Supplementary Material

In this document, section 1 and the appendices contain working notes from the preliminary work on the transformations between Jacobi coordinates and mixed Jacobi coordinates for the ABC model described in the main paper, as well as more brief discussions on Delves and APH hypersperical coordinates and tangent sphere coordinates. These are included as a guide for helpful reference. This preliminary work is important for the more general many-body work planned for realistic calculations as these types of coordinate transformations, with collision vector coordinates associated with DVR basis functions for each arrangement, will be needed for the more complicated case. Test programs under development for 3-dimensional finite mixed-basis volume integrals and surface transformations may be found in public repository https://github.com/ElliottKasoar/fortran/tree/parallel.

Section 2 gives some further details and further plots of the $\{\mathrm{p,p,\bar{p}}\}$ calculations described in the main paper. Section 3 gives further details of how short range (strong) interactions may be included in the calculations.

1 COORDINATE SYSTEMS AND TRANSFORMATIONS

1.1 Jacobi coordinates: useful relations

For three bodies with masses M_α, where $\alpha = a, b, c$, and positions relative to an origin fixed in the lab $\boldsymbol{x}_\alpha$, Jacobi coordinates are defined by [1]:

$$\boldsymbol{R}_\alpha = \boldsymbol{x}_\alpha - \frac{M_\beta \boldsymbol{x}_\beta + M_\gamma \boldsymbol{x}_\gamma}{M_\beta + M_\gamma}$$

$$\boldsymbol{r}_\alpha = \boldsymbol{x}_\beta - \boldsymbol{x}_\gamma$$

These coordinates, illustrated in Figure 3 of the main paper, are most convenient when particle α is free, while particles β and γ are bound together [1].

Total system mass, M, and three-body reduced mass, μ:

$$M = M_\alpha + M_\beta + M_\gamma$$

$$\mu = \left(\frac{M_\alpha M_\beta M_\gamma}{M} \right)^{1/2}$$

Internal reduced masses, m_α, and reduced channel masses, μ_α [2]:

$$m_\alpha = M_\beta M_\gamma / (M_\beta + M_\gamma)$$

$$\mu_\alpha = M_\alpha M_\beta M_\gamma / (m_\alpha M)$$

Mass scaled coordinates [1]:

$$\boldsymbol{S}_\alpha = d_\alpha \boldsymbol{R}_\alpha$$

$$\boldsymbol{s}_\alpha = d_\alpha^{-1} \boldsymbol{r}_\alpha$$

where d_α are dimensionless scaling factors

$$d_\alpha = \left[\frac{M_\alpha}{\mu}\left(1 - \frac{M_\alpha}{M}\right)\right]^{1/2}$$

Angle between Jacobi vectors [3]:

$$\gamma_\alpha = \cos^{-1}\left(\frac{\boldsymbol{S}_\alpha \cdot \boldsymbol{s}_\alpha}{S_\alpha S_\alpha}\right) = \cos^{-1}\left(\frac{\boldsymbol{R}_\alpha \cdot \boldsymbol{r}_\alpha}{R_\alpha r_\alpha}\right)$$

Transform between arrangements [2]:

$$\begin{aligned}\begin{pmatrix}\boldsymbol{r}_a \\ \boldsymbol{R}_a\end{pmatrix} &= \begin{pmatrix}-M_A/(M_A+M_B) & 1 \\ -M_B(M_A+M_B+M_C)/(M_B+M_A)(M_B+M_C) & -M_C/M_B+M_C)\end{pmatrix}\begin{pmatrix}\boldsymbol{r}_c \\ \boldsymbol{R}_c\end{pmatrix} \\ &= \begin{pmatrix}-M_A/(M_A+M_C) & -1 \\ M_C(M_A+M_B+M_C)/(B+C)(M_A+M_C) & -M_B/M_B+M_C)\end{pmatrix}\begin{pmatrix}\boldsymbol{r}_b \\ \boldsymbol{R}_b\end{pmatrix}\end{aligned}$$

or for scaled coordinates [1]

$$\begin{pmatrix}\boldsymbol{S}_\beta \\ \boldsymbol{s}_\beta\end{pmatrix} = \boldsymbol{T}(\chi_{\beta\alpha})\begin{pmatrix}\boldsymbol{S}_\alpha \\ \boldsymbol{s}_\alpha\end{pmatrix}$$

where $\boldsymbol{T}$ is a 6x6 matrix

$$\boldsymbol{T}(\chi_{\beta\alpha}) = \begin{pmatrix}\cos(\chi_{\beta\alpha})\mathbf{1} & \sin(\chi_{\beta\alpha})\mathbf{1} \\ -\sin(\chi_{\beta\alpha})\mathbf{1} & \cos(\chi_{\beta\alpha})\mathbf{1}\end{pmatrix}$$

where $\mathbf{1}$ is the 3x3 unit matrix.

For the symmetric definition of the three coordinates, the kinematic angles $\chi_{\beta\alpha}$ for cyclic order are negative, obtuse angles [1]

$$\cos\chi_{\beta\alpha} = -\frac{\mu}{d_\alpha d_\beta M_\gamma}$$

$$\sin\chi_{\beta\alpha} = -\frac{1}{d_\alpha d_\beta}$$

with useful identities including

$$\chi_{\alpha\alpha} = 0$$

$$\chi_{\alpha\beta} = -\chi_{\beta\alpha}$$

$$\chi_{\alpha\beta} + \chi_{\beta\gamma} + \chi_{\gamma\alpha} = 2\pi$$

Transforming between BF axis systems [1]:

$$\begin{pmatrix}\boldsymbol{S}^2_\alpha \\ \boldsymbol{s}^2_\alpha\end{pmatrix} = \boldsymbol{R}(2 \leftarrow 1)\begin{pmatrix}\boldsymbol{S}^1_\alpha \\ \boldsymbol{s}^1_\alpha\end{pmatrix}$$

where the superscript represents the axis system used and $\boldsymbol{R}(2 \leftarrow 1)$ is a 2×2 block diagonal matrix with the rotation matrix $\boldsymbol{R}$ on each diagonal

$$\boldsymbol{R} = \begin{pmatrix} \cos\Psi\cos\Theta\cos\Phi - \sin\Psi\sin\Phi & \sin\Psi\cos\Theta\cos\Phi + \cos\Psi\sin\Phi & -\sin\Theta\cos\Phi \\ -\cos\Psi\cos\Theta\sin\Phi - \sin\Psi\cos\Phi & -\sin\Psi\cos\Theta\sin\Phi + \cos\Psi\cos\Phi & \sin\Theta\sin\Phi \\ \cos\Psi\sin\Theta & \sin\Psi\sin\Theta & \cos\Theta \end{pmatrix}$$

where Ψ, Θ and Φ are Euler angles that carry system 1 into system 2.

