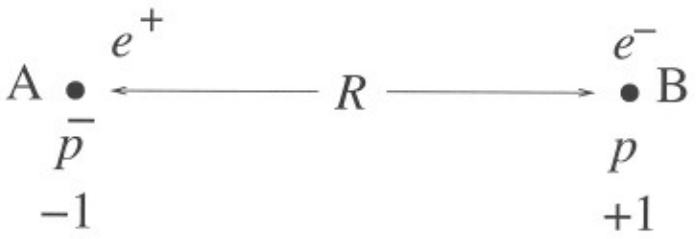
The Interaction of Antihydrogen with Simple Atoms and Molecules

E.A.G. Armour[a†], A.C. Todd[a], S. Jonsell[b], Y. Liu[a],
M.R. Gregory[a] and M. Plummer[c]

[a] *School of Mathematical Sciences, Nottingham University, Nottingham NG7 2RD, UK*
[b] *Department of Physics, University of Wales Swansea, Swansea SA2 8PP, UK*
[c] *CLRC Daresbury Laboratory, Warrington WA4 4AD, UK*

† *edward.armour@nottingham.ac.uk*

Hydrogen–Antihydrogen



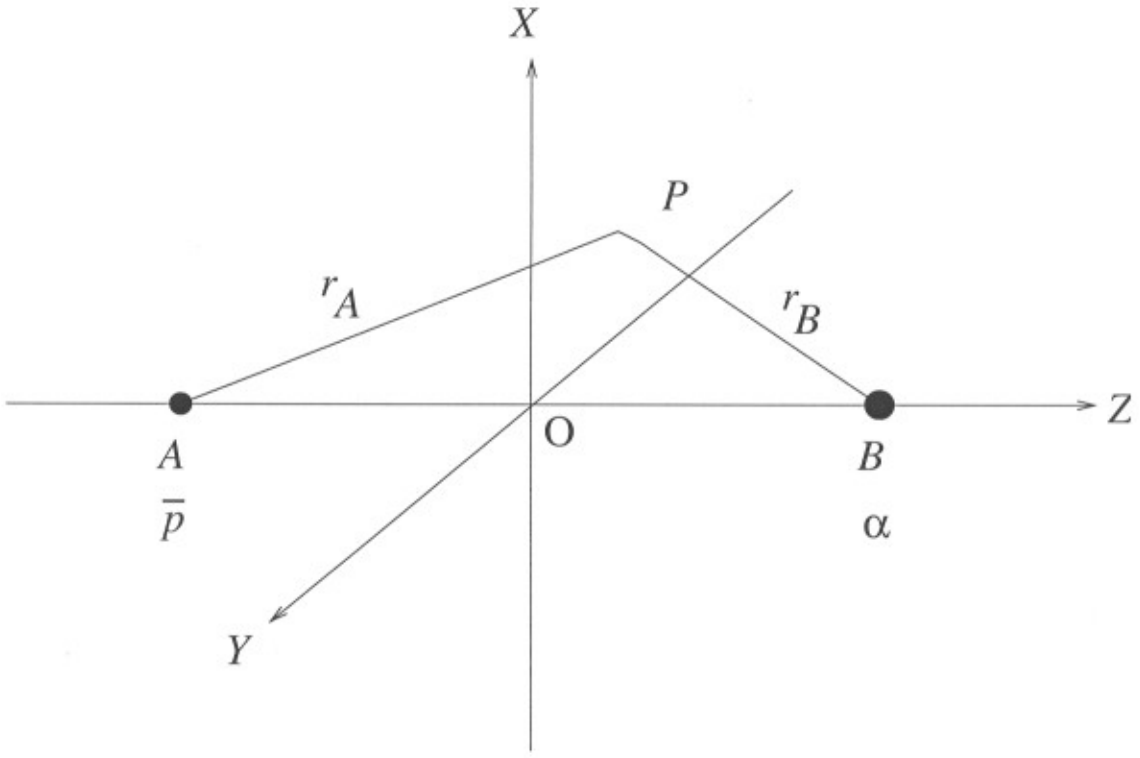
At $R = 0$, the system has no charge.

There is a critical radius, R_C such that if $R < R_C$, the nuclei are unable to bind the electron and the positron. They separate from the nuclei and form positronium (Ps) in its ground state.

$R_c \approx 0.744\ a.u.$[†]

† Strasburger, *J. Phys. B* **35**, L435 (2002).

