the exact form of the target potential.

This had the very considerable advantage that it was possible to include the key correlation functions in Table 1 containing $C(1, 1) = \rho_{12} = \frac{2}{\pi} \tau_{12}$ without calculating integrals involving $\frac{\rho_{12}}{\rho_{23}}$. These functions are Hylleraas-type functions that correlate the positron and the electrons. They play a very important role in improving the accuracy of the wave function at points at which the positron and an electron coincide that are the key to calculating $Z_{\text{eff}}(k)$ accurately. However, the complexity of the calculation only made it possible to use a target wave function that took into account 50% of the correlation energy of the H$_2$ molecule. This percentage is given by

$$\left(\frac{E_{\text{SCF}} - E_t}{E_{\text{SCF}} - E_{\text{ex}}}\right) \times 100$$  \hspace{1cm} (11)

where $E_{\text{SCF}}$ is the SCF energy of H$_2$ and $E_{\text{ex}}$ is the exact, non-relativistic energy of H$_2$ at $R = 1.4a_0$.

$Z_{\text{eff}}(k)$ is known to have a value of 14.6 for thermal positrons at 297K [7]. At this temperature, $kT = 26$ meV. Inclusion in the basis set of Hylleraas-type functions that correlate the positions of the positron and the electrons raised this to $\sim 10.2$ [6].
Our calculations [8] have been carried out without using the method of models. Inclusion of Hylleraas-type functions required the evaluation of integrals containing \( \rho_{12}/\rho_{23} \), in addition to those containing \( \rho_{13}^2 \) and \( \rho_{12}/\rho_{23} \) that were required when using the method of models. These evaluations were carried out using the Neumann expansion

\[
\frac{1}{\rho_{ij}} = \sum_{\tau=0}^{\infty} \sum_{\nu=0}^{\tau} D_{\nu}^\tau(\lambda_\nu)(\lambda_\nu)(\lambda_\nu)P_{\nu}^\mu(\mu_i)P_{\nu}^\mu(\mu_j) \cos[\nu(\phi_i - \phi_j)] \tag{12}
\]

where \( \lambda_\nu \) is the lesser of \( \lambda_i \) and \( \lambda_j \) and \( \lambda_\nu \) is the greater of \( \lambda_i \) and \( \lambda_j \), \( D_{\nu}^\tau \) is a coefficient and \( P_{\nu}^\mu(x) \) and \( Q_{\nu}^\mu(x) \) are the first and second solutions, respectively, to the associated Legendre equation.

The program used to evaluate the integrals containing \( \rho_{12}/\rho_{23} \) is to be published in Computer Physics Communications [9].

When carrying out the calculations without using the method of models, we were able to make the following improvements.

1. We used a target wave function that took into account up to 99.7% of the correlation energy of \( \text{H}_2 \).
2. The basis set used contained up to 297 short-range correlation functions as opposed to less than 100 in the calculation using the method of models.
3. We included Hylleraas-type functions in the basis set to take into account electron-electron correlation. These were not included in the calculations using the method of models.

We used two target functions, \( \phi_{1A} \) and \( \phi_{1B} \). \( \phi_{1A} \) was calculated using 144 basis functions, none of which were Hylleraas-type functions. It took into account 96.8% of the correlation energy of \( \text{H}_2 \). \( \phi_{1B} \) was calculated using the same 144 basis functions and one Hylleraas-type function containing \( \rho_{23} \) as a linear factor. It took into account 99.7% of the correlation energy.

The value of \( Z_{\text{eff}}(k) \) is given by the relation

\[
Z_{\text{eff}}(k) = \frac{1}{3} \sum_{i=2}^{3} \delta(r_1 - r_i)|\Psi_{\text{trial}}(k)|
\tag{13}
\]

where \( \Psi_{\text{trial}}(k) \) is the trial function obtained by the complex Kohn method for incident positrons with wave number \( k \). \( \Psi_{\text{trial}}(k) \) is normalised so that the incident positrons have density one per unit volume. \( r_i \) is the position vector of particle \( i \). The bar indicates averaging over all molecular orientations. The results obtained for \( Z_{\text{eff}}(k) \) at \( k = 0.04 \) are given in [8].