A 3D volume element $d\tau$ can be defined for a variety of integration variables [4]:

$$\begin{aligned} d\tau &= r_\alpha^2 R_\alpha^2 \sin\gamma_\alpha dr_\alpha dR_\alpha d\gamma_\alpha \\ &= r_{\alpha'}^2 R_{\alpha'}^2 \sin\gamma_{\alpha'} dr_{\alpha'} dR_{\alpha'} d\gamma_{\alpha'} \\ &= r_\alpha^2 r_{\alpha'}^2 \sin\overline{\gamma}_{\alpha'\alpha} dr_\alpha dr_{\alpha'} d\overline{\gamma}_{\alpha'\alpha} \\ &= \left(\frac{\mu_\alpha\mu_{\alpha'}}{m_\alpha m_{\alpha'}}\right)^{3/2} R_\alpha^2 R_{\alpha'}^2 \sin\gamma_{\alpha'\alpha} dR_\alpha dR_{\alpha'} d\gamma_{\alpha'\alpha} \end{aligned}$$

where $\gamma_{\alpha'\alpha}$ is the angle between $\hat{\boldsymbol{R}}_{\alpha'}$ and $\hat{\boldsymbol{R}}_\alpha$ and $\overline{\gamma}_{\alpha'\alpha}$ is the angle between $\boldsymbol{r}_\alpha$ and $\boldsymbol{r}_{\alpha'}$. Similarly, integrals may be defined using different coordinates [2]:

$$\int d_3\boldsymbol{r}_\alpha d_2\hat{\boldsymbol{R}}_\alpha = \int_0^\infty dr_\alpha r_\alpha^2 \int_0^\pi d\gamma_\alpha \sin\gamma_\alpha \int_0^{2\pi} d\Phi_\alpha \int_0^{2\pi} d\Psi_\alpha \int_0^\pi d\Theta_\alpha \sin\Theta_\alpha$$

$$\int_0^\infty dr_\alpha r_\alpha^2 \int_0^\pi d\gamma_\alpha \sin\gamma_\alpha = \left(\frac{\mu_\alpha\mu_\beta}{m_\alpha m_\beta}\right)^{3/2} \int_0^\infty dR_\beta R_\beta^2 \int_0^{\pm\pi} \sin\gamma_{\alpha\beta} d\gamma_{\alpha\beta}$$

where $\pm\pi$ depends on whether $\gamma_{\alpha\beta} > 0$ or < 0. r_α, r_β, γ_α, γ_β in terms of $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$ [2]:

$$r_\alpha = \mu_\alpha \left[\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta}{m_\beta}\right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta}\right]^{1/2}$$

$$r_\beta = \mu_\beta \left[\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{R_\alpha}{m_\alpha}\right)^2 + 2\frac{R_\beta R_\alpha}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta}\right]^{1/2}$$

$$\cos\gamma_\alpha = sgn(\gamma_{\beta\alpha})\mu_\alpha \left(\frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}\right) \Big/ r_\alpha$$

$$\cos\gamma_\beta = sgn(\gamma_{\alpha\beta})\mu_\beta \left(\frac{R_\beta}{M_\gamma} + \frac{R_\alpha}{m_\alpha}\cos\gamma_{\alpha\beta}\right) \Big/ r_\beta$$

1.1.1 Finite integrals transformations from mixed to single Jacobi coordinates

We want to interface the inner region with the two external regions (eventually $H_2 + \bar{H}$ and products, but first) $H_2^+ + \bar{p}$ and Pn + H. We can define the two R-matrix boundaries as $R_\alpha = A_\alpha$ and $R_\beta = A_\beta$, from which we can use the PFARM code to propagate to asymptotic distances and fit to K-matrices (phase shifts), transforming to $R_\alpha, r_\alpha, \gamma_\alpha$ and $R_\beta, r_\beta, \gamma_\beta$ at the R_α and R_β boundaries respectively.

At the $R_\alpha = A_\alpha$ boundary:

$$\int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_0^{A_\beta} dR_\beta R_\beta^2 \int_0^{\theta_{\alpha\beta}} d\gamma_{\alpha\beta} \sin\gamma_{\alpha\beta} = \left(\frac{\mu_\alpha\mu_\beta}{m_\alpha m_\beta}\right)^{-3/2} \int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_0^{a_\alpha} dr_\alpha r_\alpha^2 \int_{\theta_{\alpha,min}}^{\theta_{\alpha,max}} d\gamma_\alpha \sin\gamma_\alpha$$

where

$$a_\alpha = \mu_\alpha \left(\frac{R_\alpha}{M_\gamma} + \frac{A_\beta}{m_\beta}\right)$$

$\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ can be obtained by respectively maximising and minimising:

$$\cos\theta_\alpha = sgn(\gamma_{\beta\alpha})\frac{\mu_\alpha}{r_\alpha}\left(\frac{R_\alpha}{M_\gamma} + \cos\gamma_{\alpha\beta}\left(-\frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 + \left(\frac{R_\alpha}{M_\gamma}\right)^2(\cos^2\gamma_{\alpha\beta} - 1)}\right)\right)$$

Similarly, at the $R_\beta = A_\beta$ boundary:

$$\int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_0^{A_\beta} dR_\beta R_\beta^2 \int_0^{\theta_{\alpha\beta}} d\gamma_{\alpha\beta} \sin\gamma_{\alpha\beta} = \left(\frac{\mu_\alpha\mu_\beta}{m_\alpha m_\beta}\right)^{-3/2} \int_0^{A_\beta} dR_\beta R_\beta^2 \int_0^{a_\beta} dr_\beta r_\beta^2 \int_{\theta_{\beta,min}}^{\theta_{\beta,max}} d\gamma_\beta \sin\theta\beta$$

where

$$a_\beta = \mu_\beta \left(\frac{R_\beta}{M_\gamma} + \frac{A_\alpha}{m_\alpha}\right)$$

$\theta_{\beta,min}$ and $\theta_{\beta,max}$ can be obtained by respectively maximising and minimising:

$$\cos\theta_\beta = sgn(\gamma_{\alpha\beta})\frac{\mu_\beta}{r_\beta}\left(\frac{R_\beta}{M_\gamma} + \cos\gamma_{\alpha\beta}\left(-\frac{R_\beta}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\beta}{\mu_\beta}\right)^2 + \left(\frac{R_\beta}{M_\gamma}\right)^2(\cos^2\gamma_{\alpha\beta} - 1)}\right)\right)$$

See Appendix 2 for examples of transformations at coordinates that may used for integration limits. We may illustrate the geometrical constraints on γ_a limits in a single arrangement arising from the transformed mixed-basis limits using the program jacobi.f90 under development at https://github.com/ElliottKasoar/fortran/tree/parallel. The progam calculates the correct limits on the fly and compares results for test integrals (using both Simpson's rule and Monte Carlo techniques. With integral limits taken to be $0 \leq R_\alpha \leq 3$, $0 \leq R_\beta \leq 5$, $0 \leq \gamma_{ab} \leq \pi$, Fig. S1 shows the variation of $\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ with r_α for a typically large R_α value (around R_α = 2.7) and Fig. S2 shows the the restricted variation of $\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ with R_α for a typically large r_α value (around $r_\alpha \geq 6$). The preliminary 3-dimensional plot Fig. S3 is included for completeness and has some noise at r_α = 0 and r_α = 8 which will be corrected.