Prolate Spheroidal Coordinates (λ, μ, ϕ)



A has coordinates $\left(0, 0, -\frac{R}{2}\right)$

B has coordinates $\left(0, 0, \frac{R}{2}\right)$

$R =$ internuclear distance

$$\lambda = \frac{r_A + r_B}{R}$$

$$\mu = \frac{r_A - r_B}{R}$$

ϕ is the usual azimuthal angle of spherical polar coordinates.

$H\bar{H}$ scattering at very low energies

Possible processes to be considered

(1) Elastic scattering.

(2) Direct antiproton-proton annihilation through the strong interaction.

Armour, Liu and Vigier, *J. Phys. B* **38**, L47 (2005).

Jonsell, Saenz, Froelich, Zygelman and Dalgarno, *J. Phys.* **37**, 1195 (2004).

(3) Direct positron-electron annihilation through the electromagnetic interaction.

(4) A rearrangement may take place into

$$p\bar{p} \text{ (protonium)} + e^+e^- \text{ (positronium)}.$$

This is always followed by $p\bar{p}$ and e^+e^- annihilation.

Application of the Kohn variational method to the calculation of cross sections for rearrangement channels

$$\mathrm{H} + \bar{\mathrm{H}} \rightarrow \underset{\text{(Protonium)}}{\mathrm{Pn}(p\bar{p})} + \underset{\text{(Positronium)}}{\mathrm{Ps}(e^+e^-)}$$

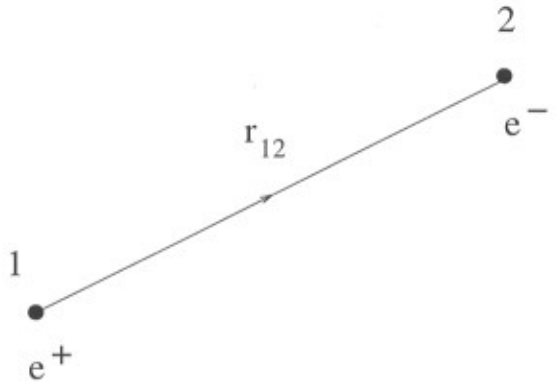
Armour and Chamberlain, *J. Phys. B* **35**, L489 (2002).

Very low energies – only s-wave included. Two types of channel had to be taken into account.

Overlap and Hamiltonian matrix elements had to be calculated between all the basis functions in the Kohn trial function, which was very flexible.

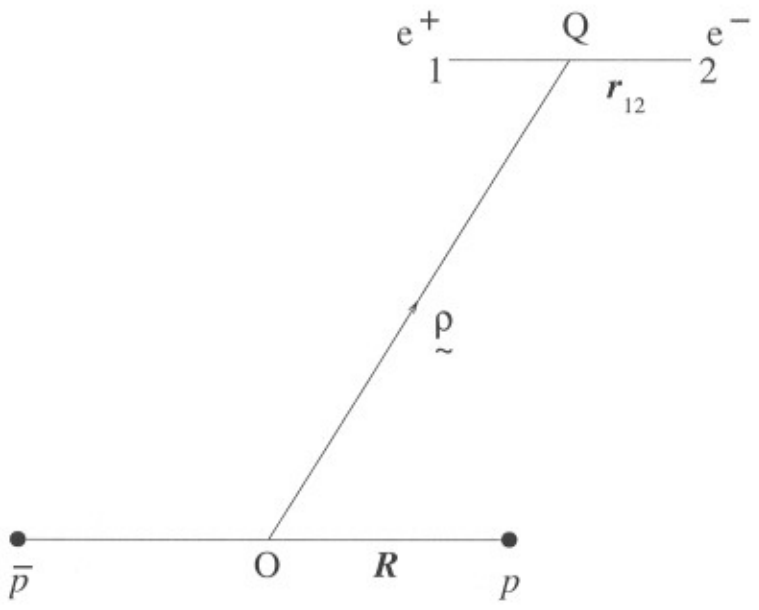
Entrance channel basis functions

Coordinates – prolate spheroidal coordinates: $\lambda_1, \mu_1, \lambda_2, \mu_2$, $\phi = \phi_1 - \phi_2$ and R, the internuclear distance Hylleraas-type basis functions included linear in r_{12}.



Rearrangement channel basis functions

Coordinates: ρ, r_{12} and R.



O is the C of M of $p\bar{p}$.

Q is the C of M of e^+e^-.