Recently, we have taken into account the motion of the nuclei in our calculations. As a first step we have determined how \( Z_{\text{eff}}(k) \) at \( k = 0.04 \) varies with the internuclear distance, \( R \). The results obtained both with and without the use of the method of models are given in Table 2. It can be seen that the results obtained using the method of modules are larger than those obtained without using this method. The vibrationally averaged value of \( Z_{\text{eff}}(k) \), obtained using a Morse function, is 13.5 when obtained using the method of models and 9.7 without using this method [10].

The value obtained with the method of models is closer to the experimental value of 14.6 than that obtained without using it. In a very recent, very accurate calculation of \( Z_{\text{eff}}(k) \) at very low energies, Zhang et al [11] find similar behaviour to the values we obtain using the method of models as \( R \) increases beyond 1.6a_0. It may be relevant that results obtained by the method of models have been found to have better convergence behaviour than those obtained without using this method [12, 8].
2.2. Investigation of the cause of large $Z_{\text{eff}}(k)$ values

It is of interest to consider a model system which makes it possible to use the Kohn method to investigate how $Z_{\text{eff}}(k)$ might be greatly increased through resonances due to the existence of vibrationally excited quasi-bound states of the positron and the molecule. It is such states that are considered by Gribakin [13] to be responsible for the very large $Z_{\text{eff}}(k)$ values that have been observed in low-energy, positron scattering by some organic molecules [14].

No positron H$_2$ bound state exists. However, we can increase the ‘positron’ mass $m_p$ to produce a weakly bound state.

Let us begin by applying the Born-Oppenheimer (B–O) approximation. The leptonic Hamiltonian is

\[
\hat{H}_{\text{lep}} = -\frac{1}{2m_p} \nabla^2_1 - \frac{1}{2} \nabla^2_2 - \frac{1}{2} \nabla^2_3 + \frac{1}{r_{A1}} + \frac{1}{r_{B1}} - \frac{1}{r_{A2}} - \frac{1}{r_{B2}} - \frac{1}{r_{A3}} + \frac{1}{r_{B3}} - \frac{1}{r_{12}} - \frac{1}{r_{13}} + \frac{1}{R},
\]

(14)

where $A$ and $B$ are the nuclei. The potential is made up of the Coulomb interactions between all five particles. The nuclei are fixed at internuclear distance $R$. The leptonic coordinates are fixed relative to the nuclei. For details of the relationship between molecule fixed coordinates and non-rotating coordinates, see, for example, Armour and Jonsell [15].

The Schrödinger equation for the leptons is

\[
\hat{H}_{\text{lep}} \Psi_{\text{lep},m}(r_1, r_2, r_3; R) = E_m(R) \Psi_{\text{lep},m}(r_1, r_2, r_3; R)
\]

(15)

In principle, this equation can be solved exactly. Suppose a weakly bound state is found for a range of $R$ values surrounding the equilibrium $R$ value of H$_2$.

There are two possibilities.

(1) The state is bound for all $R$ values for which the associated vibrational wave function has an appreciable non-zero value.

(2) The state is only bound for a subset of the above $R$ values.

We will only consider possibility (1). Denote the bound state by $m = 0$. There will also be continuum solutions to the Schrödinger (15). Denote them by $m = 1$. They will have energy

\[
E_1(R) = E_p + E_{\text{mo}1}(R),
\]

(16)

where $E_p$ is the energy of the incident positron and $E_{\text{mo}1}(R)$ is the electronic energy of H$_2$ at a given $R$ value. In our earlier calculations, we obtained approximate solutions of this type at a given $R$ value, in most cases the H$_2$ equilibrium value 1.4\AA.

In the B–O approximation, we obtain normalised bound states

\[
\{\Psi_{\text{lep},0}(r_1, r_2, r_3; R)\chi_{n0}(R)\}, \quad n = 0, 1, 2, \ldots
\]

where $\chi_{n0}(R)$ is a vibrational wave function associated with the potential $E_0(R)$, with appropriate angular momentum.