1.1.2 Finite integrals transformations from single to mixed Jacobi coordinates

Transforming from $(R_\alpha, r_\alpha, \gamma_\alpha)$ to $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$:

$$\int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_0^{a_\alpha} dr_\alpha r_\alpha^2 \int_0^{\theta_\alpha} d\gamma_\alpha \sin\gamma_\alpha = \left(\frac{\mu_\alpha\mu_\beta}{m_\alpha m_\beta}\right)^{3/2} \int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_0^{A_\beta} dR_\beta R_\beta^2 \int_{\theta_{\alpha\beta,min}}^{\theta_{\alpha\beta,max}} d\gamma_{\alpha\beta} \sin\gamma_{\alpha\beta}$$

Transforming from $(R_\beta, r_\beta, \gamma_\beta)$ to $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$:

$$\int_0^{A_\beta} dR_\beta R_\beta^2 \int_0^{a_\beta} dr_\beta r_\beta^2 \int_0^{\theta_\beta} d\gamma_\beta \sin\gamma_\beta = \left(\frac{\mu_\alpha \mu_\beta}{m_\alpha m_\beta}\right)^{3/2} \int_0^{A_\beta} dR_\beta R_\beta^2 \int_0^{A_\alpha} dR_\alpha R_\alpha^2 \int_{\theta_{\alpha\beta,min}}^{\theta_{\alpha\beta,max}} d\gamma_{\alpha\beta} \sin\gamma_{\alpha\beta}$$

See Appendix 3 for examples of transformations of coordinates that may used for integration limits.

1.1.3 Transformation of surface amplitudes at the boundary

In a general R-matrix calculation with boundary a_0, surface amplitudes are defined as

$$a_0^{-1} w_{ik}^\Gamma = \langle \bar{\Phi}_i^\Gamma | \Psi_k^\Gamma \rangle'_{r=a_0}$$

where Γ represents the conserved channel quantum numbers, $\bar{\Phi}_i^\Gamma$ are channel functions, Ψ_k^Γ are basis states for the scattering wavefunction, and the prime on the Dirac brackets means that integration is carried out over all space and spin coordinates except the radial coordinate, r.

The surface amplitudes will be calculated in the inner region, and so in our case will be defined for mixed Jacobi coordinates. However, the propagation of the R-matrix in the external region will be carried out in single Jacobi coordinates. A transformation of the surface amplitudes at the boundary will therefore be necessary in order to obtain

$$a_0^{-1} w_{ik}^{\Gamma\prime} = \langle \bar{\Phi}_i^{\Gamma\prime} | \Psi_k^\Gamma \rangle'_{r=a_0}$$

where the further primes indicate equivalent functions in single Jacobi coordinates.

Since a basis state, $|b_k\rangle$, may be written in terms of an expansion of another complete basis, $|a_n\rangle$:

$$|b_k\rangle = \sum_{n=1}^{N} |a_n\rangle \langle a_n | b_k \rangle$$

the transformed amplitudes may be written as

$$\begin{aligned} a_0^{-1} w_{ik}^{\Gamma\prime} &= \sum_n \langle \bar{\Phi}_i^{\Gamma\prime} | \bar{\Phi}_n^\Gamma \rangle'_{r=a_0} \langle \bar{\Phi}_n^\Gamma | \Psi_k^\Gamma \rangle'_{r=a_0} \\ &= \sum_n \langle \bar{\Phi}_i^{\Gamma\prime} | \bar{\Phi}_n^\Gamma \rangle'_{r=a_0} a_0^{-1} w_{nk}^\Gamma \end{aligned}$$

and so

$$w_{ik}^{\Gamma\prime} = \sum_n \langle \bar{\Phi}_i^{\Gamma\prime} | \bar{\Phi}_n^\Gamma \rangle'_{r=a_0} w_{nk}^\Gamma$$

1.2 Delves hyperspherical coordinates: useful relations

While the hyperradius is shared between all arrangements, the five hyperangles and axes are those of one of three possible arrangements, and so the three arrangements are not treated symmetrically [1].

hyperradius, ρ, and Delves hyperangle, θ_{D_α} [1]:

$$\rho = (S_\alpha^2 + s_\alpha^2)^{1/2}$$

$$\theta_{D_\alpha} = \tan^{-1}(s_\alpha / S_\alpha)$$

with four space-fixed or body-fixed angles completing the set. Note that unlike θ_{D_α} and γ_α (in the BF system), ρ is shared by all three Jacobi coordinates, i.e.

$$\rho = (S_a^2 + s_a^2)^{1/2} = (S_b^2 + s_b^2)^{1/2} = (S_c^2 + s_c^2)^{1/2}$$

Transforming from hyperspherical coordinates to Jacobi [3]:

$$S_\alpha = \rho \cos\theta_{D_\alpha}$$

$$s_\alpha = \rho \sin\theta_{D_\alpha}$$

Integration:

$$\begin{aligned}\int d\boldsymbol{S}_\alpha d\boldsymbol{s}_\alpha &= \int_0^\infty dS_\alpha S_\alpha^2 \int_0^\infty ds_\alpha s_\alpha^2 \int d\hat{S}_\alpha \int d\hat{s}_\alpha \\ &= \frac{1}{4}\int_0^\infty d\rho\rho^5 \int_0^{\pi/2} d\theta_{D_\alpha} \sin^2(2\theta_{D_\alpha}) \int d\hat{S}_\alpha \int d\hat{s}_\alpha\end{aligned}$$

where in the SF system

$$d\hat{S}_\alpha d\hat{s}_\alpha = \sin\vartheta_{S_\alpha} d\vartheta_{S_\alpha} d\varphi_{S_\alpha} \sin\vartheta_{s_\alpha} d\vartheta_{s_\alpha} d\varphi_{s_\alpha}$$

and in the BF system

$$d\hat{S}_\Psi d\hat{s}_\alpha = d\Psi_\alpha \sin\Theta_\alpha d\Theta_\alpha d\Phi_\alpha \sin\gamma_\alpha d\gamma_\alpha$$

where ϑ and φ are spherical polar angles of their respective subscripted vectors, Ψ, Θ and Φ are Euler angles, and γ_α is the angle between $\boldsymbol{S}_\alpha$ and $\boldsymbol{s}_\alpha$, such that both angular integrations cover $(4\pi)^2$ sr.