Method of evaluation of matrix elements

Within a channel

By analytical integration or 1D numerical integration.

Entrance channel – prolate spheroidal coordinates.

Neumann expansion

$$\frac{1}{r_{12}} = \frac{2}{R} \sum_{\tau=0}^{\infty} \sum_{\nu=0}^{\tau} D_{\tau\nu} P_\tau^\nu(\lambda_<) Q_\tau^\nu(\lambda_>) P_\tau^\nu(\mu_1) P_\tau^\nu(\mu_2) \cos[\nu(\phi_1 - \phi_2)]$$

$\lambda_>$ = greater of λ_1 and λ_2

$\lambda_<$ = lesser of λ_1 and λ_2

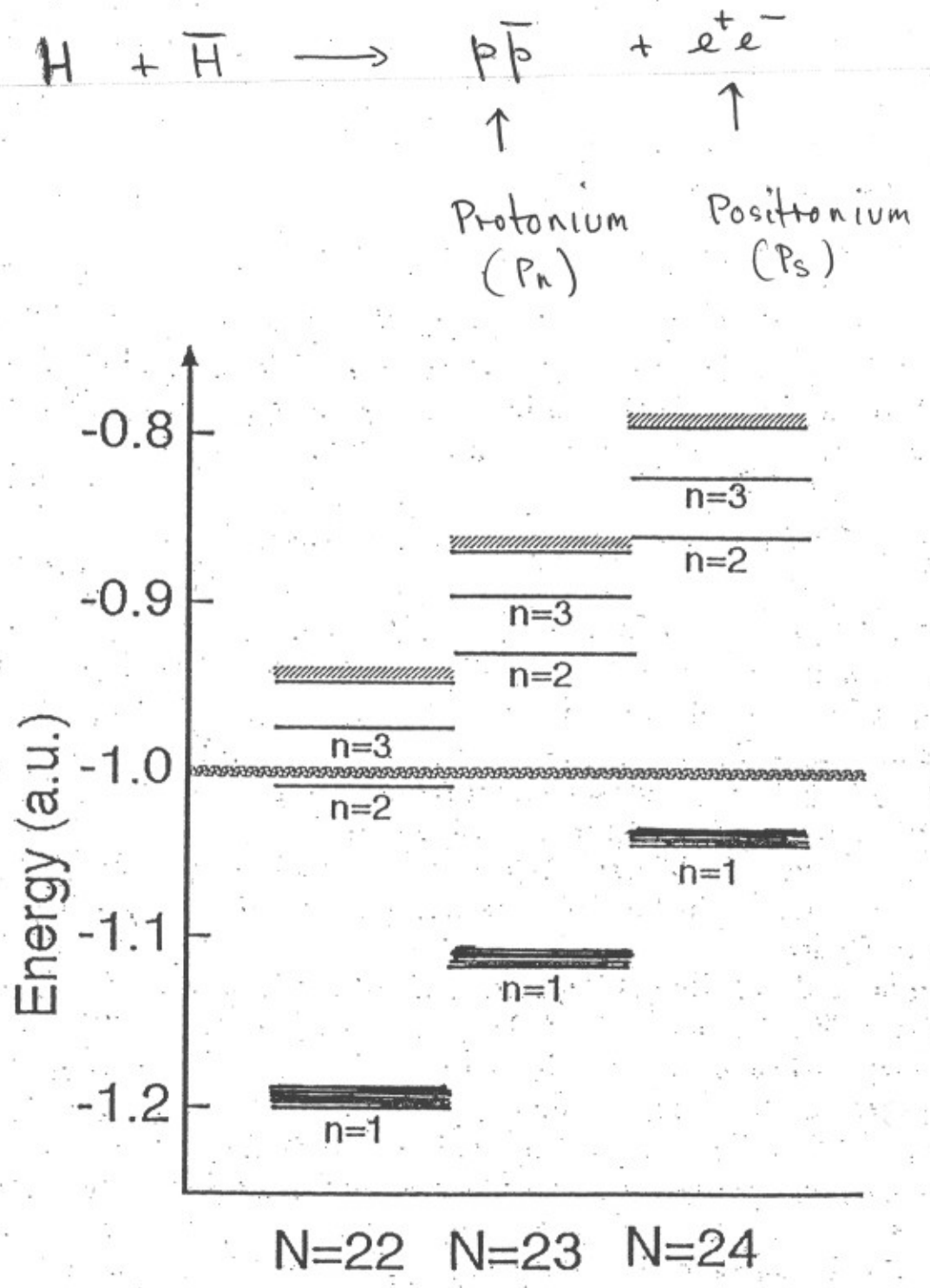
$P_\tau^\nu(\lambda)$ and $Q_\tau^\nu(\lambda)$, the first and second solutions, respectively, or the associated Legendre equation.