The bound state with $n = 0$, i.e. corresponding to the vibrational ground state, will be below the continuum. But when $n > 0$, the states will be in the continuum of states $\{\Psi_{\text{lep},1}(r_1, r_2, r_3; R)\chi_{10}(R)\}$. However, no interaction with the continuum will occur if we remain within the B–O approximation. Coupling will only occur if we go beyond the B–O approximation. These bound states will then become quasi-bound.
In Gribakin’s theory [16], it is the existence of a permanent molecular dipole moment that brings about coupling between the quasi-bound states and the continuum. \( \text{H}_2 \) does not have a permanent dipole moment. However, such a dipole moment could be introduced into our model by changing the unit charges on the nuclei to \( 1+Z \) and \( 1-Z \), where \( 0 < Z < 1 \). We have not thought it necessary to do this as the coupling between the quasi-bound states and the continuum is due to the breakdown of the B–O approximation. Further investigation is necessary to find out if any relationship between this and a permanent dipole moment can be derived.

We have carried out a preliminary Kohn calculation to investigate the effect on \( Z_{\text{eff}}(k) \) of the coupling between the lowest quasi-bound state, \( \Psi_{\text{lep},0}\chi_{01} \) with zero angular momentum and the continuum due to the breakdown of the B–O approximation. We take the target \( \text{H}_2 \) to be in its ground state with zero total angular momentum. We find analytically that resonant behaviour occurs when the energy \( E \) of \( e^+\text{H}_2 \) satisfies the relation

\[
E = E_{01} + B,
\]

where \( E_{01} \) is the energy of the quasi-bound state, as calculated using the B–O approximation. \( B \) is a level shift equal to the first order correction to \( E_{01} \) due to the inclusion of the terms neglected in the B–O approximation.

If we use a basis set containing \( \Psi_{\text{lep},0}\chi_{01} \) with all other basis functions orthogonal to it, we find from the Kohn equations that the coefficient of \( \Psi_{\text{lep},0}\chi_{01} \) in the scattering wave function is of \( O(\mu_M) \), when \( E \) satisfies (17). The contribution to \( Z_{\text{eff}}(k) \) at this \( E \) value from this quasi-bound state is thus of \( O(\mu_M^2) \). As \( \mu_M = 918 \), at this \( E \) value \( Z_{\text{eff}}(k) \) is likely to have a large value.

This theory should be extendable to organic molecules that have weakly bound positron-molecule states associated with very large values of \( Z_{\text{eff}}(k) \).

2.3. Examination of singular behaviour in generalised Kohn calculations

Running parallel to our calculations of \( Z_{\text{eff}}(k) \), we have carried out an examination of singularities that can arise when carrying out calculations using the generalised Kohn method in which a parameter \( \tau \) is added to \( c(\lambda_1 - 1) \) in the arguments of the sine and cosine factors in equations (5) and (6) and \( T \) in equation (4) is taken to be equal to the modified \( C \) factor. A detailed study is made of the structure of the Kohn equations and the behaviour of the phase shift as \( \tau \) is varied. A method is developed for determining an optimum choice of \( \tau \) to avoid anomalous behaviour due to the singularities. This optimum choice is shown to give a phase shift value that is the same as that obtained by taking the real part of the phase shift calculated using the complex Kohn method [10, 17, 18].

3. Helium-antihydrogen scattering

The calculations that we have carried out on \( \text{He}\bar{\text{H}} \) scattering are a continuation of those described in [4]. We are interested in the rearrangement reactions

\[
\text{He} + \bar{\text{H}} \rightarrow \text{He}^+ \bar{p} + \text{Ps} \quad (18)
\]
\[
\text{He} + \bar{\text{H}} \rightarrow \text{He}^+ \bar{p} + e^+ \quad (19)
\]
\[
\text{He} + \bar{\text{H}} \rightarrow \alpha \bar{p} + \text{Ps}^- \quad (20)
\]
We calculate the entrance channel wave function using the B–O approximation and
the Rayleigh-Ritz variational method. The coordinates we use are prolate spheroidal
coordinates, as in the \( e^+H_2 \) calculation. We take \( \vec{p} \) to be at \( A \) and \( \alpha \) at \( B \) in Figure 1.