1.2.1 Coordinate transformations for finite integrals

α:

$$\int_0^{\rho_{max}} d\rho\rho^5 \int_0^{\theta_{max}} d\theta_{D_\alpha} \sin^2(2\theta_{D_\alpha}) = 4\int_0^{A_\alpha} dS_\alpha S_\alpha^2 \int_0^{a_\alpha} ds_\alpha s_\alpha^2$$

where

$$A_\alpha = \rho_{max} \cos\theta_{max}$$

$$a_\alpha = \rho_{max} \sin\theta_{max}$$

1.3 APH coordinates

1.3.1 Notes

Adiabatically adjusting, principal axes hyperspherical (APH) coordinates: $(\rho, \theta, \chi_i, \alpha_Q, \beta_Q, \gamma_Q)$. The BF_Q axes are fixed on the instantaneous principle axes of inertia, and are related to the BF_α axes by a rotation about their common BF y axis. The internal coordinates treat all arrangements equally and swing smoothly during the course of the reaction [1].

1.3.2 Transformation to Jacobi coordinates

In terms of scaled Jacobi coordinates [1]:

$$\rho = (S_\alpha^2 + s_\alpha^2)^{1/2}$$

$$\sin(2\chi_\alpha) = \frac{2\boldsymbol{S}_\alpha \cdot \boldsymbol{s}_\alpha}{\sqrt{(S_\alpha^2 - s_\alpha^2)^2 + (2\boldsymbol{S}_\alpha \cdot \boldsymbol{s}_\alpha)^2}}$$

$$\cos(2\chi_\alpha) = \frac{S_\alpha^2 - s_\alpha^2}{\sqrt{(S_\alpha^2 - s_\alpha^2)^2 + (2\boldsymbol{S}_\alpha \cdot \boldsymbol{s}_\alpha)^2}}$$

$$\tan\theta = \frac{\sqrt{(S_\alpha^2 - s_\alpha^2)^2 + (2\boldsymbol{S}_\alpha \cdot \boldsymbol{s}_\alpha)^2}}{2S_\alpha s_\alpha \sin\gamma_\alpha}$$

where $\chi_\alpha = \chi_i - \chi_{\alpha i}$ (i.e. the three choices of α are equivalent and differ only in origin), and ρ and θ are both independent of α.

Obtaining Jacobi coordinates from APH coordinates [1]:

$$S_\alpha = \frac{\rho}{\sqrt{2}}\sqrt{1 + \sin\theta\cos(2\chi)}$$

$$s_\alpha = \frac{\rho}{\sqrt{2}}\sqrt{1 - \sin\theta\cos(2\chi)}$$

$$\cos\gamma_\alpha = \frac{\sin\theta\sin(2\chi_\alpha)}{\sqrt{1 - \sin^2\theta\cos^2(2\chi)}}$$

Changing of variables for full integration:

$$\int d\boldsymbol{S}_\alpha d\boldsymbol{s}_\alpha = \frac{1}{16}\int_0^\infty d\rho\rho^5 \int_{-\pi}^{\pi} d\chi_\alpha \int_0^{\pi/2} d\theta \sin 2\theta \int_0^{2\pi} d\alpha_Q \int_0^{\pi} d\beta_Q \sin\beta_Q \int_0^{2\pi} d\gamma_Q$$

where α_Q, β_Q and γ_Q are Euler angles and the integration over χ_α covers configuration space twice to handle inversion, which is taken into account through the normalisation.

1.3.3 Transforming to Delves hyperspherical coordinates

As is the case for all hyperspherical coordinate systems, the Delves hyperradius, ρ_D, and APH hyperradius, ρ_{APH} are equal:

$$\rho_D = \rho_{APH}$$

and hence both are otherwise referred to as ρ.

Rotational frame transformations may be used to convert between the two sets of hyperangles. β_{Q_α} is the rotation about the common BF y axis that carries the BF_α axes into the BF_Q axes system:

$$\sin\beta_{Q_\alpha} = \frac{s_\alpha \sin\chi_\alpha \sin\gamma_\alpha}{Q}$$

$$\cos\beta_{Q_\alpha} = \frac{S_\alpha\cos\chi_\alpha + s_\alpha\sin\chi_\alpha\cos\gamma_\alpha}{Q}$$

where

$$Q = \sqrt{s_\alpha^2 \sin^2\chi_\alpha \sin^2\gamma_\alpha + (S_\alpha \cos\chi_\alpha + s_\alpha \sin\chi_\alpha \cos\gamma_\alpha)^2}$$

The Delves hyperangle can be written in terms of APH angles:

$$\begin{aligned}\theta_{D_\alpha} &= \tan^{-1}(s_\alpha/S_\alpha) \\ &= \tan^{-1}\left(\frac{\rho/\sqrt{2}\sqrt{1-\sin\theta cos(2\chi)}}{\rho/\sqrt{2}\sqrt{1+\sin\theta cos(2\chi)}}\right) \\ &= \tan^{-1}\left(\sqrt{\frac{1-\sin\theta cos(2\chi)}{1+\sin\theta cos(2\chi)}}\right)\end{aligned}$$

Change of variables for integration:

$$\frac{1}{16}\int_{-\pi}^{\pi} d\chi_\alpha \int_0^{\pi/2} d\theta \sin 2\theta \int_0^{2\pi} d\alpha_Q \int_0^{\pi} d\beta_Q \sin\beta_Q \int_0^{2\pi} d\gamma_Q = \frac{1}{4}\int_0^{\pi/2} d\theta_{D_\alpha} \sin^2(2\theta_{D_\alpha}) \int d\hat{S}_\alpha \int d\hat{s}_\alpha$$

1.4 Tangent-sphere coordinates

1.4.1 Notes

These coordinates are designed to smoothly connect the (Delves) hyperspherical coordinates in the rearrangement region to Jacobi coordinates in the non-rearrangement region, providing a single propagation variable that varies continuously and smoothly between the two regions. This eliminates the need for algebraic or numerical matching procedures [3].

For each arrangement, there are orthogonal coordinates $(v_\alpha, w_\alpha, \gamma_\alpha)$, where γ_α is the rotational angle of the diatom, as in Delves hyperspherical coordinates and Jacobi coordinates [3].