Matrix elements between channels

Positron and electron coordinates in the entrance channel – prolate spheroidal coordinates.

In the rearrangement channels: ρ and r_{12}.

This required 5D numerical integration.



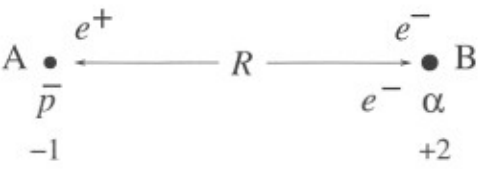
Scattering thresholds with Pn principal quantum number N=22–24, and positronium principal quantum number n. The lines show the sum of the protonium and positronium binding energies. Any final state with energy below −1 a. u., corresponding to zero collision energy, can be formed in hydrogen–antihydrogen collisions.

N	Complex optical potential method[†]	Kohn method This calculation
24	0.32	0.21
23	0.48	0.45
22	0.14	0.01
21	0.10	
20	0.04	
19	0.03	
18	0.003	

Cross sections for rearrangement into $p\bar{p}$ with $L = 0$ and N as shown + ground-state positronium. Units are $a_0^2 \epsilon^{-\frac{1}{2}}$, where ϵ is the collision energy.

[†] Zygelman, Saenz, Froelich and Jonsell., *Phys. Rev. A* **69**, 042715 (2004).

Helium–Antihydrogen



$\propto \bar{p}$ has charge +1.

At $R = 0$, the system reduces to Positronium hydride (PsH).

This is a **bound** system with binding energy, 1.06 eV.

Y. K. Ho, PRA **34**, 609 (1986), Z.-C. Yan and Y. K. Ho, PRA **59**, 2697 (1999).

This contrasts with $H\bar{H}$.

Our calculation of the BO potential between He and $\bar{\mathrm{H}}$

Basis Set

$$\begin{aligned}\psi_i &= S_{23} N \lambda_1^{a_i} \lambda_2^{b_i} \lambda_3^{c_i} \mu_1^{d_i} \mu_2^{e_i} \mu_3^{f_i} C(s_i, t_i) \\ &\times \exp[-\alpha_1 \lambda, -\alpha_2 \lambda_2 - \alpha_3 \lambda_3 + \beta_1 \mu_1 + \beta_2 \mu_2 + \beta_3 \mu_3]\end{aligned}$$

Particle 1: positron.

Particles 2 and 3: electrons.

S_{23} is the electron symmetriser.

Electrons are in a singlet spin state.

N is a normalisation constant.

$a_i, b_i, c_i, d_i, e_i, f_i$ are non-negative integers.

$\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3$ are non-linear parameters.

Types of Basis Function

s_i	t_i	$C(s_i, t_i)$	Type
0	0	1	Product of σ functions
1	1	ρ_{12}	Positron-electron Hylleraas-type
1	2	ρ_{23}	Electron-electron Hylleraas-type
2	1	$\frac{2}{R}(x_1x_2 + y_1y_2)$	Positron-electron configuration interaction (CI) product of π functions
2	2	$\frac{2}{R}(x_2x_3 + y_2y_3)$	Electron-electron CI, product of π functions

R is the internuclear distance.

The distance between particles i and j,

$$r_{ij} = \frac{R}{2}\rho_{ij}.$$

Calculation of the wave function for $He + \bar{H}$ in the Born–Oppenheimer approximation at a given value of the internuclear distance, R

Much more complicated than for $H + \bar{H}$ as we now have 3 light particles.

Inclusion of Hylleraas-type functions

Electron-electron correlation

Inclusion of linear r_{23}, the distance between the electrons, particles 2 and 3.

We needed to evaluate integrals containing $\frac{r_{ij}}{r_{ik}}$ and $r_{ij}r_{ik}$, as well as r_{ij}.

This was done using a double Neumann expansion.

Positron-electron correlation

Inclusion of linear r_{12} and r_{13} (particle 1 is the positron). We need to evaluate all of the above types of integrals.

Also, those containing $\frac{r_{ij}r_{ik}}{r_{jk}}$.