The basis functions we use to calculate the leptonic part of the entrance wave function
given in \( \text{Table 1} \). Cross sections for reactions (18) and (19) and preliminary results for (20) are
given in \( \text{Table 1} \). We wish to describe further calculations that we have carried out for
reaction (20). We would like eventually to carry out calculations on these reactions
using the Kohn variational method, as in the case of the HH rearrangement reaction
\( [3] \).

\[ H + \bar{H} \rightarrow Pn + Ps, \]

where \( Pn \) is protonium \((p\bar{p})\). However, such a calculation would be very complicated
to carry out. For this reason, we have used a method involving the \( T \)-matrix and a
distorted wave approximation.

The rearrangement cross section, \( \sigma_{3i} \), for the third \( \text{HeH} \) reaction, i.e. reaction
(20), is of the form

\[ \sigma_{3i} = \frac{(2\pi)^3}{\hbar v_i} \int \delta(E_i - E_3)|T_{3i}|^2dk_3, \]

where \( v_i \) is the relative speed of the colliding particles \( \text{He} \) and \( \bar{H} \), \( k_3 \) is the wave vector
of the relative motion of \( \alpha \bar{p} \) and \( Ps^- \) and \( E_i \) and \( E_3 \) are the total energies of the initial
and final states, respectively. \( T_{3i} \) is the \( T \)-matrix element

\[ T_{3i} = \langle \Phi_3|V_3|\Psi_{k_i}^{(+)} \rangle, \]

where \( \Psi_{k_i}^{(+)} \) is the exact scattering wave function for the incident energy under
consideration and \( k_i \) is the associated wave vector. \( V_3 \) is the potential that couples
the two systems resulting from the scattering, i.e. \( \alpha \bar{p} \) and \( Ps^- \). \( \Phi_3 \) is the appropriate
wave function to represent \( \alpha \bar{p} \) and \( Ps^- \) in the rearrangement channel.

It is not possible to determine \( \Psi_{k_i}^{(+)} \). Thus we used the form of the distorted wave
approximation introduced by Jonsell \textit{et al} \( [19] \) in their calculation of rearrangement
cross sections for HH scattering. In this method, \( \Psi_{k_i}^{(+)} \) is approximated by the
wave function for the entrance channel, calculated using the Born-Oppenheimer
approximation.
The leptonic wave function for the incident channel, \( \psi_{\text{BO}}(r; R) \), was calculated using the basis functions (21) and the variational method as described in [4]. \( r \) represents the coordinates of the leptons and \( R \) is the internuclear vector. The continuum wave functions, \( \chi(R) \), for the relative motion of He and \( \bar{\text{H}} \) was calculated using the very accurate B–O potential of Strasburger and Chojnacki [20]. The approximate wave function we used in place of the exact wave function \( \Psi_{k_i}^{(+)} \) in (24) is \( \psi_{\text{BO}}(r; R) \chi(R) \).

The wave function, \( \Phi_3 \), used to represent the rearrangement channel was of the form

\[
\Phi_3 = \eta(\rho) \phi_{\text{Ps}^-(r_{12}, r_{13}, r_{23})} \chi_{\alpha p}(R)
\]

where \( \chi_{\alpha p}(R) \) is an \( \alpha \bar{p} \) bound state wave function. This is taken to be an s-state. \( \phi_{\text{Ps}^-}(r_{12}, r_{13}, r_{23}) \) was taken to be the 15 term ground-state Ps\(^-\) wave function calculated by Ho [21]. The energy value of this ground state obtained using this wave function is \(-0.26161\). The exact value is \(-0.26201\) [22]. \( \eta(\rho) \) is the wave function for the Ps\(^-\) centre of mass motion, where \( \rho \) is the position vector of the centre of mass of \( \alpha \bar{p} \). If \( \eta(\rho) \) is an s-wave, it is a function of \( \rho \) only. For higher partial waves, it will depend on the spherical polar angles \( \theta_\rho \) and \( \phi_\rho \) of \( \rho \). These angles must be in terms of fixed-axes that do not rotate with \( R \). \( \eta(\rho) \) can be expressed in this way using the rotation properties of spherical harmonics.