1.4.2 Useful relations

The hyperradius ρ_{max} is the outer constant-ρ contour of the (Delves) hyperspherical coordinate region, large enough to enclose all rearrangement processes, beyond which the coordinate system is changed [3]:

$$\rho_{max} = \max\left(\rho_{AB}^{max}, \rho_{BC}^{max}, \rho_{AC}^{max}\right)$$

where

$$\rho_{AB}^{max} = \frac{1}{\sin\chi_{AB}}\sqrt{(s_A^{max})^2 + 2s_A^{max}s_B^{max}\cos\chi_{AB} + (s_B^{max})^2}$$

Tangent-sphere from Delves hyperspherical [3]:

$$v_\alpha = \frac{\rho\cos\theta_\alpha - \rho_{max}}{\rho^2 + \rho_{max}^2 - 2\rho\rho_{max}\cos\theta_\alpha}$$

$$w_\alpha = \frac{\rho^2 + \rho_{max}^2 - 2\rho\rho_{max}\cos\theta_\alpha}{\rho\sin\theta_\alpha}$$

Tangent-sphere from Jacobi coordinates [3]:

$$v_\alpha = \frac{S_\alpha - \rho_{max}}{s_\alpha^2 + (S_\alpha - \rho_{max})^2}$$

$$v_\alpha = \frac{s_\alpha^2 + (S_\alpha - \rho_{max})^2}{s_\alpha}$$

Jacobi coordinates from tangent-sphere [3]:

$$S_\alpha = \frac{v_\alpha w_\alpha^2}{1 + v_\alpha^2 w_\alpha^2} + \rho_{max}$$

$$s_\alpha = \frac{w_\alpha}{1 + v_\alpha^2 w_\alpha^2}$$

Volume element:

$$\frac{w_\alpha^4 (v_\alpha w_\alpha^2 + \rho_{max} + v_\alpha^2 w_\alpha^2 \rho_{max})^2}{(1 + v_\alpha^2 w_\alpha^2)^6} dw_\alpha dv_\alpha d\hat{S}_\alpha d\hat{s}_\alpha$$

2 BOUND-STATE CALCULATIONS

The bound-state calculations on the {p,p,$\bar{\text{p}}$} system used bondlength-bondangle coordinates (that is the two proton-antiproton distances, r_1 and r_2 and the angle between these two 'bonds', θ). Spherical oscillator basis functions are used for the radial motions (with the parameter α set to zero to allow non-zero amplitudes at $r = 0$) and Legendre polynomials for the angular motion [5]. The spherical oscillator basis functions consist of products of a Gaussian and associated Laguerre polynomials, all defined in terms of the quantity $y = \beta r^2$. The polynomial part of the (direct product) basis set consists of 6327 symmetrised functions up to 36th order in y and 8th order in $\cos\theta$.

The calculations are restricted to total angular momentum $J = 0$ (including the angular momentum of the overall rotation of the system but excluding the spins of the protons and antiproton) and to be (spacially) symmetric with respect to interchange of the protons.

The stabilization diagram for the {p,p,$\bar{\text{p}}$} system for the complete range of stabilization parameter values studied ($\beta^{-1/2}$ = 0.000859 to 0.008125 a_0) is given in Fig. S4. See also Fig. 4 in the main text where the narrower ranges of $\beta^{-1/2}$ = 0.002 to 0.005 a_0 and energy = -40 to -140 E_h are used. The present calculated energies of the {p,p,$\bar{\text{p}}$} bound state and lowest-lying s-wave resonances are compared with the literature results (mass-scaled from Ps^-/Ps + e^-) in Table S1 below; the $\beta^{-1/2}$ values corresponding to each energy are also given. The complete set of data is tabulated in a separate file `stable.csv`.

The one bound state is 'variationally' (if we ignore the quadrature errors) optimized for $\beta^{-1/2}$ = 0.0009 a_0. The apparent energies of the resonances also vary with β. We note that the form of basis set used here is quite restrictive with effectively just this one parameter adjusting the length scale of the whole basis set.

Figures S5-S9 show radial density plots for the lowest energy state (the true bound state, state 1), state 10 (an ordinary scattering state), and states 11, 12 and 20 (the three lowest energy s-wave resonances) - all for $\beta^{-1/2}$ = 0.003416 a_0.

3 STRONG INTERACTION

If proton-antiproton annihilation is assumed to occur at coalescence of the two particles, the probability of annihilation can be calculated by considering a pseudopotential [6]:

$$V_a^{p\bar{p}} = A^{p\bar{p}}\delta(\boldsymbol{R})$$

where the annihilation constant, $A^{p\bar{p}}$ may be determined from experimental data, such as the width of bound protonium states [6]:

$$\Gamma_{1s} = A^{p\bar{p}}|\widetilde{\phi}_{100}(0)|^2$$

The rate of in-flight annihilation can then be calculated [6]:

$$\lambda_a^{p\bar{p}} = \langle\chi_{\boldsymbol{k}_i}(\boldsymbol{R})|\, V_a^{p\bar{p}}\,|\chi_{\boldsymbol{k}_i}(\boldsymbol{R})\rangle = A^{p\bar{p}}|\chi_{\boldsymbol{k}_i}(0)|^2$$

where $\chi_{\boldsymbol{k}_i}(\boldsymbol{R})$ is the scattering function for the proton-antiproton pair, without considering the pseudopotential. Only the $J = 0$ partial waves are non-zero at the origin, so only s-waves contribute to this rate [6]. This treatment is equivalent to first-order perturbation theory for an effective annihilation potential proportional to $\delta(\boldsymbol{R})$, so is not sufficient for large perturbations [7].

A nonpertubative method for incorporating the strong interaction is to use an optical model potential, which describes annihilation through the complex component of the optical potential. This approach often makes use of significantly simplified proton mass densities, with free parameters adjusted to reproduce experimental results [8].

A further alternative is to represent the strong interaction through a single complex parameter - the Coulomb-corrected strong force scattering length [8]. Since the range of the strong force ($R_{si} \sim 10^{-5}a_0$) is significantly shorter than typical atomic distances ($R_a \sim a_0$), where a_0 is the Bohr radius, there is a range of internuclear distances short enough for the Born-Oppenheimer potential to be dominated by the Coulomb interaction, that is larger than the range of the strong interaction [7].

The wavefunction for nuclear motion, $\chi_{\epsilon_i,0}(kR)$, can therefore be written as [7]:

$$\chi_{\epsilon_i,0}(kR) = N[F_0(kR) + \tan\delta_{si}G_0(kR)] \qquad\qquad R_{si} << R << R_a$$

where F_0 is the zero-angular momentum regular Coulomb wavefunction, which the nuclear motion wavefunction would be proportional to in the absence of the strong interaction, G_0 is the zero-angular momentum irregular Coulomb wavefunction, δ_{si} is the (complex) phase shift induced by the strong interaction, and N is a normalisation constant. The imaginary component of the phase shift permits annihilation, in a similar manner to the optical potential [7].

At atomic length scales ($R \sim R_a$), leptonic interactions cannot be neglected, so the above form of the wavefunction for nuclear motion is not valid [9]. Instead, this form may be used as the short-range boundary condition, replacing solely the regular Coulomb wavefunction ($\delta_{si} = 0$). This allows the

interaction potential to be integrated using standard methods, simplifying calculations significantly in comparison to using an optical model potential [8].