This was done using a triple Neumann expansion.

An algorithm was used to select the best 200 basis functions from a set of 2314 at each value of R, the internuclear distance. The algorithm also optimised the values of the exponents α_1, α_2, α_3, β_1, β_2, β_3.

Comparison of the results with those obtained by Strasburger, Chojnacki and Sokolowska, *Phys. Rev. Lett.* **88**, 163201 (2002) and *J. Phys. B* **38**, 3091 (2005), using basis functions, $\{\chi_i\}$, made up of explicitly correlated Gaussian functions.

$$\chi_{ip} = S_{23} \exp \left[-\sum_{i=1}^{3} \alpha_{ip}(\boldsymbol{r}_i - \boldsymbol{R}_{ip}) - \sum_{i>j}^{3} \beta_{ijp}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \right]$$

where α_{ip}, β_{ijp} and $\boldsymbol{R}_{ip}$ are independent non-linear parameters. S_{23} is the electron symmatriser.

Comparison of Results

Internuclear distance, R	Leptonic energy value This calculation	Leptonic energy value Strasburger *et al.*	Difference
0.1	−0.793417	−0.802881	0.0095
0.5	−1.070414	−1.076846	0.0064
1.0	−1.634494	−1.636474	0.0020
1.5	−2.099359	−2.100153	0.0008

All units are hartree atomic units.

Our calculation: 200 hundred selected basis functions.

Strasburger *et al.*: 768 basis functions.

Increasing out basis set beyond 200 functions did not bring about much improvement in our energy values.

Calculation of rearrangment cross sections

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \mathrm{He}^{+}\bar{p} + \mathrm{Ps} \tag{1}$$

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \mathrm{He}\,\bar{p} + e^{+} \tag{2}$$

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \alpha\bar{p} + \mathrm{Ps}^{-} \tag{3}$$

Cross sections can be determined from the T-matrix

$$\langle \psi_j \mid V_j \mid \Psi_{ex} \rangle \quad (j = 1, 2, 3).$$

Ψ_{ex} – exact scattering wave function.

ψ_j – the rearrangement channel j wave function.

V_j – potential connecting the systems in channel j.

Distorted wave approximation using the Born–Oppenheimer approximation

Jonsell, Saenz, Froelich, Zygelman and Dalgarno, *Phys. Rev. A* **64**, 052712 (2001).

Replace the exact scattering wave function, Ψ_{ex}, by Ψ_{BO}, the wave function for elastic scattering, calculated using the Born–Oppenheimer approximation. In this approximation, the T-matrix is taken to be

$$\langle \psi_j \mid V_j \mid \Psi_{\mathrm{BO}} \rangle.$$

Calculations for the rearrangement process

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \mathrm{He}^{+}\bar{p} + \mathrm{Ps}$$

A preliminary report on this calculation was given in: Armour, Jonsell, Liu and Todd, *Nucl. Instr. and Meth. B* **247**, 127 (2006).

In this case, V_1 is the potential describing the interaction between $\mathrm{He}^{+}\bar{p}$ and Ps. It is of the form

$$\mathrm{V}_1 = -\frac{1}{r_{A1}} + \frac{2}{r_{B1}} + \frac{1}{r_{A2}} - \frac{2}{r_{B2}} - \frac{1}{r_{13}} + \frac{1}{r_{23}}.$$

A is the $\bar{p}$, B is the He nucleus.

Particle 1 – positron.

Particles 2, 3 – electrons.

Electron 2 is taken to be in the Ps and electron 3 in the $\mathrm{He}^{+}\bar{p}$.

Exchange is allowed for at a later stage.

The T-matrix element is of the form

$$\langle \psi_1 \mid V_1 \mid \Psi_{\mathrm{BO}} \rangle$$

where Ψ_{BO} is the entrance channel wave function representing the incoming He and $\bar{\mathrm{H}}$. It is of the form

$$\Psi_{\mathrm{BO}}(\boldsymbol{r}, \boldsymbol{R}) = \psi_{\mathrm{BO}}(\boldsymbol{r}; R)\chi(\boldsymbol{R})$$

$\boldsymbol{r} \equiv$ coordinates of the light particles

$\boldsymbol{R} \equiv$ internuclear vector

$\psi_{\mathrm{BO}}(\boldsymbol{r}; \boldsymbol{R})$ – positron and electron BO wave function calculated earlier. It is a function of $\boldsymbol{R}$.