The \( T \)-matrix element (24) in the distorted wave approximation can be expressed in the form

\[
T_{3i} = \int \chi_{\alpha p}^*(R) \ell_{3i}(R) \chi(R) \, dR
\]

where \( \ell_{3i}(R) = \langle \eta(\rho) \phi_{\alpha p^-} | r_{12}, r_{13}, r_{23} \rangle | V_3 \psi_{\text{BO}}(r; R) \rangle \)

is the leptonic \( T \)-matrix. The integration in the expression for \( t_{3i}(R) \) is over the leptonic coordinates. \( t_{3i}(R) \) was evaluated using 8D numerical integration, rather than 9D, as the symmetry about the internuclear axis made it possible to reduce the dimension of the integrals by one.

An interesting question arises regarding the form of \( V_3 \) in the \( T \)-matrix, \( T_{3i} \). The potential between \( \alpha \bar{p} \) and Ps\(^-\) is, in an obvious notation,

\[
V = \frac{2}{r_{\alpha 1}} - \frac{2}{r_{\alpha 2}} - \frac{2}{r_{\alpha 3}} + \frac{1}{r_{\rho 1}} + \frac{1}{r_{\rho 2}} + \frac{1}{r_{\rho 3}}.
\]

As

\[
V \sim \rho \rightarrow \infty \frac{-1}{\rho},
\]

it is of attractive Coulomb form asymptotically. As is well-known, such a potential affects the form of the scattering wave function, \( \eta(\rho) \), asymptotically.

We are in the process of considering the following forms for \( V_3 \) and \( \eta(\rho) \):

1. \( V_3 = V \) and \( \eta(\rho) = F_c(\rho) \), where \( F_c(\rho) \) is the Coulomb wave function in a potential \( -\frac{1}{\rho} \)

2. \( V_3 = V + \frac{1}{\rho} \) and \( \eta(\rho) = F_c(\rho) \)

3. \( V_3 = V + \frac{1}{\rho} + \frac{\mu}{k^2(1 + \cos w)\rho^2} \),
where \( \mu \) is the reduced mass of \( \alpha \bar{p} \) and Ps\(^- \), \( k \) is the wave number of the relative motion and \( w \) is the angle between the directions of \( k \) and \( \rho \).

\[
\eta(\rho) = \exp\left\{ i \left[ k \cdot \rho + \frac{\mu}{k} \ln(k\rho + k \cdot \rho) \right] \right\}.
\]

This is a method of taking into account the Coulomb form of \( V \) asymptotically that we are currently investigating. It is related to the methods developed by Mulherin and Zinnes [23], Rosenberg [24] and Belkić et al [25].

Another possible way of treating the Coulomb form of \( V \) that we are considering is the surface-integral formulation of scattering theory of Kadyrov et al [26].

We have obtained rearrangement cross sections for \( s \)-wave scattering using the first form of \( V_3 \) and \( \eta(\rho) \) above. This is not a very satisfactory choice from a theoretical point of view. However, it is the easiest to use and should give a reasonable estimate of the size of the cross sections. We estimate that higher partial waves must be included for energies \( \sim 10^{-6} \) a.u.

The results obtained for the cross sections are given in Table 3. An error in the calculation described in the second paper in [4] has been corrected. The threshold energy is between \( \alpha \bar{p} \) states with principal quantum number \( N_\rho = 30 \) and \( N_\rho = 31 \).