Since atomic scattering energies ($\sim$ eV) are much smaller than typical nuclear energies ($\sim$ MeV), the zero-energy limit of δ_{si} may be used, which can then be related to the Coulomb-corrected scattering length of the strong interaction [7]:

$$\frac{1}{a_{si}} = -\frac{2\pi}{b_\mu} \lim_{k\to 0} \cot \delta_{si}(k)$$

where b_μ is the Coulomb parameter, and a_{si} may be determined through fitting to experimental data.

REFERENCES

[1]R.T. Pack and G. A. Parker, Quantum reactive scattering in three dimensions using hyperspherical (APH) coordinates. Theory, *J. Chem. Phys.* **87**, 3888 (1987).

[2]W. H. Miller, Coupled Equations and the Minimum Principle for Collisions of an Atom and a Diatomic Molecle, Including Rearrangements, *J. Chem. Phys.* **50**, 407 (1969).

[3]G. A. Parker, M. Keil and M. A. Morrison, Quantum reactive scattering in three dimensions: Using tangent-sphere coordinates to smoothly transform from hyperspherical to Jacobi regions, *J. Chem. Phys.* **113**, 957 (2000).

[4]J. Z. H. Zhang and W. H. Miller, Quantum reactive scattering via the S-mstrix version of the Kohn variational principle *J. Chem. Phys.* **88**, 6233 (1988).

[5]J. Tennyson, S. Miller and C. R. Le Sueur, TRIATOM: programs for the calculation of ro-vibrational spectra of triatomic molecules, *Comp.Phys. Commun.* **75**, 339 (1993).

[6]S. Jonsell, A. Saenz, P. Froelich, B. Zygelman and A. Dalgarno, Stability of hydrogen-antihydrogen mixtures at low energies, *Phys. Rev. A*, **64**, 052712 (2001).

[7]S. Jonsell, E. A. G. Armour, M Plummer, Y Liu and A C Todd, Helium–antihydrogen scattering at low energies, *New J. Phys.* **14**, 035013 (2012).

[8]S. Jonsell, A. Saenz, P. Froelich, B. Zygelman, and A. Dalgarno, Including the strong nuclear force in antihydrogen-scattering calculations, *Canad. J. Phys* **83**, 435 (2005).

[9]S. Jonsell, A. Saenz, P. Froelich, B. Zygelman, and A. Dalgarno, Hydrogen–antihydrogen scattering in the Born–Oppenheimer approximation, *J. Phys. B: At. Mol. Opt. Phys* **37**, 1195 (2004).

[10]Y. Zhou and C. D. Lin, Comparative Studies of Excitations and Resonances in H^-, Ps^-, and e^+ + H Systems, *Phys. Rev. Lett.* **75**, 2296 (1995).

APPENDICES

1 DERIVATIONS

$$r_\alpha = \mu_\alpha \left[\left(\frac{R_\alpha}{M_\gamma} \right)^2 + \left(\frac{R_\beta}{m_\beta} \right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta} \cos\gamma_{\alpha\beta} \right]^{1/2} \tag{S1}$$

$$r_\beta = \mu_\beta \left[\left(\frac{R_\beta}{M_\gamma} \right)^2 + \left(\frac{R_\alpha}{m_\alpha} \right)^2 + 2\frac{R_\beta R_\alpha}{M_\gamma m_\beta} \cos\gamma_{\alpha\beta} \right]^{1/2} \tag{S2}$$

$$\cos\gamma_\alpha = sgn(\gamma_{\beta\alpha})\mu_\alpha \left(\frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}\right) \Big/ r_\alpha \tag{S3}$$

$$\cos\gamma_\beta = sgn(\gamma_{\alpha\beta})\mu_\beta \left(\frac{R_\beta}{M_\gamma} + \frac{R_\alpha}{m_\alpha}\cos\gamma_{\alpha\beta}\right) \Big/ r_\beta \tag{S4}$$

From equation S1:

$$\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 = \left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta}{m_\beta}\right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta} \tag{S5}$$

From equation S3:

$$\begin{aligned}
\cos^2\gamma_\alpha \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 &= \left(\frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}\right)^2 \\
&= \left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta\cos\gamma_{\alpha\beta}}{m_\beta}\right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta} \\
&= \left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta\cos\gamma_{\alpha\beta}}{m_\beta}\right)^2 + \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - \left(\frac{R_\alpha}{M_\gamma}\right)^2 - \left(\frac{R_\beta}{m_\beta}\right)^2 \\
&= \left(\frac{R_\beta\cos\gamma_{\alpha\beta}}{m_\beta}\right)^2 + \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - \left(\frac{R_\beta}{m_\beta}\right)^2
\end{aligned}$$

Therefore

$$\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 (\cos^2\gamma_\alpha - 1) = \left(\frac{R_\beta}{m_\beta}\right)^2 (\cos^2\gamma_{\alpha\beta} - 1)$$

$$\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 \sin^2\gamma_\alpha = \left(\frac{R_\beta}{m_\beta}\right)^2 \sin^2\gamma_{\alpha\beta}$$

$$\sin\gamma_{\alpha\beta} = \pm\frac{r_\alpha m_\beta}{\mu_\alpha R_\beta}\sin\gamma_\alpha$$

and similarly

$$\sin\gamma_{\alpha\beta} = \pm\frac{r_\beta m_\alpha}{\mu_\beta R_\alpha}\sin\gamma_\beta$$

From equation S5

$$\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 = \left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta}{m_\beta} + \frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta}\right)^2 - \left(\frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta}\right)^2$$

Therefore

$$R_\beta = m_\beta\left(-\frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 + \left(\frac{R_\alpha}{M_\gamma}\right)^2(\cos^2\gamma_{\alpha\beta} - 1)}\right)$$

and similarly

$$R_\alpha = m_\alpha\left(-\frac{R_\beta}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\beta}{\mu_\beta}\right)^2 + \left(\frac{R_\beta}{M_\gamma}\right)^2(\cos^2\gamma_{\alpha\beta} - 1)}\right)$$

Alternatively, from equation S3

$$sng(\gamma_{\beta\alpha})\frac{r_\alpha}{\mu_\alpha}\cos\gamma_\alpha = \frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}$$

and so from equation S1

$$sng(\gamma_{\beta\alpha})\frac{r_\alpha}{\mu_\alpha}\cos\gamma_\alpha = \frac{R_\alpha}{M_\gamma} + \frac{R_\beta M_\gamma m_\beta}{2m_\beta R_\alpha R_\beta}\left[\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - \left(\frac{R_\alpha}{M_\gamma}\right)^2 - \left(\frac{R_\beta}{m_\beta}\right)^2\right]$$

$$2sng(\gamma_{\beta\alpha})\frac{r_\alpha R_\alpha}{\mu_\alpha M_\gamma}\cos\gamma_\alpha = 2\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - \left(\frac{R_\alpha}{M_\gamma}\right)^2 - \left(\frac{R_\beta}{m_\beta}\right)^2$$