$\chi(\boldsymbol{R})$ – nuclear wave function. This was calculated using the potential of Strasburger *et al.*

ψ_1 is the wave function, in Jacobi coordinates, of non-interacting $He^+\bar{p}$ and Ps.

If the nuclei are fixed, the Schrödinger equation for the electron in $He^+\bar{p}$ is separable in prolate spheroidal coordinates.

Thus a very accurate electronic wave function and energy can be obtained within the B-O approximation.

$$V_1 = -\frac{1}{r_{A1}} + \frac{2}{r_{B1}} + \frac{1}{r_{A2}} - \frac{2}{r_{B2}} - \frac{1}{r_{13}} + \frac{1}{r_{23}}$$

The most difficult matrix elements to evaluate are those involving $-\frac{1}{r_{13}}$ and $\frac{1}{r_{23}}$.

There are 9 light particle coordinates. The Σ symmetry of the entrance and rearrangement channel wave functions makes possible direct integration over one coordinate.

That leaves 8 coordinates.

Integration over the 3 coordinates of the electron in the $He^+\bar{p}$ was carried out accurately using analytical integration and 1D numerical integration using single or double Neumann expansions, where necessary.

Integration over the remaining 5 coordinates involving the positron and the electron in the Ps was carried out numerically as it involved prolate spheroidal coordinates, the Ps centre of mass coordinate, ρ, and $e^{-\frac{1}{2}r_{12}}$ in the Ps ground state wave function.

Cross sections for the $v = 35$ state of $He^+\bar{p}$

This state is closest to threshold

Incident energy, ϵ a.u.	Cross section a_0^2	Cross section $a_0^2/\sqrt{\epsilon}$
10^{-10}	14237	0.14237
10^{-9}	4501.5	0.14235
10^{-8}	1421.0	0.14210
10^{-7}	441.9	0.1397
10^{-6}	121.5	0.1215
10^{-5}	20.57	0.0651
10^{-4}	2.30	0.023
10^{-3}	0.27	0.0085

Cross section for the $v = 34$ state

Incident energy, ϵ a.u.	Cross section a_0^2	Cross section $a_0^2/\sqrt{\epsilon}$
10^{-10}	126.1	0.001261

Overlap approximation

Introduced by Zygelman, Saenz, Froelich and Jonsell, *Phys. Rev. A* **69**, 042715 (2004).

Detailed treatment in Armour and Jonsell, *J. Phys. A* **40**, 701 (2007).

T-matrix

$$\langle \psi_1 \mid V_1 \mid \Psi_{\mathrm{BO}} \rangle$$

$\psi_1 = \sqrt{2}\psi_{\mathrm{Ps}}(\boldsymbol{\rho}, \boldsymbol{r}_{12})\phi_{\mathrm{He}^+\bar{p}}(\boldsymbol{r}_3; \boldsymbol{R})$

ψ_{Ps} – wave function for Ps

$\phi_{\mathrm{He}^+\bar{p}}$ – wave function for $\mathrm{He}^+\bar{p}$ – calculated using the Born–Oppenheimer approximation.

The factor of $\sqrt{2}$ allows for exchange.

Both the entrance and rearrangement channel wave functions are obtained using the Born–Oppenheimer approximation.

To a good approximation, we can use this to obtain an expression for the T-matrix of the form

$$\langle \psi_1 \mid V_1 \mid \Psi_{\mathrm{BO}} \rangle = \langle \chi_f(\boldsymbol{R}) \mid t_{fi}(R) \mid \chi_i(\boldsymbol{R}) \rangle$$

$\chi_i(\boldsymbol{R})$ – $\mathrm{He} + \bar{\mathrm{H}}$ nuclear wave function