In the range considered, the cross sections \( \sigma_{3l}(N_\rho) \) only differ slightly from their threshold behaviour given by

\[
\lim_{\epsilon_i \rightarrow 0^+} \left[ \epsilon_i^{\frac{3}{2}} \sigma_{3l}(N_\rho) \right] = C_N
\]

where \( \epsilon_i \) is the incident energy and \( C_N \) is a constant that depends on the \( \alpha \bar{p} \) principal quantum number, \( N_\rho \). Both \( \chi_{\alpha \rho}(R) \), for the high \( N_\rho \) values under consideration, and \( \chi(R) \) are rapidly oscillating functions of \( R \). (As they are \( s \)-states, they are only functions of \( R \).) The leptonic T-matrix elements do not depend on \( N_\rho \) and there is evidence that they vary smoothly with \( R \) [27]. Thus, as would be expected from (26) and (27), we find some structure in \( \sigma_{3l}(N_\rho) \), depending on the extent to which the oscillation in \( \chi_{\alpha \rho}(R) \) and \( \chi(R) \) are in phase at a given incident energy. As this structure is very sensitive to the values of these wave functions, we wish to do further checks before publishing graphs of \( \sigma_{3l}(N_\rho) \).

It can be seen that all the cross sections in Table 3 are less than or equal to \( \sim 10^{-3} \epsilon_i^{\frac{3}{2}} a_0^2 \). The antiproton interacts with a proton, or a nucleus containing a proton, through the strong interaction to form pions. The strong interaction is much stronger than the electromagnetic interaction that brings about the annihilation of a positron and an electron. At very low energies the cross section for antiproton loss through the strong interaction in \( \text{HeH} \) scattering is \( \sim 2.6 \epsilon_i^{\frac{3}{2}} a_0^2 \), which is very much larger than the cross sections in Table 3. It is also much larger than the cross sections for the other two rearrangement processes (18) and (19). See [4].

4. Conclusion

We have carried out detailed calculations on two scattering processes, low-energy positron-hydrogen-molecule and helium-antihydrogen scattering that contain the same three leptons.

In the calculations of \( e^+ \text{H}_2 \) scattering, we used the complex Kohn variational method to calculate \( Z_{\alpha}(k) \). We were able to avoid using the method of models [5] that was a feature of previous calculations [6]. This was possible as we were able to calculate integrals involving \( \frac{\epsilon^{\frac{3}{2}} \rho_{\alpha \rho}}{\rho_{3l}} \) [9]. The results of our calculations are given in [8].
Recently, we have examined the behaviour of $Z_{\text{eff}}(k)$ when the internuclear distance, $R$, is varied. When the nuclear motion is taken into account, we obtain a value of $Z_{\text{eff}}(k)$ considerably closer to experiment using the method of models. This is partly due to the much larger values of $Z_{\text{eff}}(k)$ that are obtained at $R > 1.6a_0$ using the method of models. Similar behaviour at $R > 1.6a_0$ has very recently been found by Zhang et al. [11] in a very accurate calculation.

We have also used a model $e^+H_2$ system and the Kohn method to investigate possible resonant behaviour due to the presence of a quasi-bound positron-$H_2$ state, associated with an excited vibrational state. A preliminary calculation shows that such a state is coupled to the continuum through a breakdown in the Born-Oppenheimer approximation, probably resulting in a large $Z_{\text{eff}}(k)$ value when a resonant condition is satisfied. This is an interesting result. It is not clear how it is related to Gribakin’s theory [13, 16] of the very large $Z_{\text{eff}}(k)$ values that have been observed in positron scattering by some organic molecules [14].

We have also carried out interesting studies of singular behaviour in the generalised Kohn method and also of the relationship between phase shifts obtained by this method and the complex Kohn method [10, 17, 18].

In previous calculations on low-energy HeH scattering [4], we carried out calculations cross sections for the rearrangement reactions (18) and (19). Preliminary calculations of cross sections were also carried out for the rearrangement reaction (20). These made use of a 15-term Ps$^-$ ground-state wave function obtained by Ho [21].