Therefore

$$R_\beta = m_\beta\sqrt{\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - 2sgn(\gamma_{\beta\alpha})\frac{r_\alpha R_\alpha}{\mu_\alpha M_\gamma}\cos\gamma_\alpha}$$

and similarly

$$R_\alpha = m_\alpha\sqrt{\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{r_\beta}{\mu_\beta}\right)^2 - 2sgn(\gamma_{\alpha\beta})\frac{r_\beta R_\beta}{\mu_\beta M_\gamma}\cos\gamma_\beta}$$

2 TRANSFORMING FROM MIXED TO SINGLE JACOBI COORDINATES

2.1 Transformation examples

In general, at $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$:

$$r_\alpha = \mu_\alpha\left[\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta}{m_\beta}\right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta}\right]^{1/2}$$

$$r_\beta = \mu_\beta\left[\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{R_\alpha}{m_\alpha}\right)^2 + 2\frac{R_\beta R_\alpha}{M_\gamma m_\alpha}\cos\gamma_{\alpha\beta}\right]^{1/2}$$

$$\cos\gamma_\alpha = sgn(\gamma_{\beta\alpha})\left(\frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}\right)\left[\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{R_\beta}{m_\beta}\right)^2 + 2\frac{R_\alpha R_\beta}{M_\gamma m_\beta}\cos\gamma_{\alpha\beta}\right]^{-1/2}$$

$$\cos\gamma_\beta = sgn(\gamma_{\alpha\beta})\left(\frac{R_\beta}{M_\gamma} + \frac{R_\alpha}{m_\alpha}\cos\gamma_{\alpha\beta}\right)\left[\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{R_\alpha}{m_\alpha}\right)^2 + 2\frac{R_\beta R_\alpha}{M_\gamma m_\alpha}\cos\gamma_{\alpha\beta}\right]^{-1/2}$$

At the lower limit of each mixed integration variable, $(R_\alpha, R_\beta, \gamma_{\alpha\beta}) = (0, 0, 0)$:

$$r_\alpha = 0$$

$$r_\beta = 0$$

γ_α and γ_β are undefined. At the upper limit of each mixed integration variable, $(R_\alpha, R_\beta, \gamma_{\alpha\beta}) = (A_\alpha, A_\beta, \pi)$:

$$\begin{aligned} r_\alpha &= \mu_\alpha \left[\left(\frac{A_\alpha}{M_\gamma} \right)^2 + \left(\frac{A_\beta}{m_\beta} \right)^2 - 2 \frac{A_\alpha A_\beta}{M_\gamma m_\beta} \right]^{1/2} \\ &= \mu_\alpha \left[\left(\frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right)^2 \right]^{1/2} \\ &= \mu_\alpha \left| \frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right| \end{aligned}$$

$$\begin{aligned} r_\beta &= \mu_\beta \left[\left(\frac{A_\beta}{M_\gamma} \right)^2 + \left(\frac{A_\alpha}{m_\alpha} \right)^2 - 2 \frac{A_\beta A_\alpha}{M_\gamma m_\alpha} \right]^{1/2} \\ &= \mu_\beta \left[\left(\frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right)^2 \right]^{1/2} \\ &= \mu_\beta \left| \frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right| \end{aligned}$$

$$\begin{aligned} \cos\gamma_\alpha &= sgn(\gamma_{\beta\alpha}) \left(\frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right) \left[\left(\frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right)^2 \right]^{-1/2} \\ &= sgn(\gamma_{\beta\alpha}) \left(\frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right) \left| \frac{A_\alpha}{M_\gamma} - \frac{A_\beta}{m_\beta} \right|^{-1} \\ &= \pm sgn(\gamma_{\beta\alpha}) \end{aligned}$$

$$\gamma_\alpha = \pi, 0$$

$$\begin{aligned} \cos\gamma_\beta &= sgn(\gamma_{\alpha\beta}) \left(\frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right) \left[\left(\frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right)^2 \right]^{-1/2} \\ &= sgn(\gamma_{\alpha\beta}) \left(\frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right) \left| \frac{A_\beta}{M_\gamma} - \frac{A_\alpha}{m_\alpha} \right|^{-1} \\ &= \pm sgn(\gamma_{\alpha\beta}) \end{aligned}$$

$$\gamma_\beta = 0, \pi$$

where the $\pm$ solutions depend on whether $A_\alpha/M_\gamma > A_\beta/m_\beta$ and $A_\beta/M_\gamma > A_\alpha/m_\alpha$.

2.2 Integration limits for single Jacobi coordinates

2.2.1 $\boldsymbol{R_\alpha}$

Limits remain unchanged: $0, A_\alpha$.

2.2.2 $\boldsymbol{R_\beta}$

Limits remain unchanged: $0, A_\beta$.

2.2.3 $\boldsymbol{r_\alpha}$

These limits are dependent on the value of R_α. Since

$$r_\alpha = \mu_\alpha \left[\left(\frac{R_\alpha}{M_\gamma} \right)^2 + \left(\frac{R_\beta}{m_\beta} \right)^2 + 2 \frac{R_\alpha R_\beta}{M_\gamma m_\beta} \cos\gamma_{\alpha\beta} \right]^{1/2}$$

and it is always possible for $R_\alpha = 0, R_\beta = 0$

$$r_{\alpha,min} = 0$$

It is also always possible for $R_\beta = A_\beta, \gamma_{\alpha\beta} = 0$ ($\cos\gamma_{\alpha\beta} = 1$), meaning for a given R_α

$$\begin{aligned} r_{\alpha,max} &= \mu_\alpha \left[\left(\frac{R_\alpha}{M_\gamma} \right)^2 + \left(\frac{A_\beta}{m_\beta} \right)^2 + 2 \frac{R_\alpha A_\beta}{M_\gamma m_\beta} \right]^{1/2} \\ &= \mu_\alpha \left[\left(\frac{R_\alpha}{M_\gamma} + \frac{A_\beta}{m_\beta} \right)^2 \right]^{1/2} \\ &= \mu_\alpha \left(\frac{R_\alpha}{M_\gamma} + \frac{A_\beta}{m_\beta} \right) \end{aligned}$$