$\chi_j(\boldsymbol{R})$ – $\mathrm{He}^+\bar{p}$ nuclear wave function

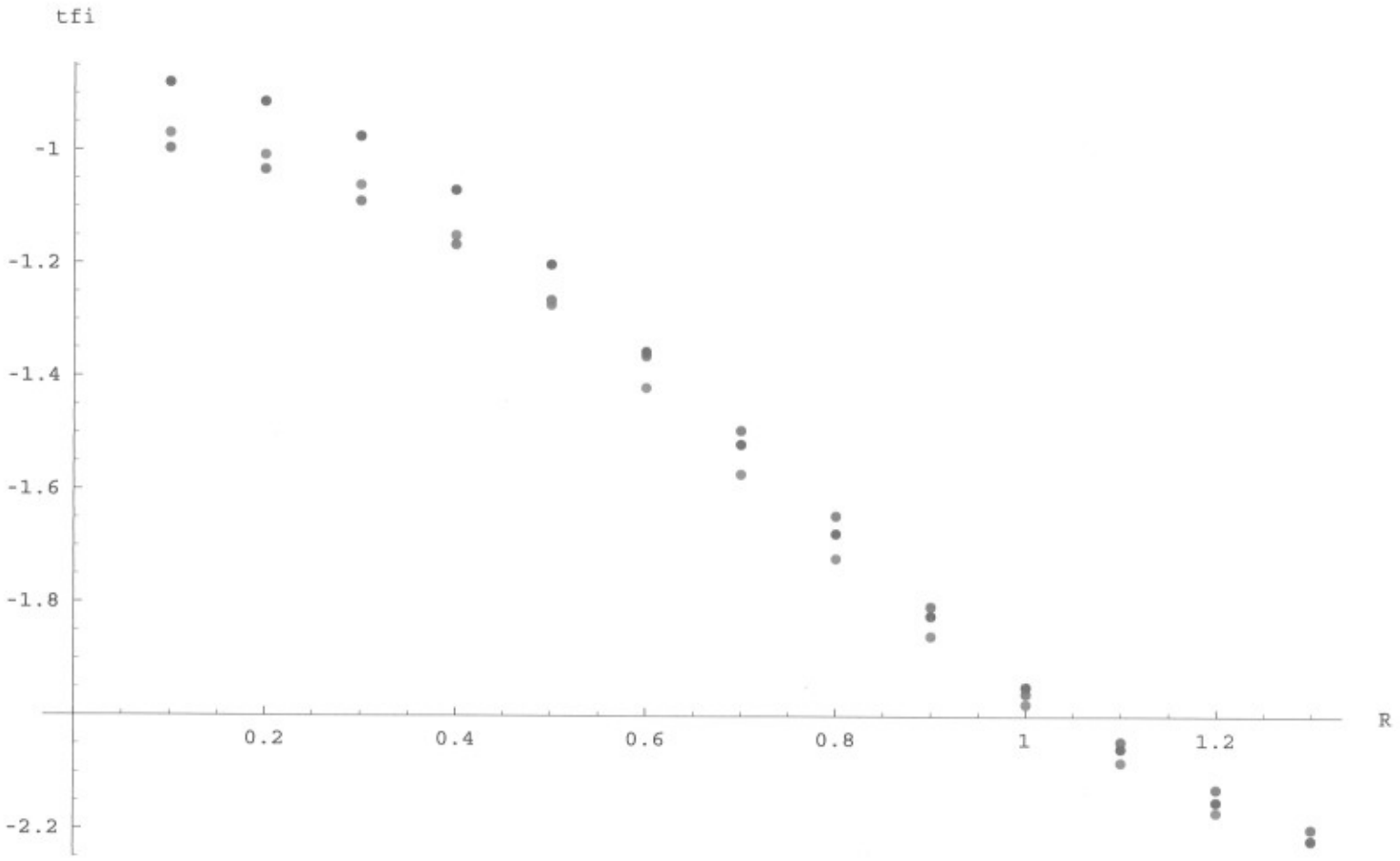
$$\langle \psi_1 \mid V_1 \mid \Psi_{\mathrm{BO}} = \langle \chi_f(\boldsymbol{R}) \mid t_{fi}(R) \mid \chi_i(\boldsymbol{R}) \rangle$$

where t_{fi} is a function of

(1) The BO energies of the leptons in the $\mathrm{He} + \bar{\mathrm{H}}$ and the electron in $\mathrm{He}^+\bar{p}$.

(2) The internal energy of Ps and the kinetic energy of its relative motion.

(3) The *overlap* of the leptonic wave functions for the entrance and rearrangement channels.



23 A

Calculations for the rearrangement process

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \mathrm{He}\bar{p} + e^+$$

where $\mathrm{He}\bar{p}$ is a complex made up of He and $\bar{p}$. In this case, the interaction potential between the $\mathrm{He}\bar{p}$ and the e^+ is

$$-\frac{1}{r_{A1}} + \frac{2}{r_{B1}} - \frac{1}{r_{12}} - \frac{1}{r_{13}}.$$

A is the $\bar{p}$, B is the He nucleus.