We have carried out further calculations for the third reaction and corrected an error in the preliminary calculations [4]. The potential between $\alpha\bar{p}$ and Ps$^-$ is of Coulomb form asymptotically. We are in the process of investigating various possible ways of taking this into account [22–25].

We obtained values for the s-wave contribution to the cross section for the first four $\alpha\bar{p}$ s-states below threshold, using the simplest method of treating the long-range Coulomb behaviour. Contributions from higher partial waves must be included for incident energies greater than about $10^{-6}$ a.u., which is in the sub-Kelvin temperature range.

In the calculations that we have carried out for reaction (20), and in [4] for reactions (18) and (19), we find that the rearrangement cross sections that we obtain are much smaller than the antiproton annihilation cross-section.

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Figure 1. Coordinate System

Table 1. Forms used for the factor $C(s_i, t_i)$ in the short-range correlation functions.

| $s_i$ | $t_i$ | $C(s_i, t_i)$ | Type of basis function |
|-------|-------|---------------|------------------------|
| 0     | 0     | 1             | Product of $\sigma$ functions |
| 1     | 1     | $\rho_{12}$   | Positron-electron Hylleraas-type |
| 1     | 2     | $\rho_{23}$   | Electron-electron Hylleraas-type |
| 2     | 1     | $\frac{2}{R}(x_1 x_2 + y_1 y_2)$ | Positron-electron configuration interaction (CI) product of $\pi$ functions |
| 2     | 2     | $\frac{2}{R}(x_2 x_3 + y_2 y_3)$ | Electron-electron CI, product of $\pi$ functions |

$R$ is the internuclear distance.
The distance between particles $i$ and $j$,

$$r_{ij} = \frac{1}{2} \rho_{ij}.$$
Table 2. The dependence of $Z_{\text{eff}}(k)$ for $k = 0.04$ on the internuclear distance $R$.

| Internuclear distance, $R$ ($a_0$) | $Z_{\text{eff}}(k)$ Calculated using the method of models $^\dagger$ | $Z_{\text{eff}}(k)$ Calculated without using the method of models $^*$ |
|-----------------------------------|-------------------------------------------------|-------------------------------------------------|
| 0.8                              | 6.4                                             | 5.0                                             |
| 0.9                              | 7.2                                             | 5.8                                             |
| 1.0                              | 8.0                                             | 6.5                                             |
| 1.2                              | 10.0                                            | 8.1                                             |
| 1.4                              | 12.6                                            | 9.6                                             |
| 1.6                              | 15.8                                            | 10.6                                            |
| 1.8                              | 19.8                                            | 11.1                                            |
| 2.0                              | 24.3                                            | 10.8                                            |
| 2.1                              | 26.7                                            | 10.5                                            |

$^\dagger$Trial function containing 279 short-range correlation functions, 18 of which correlate the positron and the electrons, and a target wave function that takes into account 57.1% of the correlation of energy of $\text{H}_2$ at $R = 1.4a_0$.

$^*$Trial function as above but with a target wave function that takes into account 96.8% of the correlation energy of $\text{H}_2$ at $R = 1.4a_0$.

Table 3. Cross sections for rearrangement into $\alpha p + \text{Ps}^-$.

| Incident energy $\epsilon_1$ (a.u.) | Cross sections $\langle \sigma_{\beta i}(N) \rangle (\epsilon_1^2 a_0^2)$ |
|--------------------------------------|-------------------------------------------------|
| $10^{-10}$                           | $0.36 \times 10^{-3}$ | $0.30 \times 10^{-3}$ | $0.004 \times 10^{-3}$ | $0.017 \times 10^{-3}$ |
| $10^{-9}$                            | $0.36 \times 10^{-3}$ | $0.30 \times 10^{-3}$ | $0.004 \times 10^{-3}$ | $0.017 \times 10^{-3}$ |
| $10^{-8}$                            | $0.31 \times 10^{-3}$ | $0.26 \times 10^{-3}$ | $0.004 \times 10^{-3}$ | $0.015 \times 10^{-3}$ |

$N$ is the principal quantum number of the s-state $\alpha p$. 
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