Particle 1 – positron. Particles 2, 3 – electrons.

This potential corresponds asymptotically to an attractive *Coulomb* potential.

We allow for this by taking V_2 in the T-matrix element

$$\langle \psi_2 \mid V_2 \mid \Psi_{\mathrm{BO}} \rangle$$

for this process to be of the form

$$V_2 = -\frac{1}{r_{A1}} + \frac{2}{r_{B1}} - \frac{1}{r_{12}} - \frac{1}{r_{13}} - V_{\mathrm{Coul}}$$

$$V_{\mathrm{Coul}} = -\frac{2}{R}\frac{\lambda_1}{\lambda_1^2 - \mu_1^2}.$$

This is the Coulomb potential of a positron and two fixed nuclei of charge -0.5 a.u., a distance R apart.

V_{Coul} removes the Coulombic behaviour from the long-range form of V_2

$$\psi_2 = \phi_{e^+}(\lambda_1, \mu_1; R)\psi_{\mathrm{He}\bar{p}}(\boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{R})$$

$\phi_{e^+}(\lambda_1, \mu_1; R)$ – 's-wave' Coulombic spheroidal wave function corresponding to the potential, V_{Coul}.

This includes the effect of V_{Coul}. Analogous to the Coulomb–Born approximation.

Brauner, Briggs and Klar, *J. Phys. B* **22**, 2265 (1989).

$\psi_{\mathrm{He}\bar{p}}(\boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{R})$ – a 'bound state' He$\bar{p}$ wave function, calculated in the Born–Oppenheimer approximation.

Todd and Armour, *J. Phys. B* **38**, 3367 (2005).

Cross sections for the $He\bar{p} + e^+$ channel

The $v = 33$ state of $He\bar{p}$ is the first below threshold.

Incident energy ϵ a.u.	$v = 29$ state		$v = 33$ state	
	Cross section a_0^2	Cross section $a_0^2/\sqrt{\epsilon}$	Cross section a_0^2	Cross section $a_0^2/\sqrt{e}$
10^{-10}	0.1908	1.91×10^{-6}	1.4955	1.50×10^{-5}
10^{-9}	0.0594	1.88×10^{-6}	0.4657	1.47×10^{-5}
10^{-8}	0.0191	1.91×10^{-6}	0.14964	1.50×10^{-5}
10^{-7}	0.0061	1.93×10^{-6}	0.0479	1.51×10^{-5}
10^{-6}	0.0016	1.64×10^{-6}	0.0129	1.29×10^{-5}
10^{-5}	0.0011	3.57×10^{-6}	0.0088	2.80×10^{-5}
10^{-4}	0.0001	1.19×10^{-6}	0.0009	9.32×10^{-6}
10^{-3}	2.47×10^{-6}	7.80×10^{-8}	1.97×10^{-5}	6.23×10^{-7}

The results for the $v = 32$ state are similar to those for the $v = 33$.

Those for the $v = 31$ and 30 states are between the results for $v = 33$ and $v = 29$.

Calculations for the rearrangement process

$$\mathrm{He} + \bar{\mathrm{H}} \longrightarrow \alpha\bar{p} + \mathrm{Ps}^-(e^+e^-e^-)$$

$$\langle \psi_3 \mid V_3 \mid \Psi_{\mathrm{BO}} \rangle$$

In this case the interaction between the $\alpha\bar{p}$ and the Ps^- is

$$-\frac{1}{r_{A1}} + \frac{2}{r_{B1}} + \frac{1}{r_{A2}} - \frac{2}{r_{B2}} + \frac{1}{r_{A3}} - \frac{2}{r_{B3}}.$$

A is the $\bar{p}$, B is the He nucleus.

Particle 1 – positron. Particles 2, 3 – electrons.

Once again the asymptotic Coulombic behaviour must be removed.

$$\psi_3 = \eta(\rho)\phi_{\mathrm{Ps}^-}(r_{12}, r_{13}, r_{32})\chi(\underset{\alpha\bar{p}}{\boldsymbol{R}})$$

$\boldsymbol{\rho}$ is the position vector of the centre of mass of the Ps^-. $\eta(\rho)$ is an s-wave Coulombic wave function.

Calculation in progress using 8D numerical integration and Ps^- wave functions, $\phi_{\mathrm{Ps}^-}(r_{12}, r_{13}, r_{23})$, supplied by Y. K. Ho (Taiwan).