2.2.4 $\boldsymbol{r_\beta}$

These limits are dependent on the value of R_β. Since

$$r_\beta = \mu_\beta \left[\left(\frac{R_\beta}{M_\gamma} \right)^2 + \left(\frac{R_\alpha}{m_\alpha} \right)^2 + 2 \frac{R_\beta R_\alpha}{M_\gamma m_\alpha} \cos\gamma_{\alpha\beta} \right]^{1/2}$$

and it is always possible for $R_\alpha = 0, R_\beta = 0$

$$r_{\beta,min} = 0$$

It is also always possible for $R_\alpha = A_\alpha, \gamma_{\alpha\beta} = 0$ ($\cos\gamma_{\alpha\beta} = 1$), meaning for a given R_β

$$\begin{aligned} r_{\beta,max} &= \mu_\beta \left[\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{A_\alpha}{m_\alpha}\right)^2 + 2\frac{R_\beta A_\alpha}{M_\gamma m_\alpha} \right]^{1/2} \\ &= \mu_\beta \left[\left(\frac{R_\beta}{M_\gamma} + \frac{A_\alpha}{m_\alpha}\right)^2 \right]^{1/2} \\ &= \mu_\beta \left(\frac{R_\beta}{M_\gamma} + \frac{A_\alpha}{m_\alpha}\right) \end{aligned}$$

2.2.5 γ_α

These limits are dependent on the value of R_α and r_α. R_α and r_α are not consistent with an arbitrary choice of $0 \leq R_\beta \leq A_\beta$ and $0 \leq \gamma_{\alpha\beta} \leq \theta_{\alpha\beta}$, so we first rewrite γ_α by eliminating R_β:

$$R_\beta = m_\beta \left(-\frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 + \left(\frac{R_\alpha}{M_\gamma}\right)^2 (\cos^2\gamma_{\alpha\beta} - 1)} \right)$$

so

$$\begin{aligned} \cos\gamma_\alpha &= sgn(\gamma_{\beta\alpha})\frac{\mu_\alpha}{r_\alpha}\left(\frac{R_\alpha}{M_\gamma} + \frac{R_\beta}{m_\beta}\cos\gamma_{\alpha\beta}\right) \\ &= sgn(\gamma_{\beta\alpha})\frac{\mu_\alpha}{r_\alpha}\left(\frac{R_\alpha}{M_\gamma} + \cos\gamma_{\alpha\beta}\left(-\frac{R_\alpha}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 + \left(\frac{R_\alpha}{M_\gamma}\right)^2 (\cos^2\gamma_{\alpha\beta} - 1)}\right)\right) \end{aligned}$$

For $0 \leq \gamma_\alpha \leq \pi$, γ_α changes monotonically with $\cos\gamma_\alpha$. Limits can therefore be obtained by minimising and maximising $\cos\gamma_\alpha$.

2.2.6 γ_β

These limits are dependent on the value of R_β and r_β. R_β and r_β are not consistent with an arbitrary choice of $0 \leq R_\alpha \leq A_\alpha$ and $0 \leq \gamma_{\alpha\beta} \leq \theta_{\alpha\beta}$, so we first rewrite γ_β by eliminating R_α:

$$R_\alpha = m_\alpha \left(-\frac{R_\beta}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\beta}{\mu_\beta}\right)^2 + \left(\frac{R_\beta}{M_\gamma}\right)^2 (\cos^2\gamma_{\alpha\beta} - 1)} \right)$$

so

$$\begin{aligned} \cos\gamma_\beta &= sgn(\gamma_{\alpha\beta})\frac{\mu_\beta}{r_\beta}\left(\frac{R_\beta}{M_\gamma} + \frac{R_\alpha}{m_\alpha}\cos\gamma_{\alpha\beta}\right) \\ &= sgn(\gamma_{\alpha\beta})\frac{\mu_\beta}{r_\beta}\left(\frac{R_\beta}{M_\gamma} + \cos\gamma_{\alpha\beta}\left(-\frac{R_\beta}{M_\gamma}\cos\gamma_{\alpha\beta} \pm \sqrt{\left(\frac{r_\beta}{\mu_\beta}\right)^2 + \left(\frac{R_\beta}{M_\gamma}\right)^2 (\cos^2\gamma_{\alpha\beta} - 1)}\right)\right) \end{aligned}$$

For $0 \leq \gamma_\beta \leq \pi$, γ_β changes monotonically with $\cos\gamma_\beta$. Limits can therefore be obtained by minimising and maximising $\cos\gamma_\beta$.

3 TRANSFORMING FROM SINGLE TO MIXED JACOBI COORDINATES

3.1 From $(R_\alpha, r_\alpha, \gamma_\alpha)$ to $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$

In general, at $(R_\alpha, r_\alpha, \gamma_\alpha)$:

$$R_\alpha = R_\alpha$$

$$R_\beta = m_\beta \sqrt{\left(\frac{R_\alpha}{M_\gamma}\right)^2 + \left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - 2sgn(\gamma_{\beta\alpha})\frac{r_\alpha R_\alpha}{\mu_\alpha M_\gamma}\cos\gamma_\alpha}$$

$$\cos\gamma_{\alpha\beta} = \frac{M_\gamma m_\beta}{2R_\alpha R_\beta}\left[\left(\frac{r_\alpha}{\mu_\alpha}\right)^2 - \left(\frac{R_\alpha}{M_\gamma}\right)^2 - \left(\frac{R_\beta}{m_\beta}\right)^2\right]$$

or

$$\cos\gamma_{\alpha\beta} = \frac{m_\beta}{R_\beta}\left(sgn(\gamma_{\beta\alpha})\cos\gamma_\alpha\frac{r_\alpha}{\mu_\alpha} - \frac{R_\alpha}{M_\gamma}\right)$$

At $(R_\alpha, r_\alpha, \gamma_\alpha) = (0, 0, 0)$:

$$R_\alpha = 0$$

$$R_\beta = 0$$

$\gamma_{\alpha\beta}$ is undefined.

At $(R_\alpha, r_\alpha, \gamma_\alpha) = (A_\alpha, a_\alpha, \pi)$

$$R_\beta = m_\beta \sqrt{\left(\frac{A_\alpha}{M_\gamma}\right)^2 + \left(\frac{a_\alpha}{\mu_\alpha}\right)^2 + 2sgn(\gamma_{\beta\alpha})\frac{a_\alpha A_\alpha}{\mu_\alpha M_\gamma}}$$

$$= m_\beta\left(\frac{A_\alpha}{M_\gamma} \pm \frac{a_\alpha}{\mu_\alpha}\right)$$

3.2 From $(R_\beta, r_\beta, \gamma_\beta)$ to $(R_\alpha, R_\beta, \gamma_{\alpha\beta})$

In general, at $(R_\beta, r_\beta, \gamma_\beta)$:

$$R_\beta = R_\beta$$

$$R_\alpha = m_\alpha \sqrt{\left(\frac{R_\beta}{M_\gamma}\right)^2 + \left(\frac{r_\beta}{\mu_\beta}\right)^2 - 2sgn(\gamma_{\alpha\beta})\frac{r_\beta R_\beta}{\mu_\beta M_\gamma}\cos\gamma_\beta}$$

$$\cos\gamma_{\alpha\beta} = \frac{M_\gamma m_\alpha}{2R_\alpha R_\beta}\left[\left(\frac{r_\beta}{\mu_\beta}\right)^2 - \left(\frac{R_\beta}{M_\gamma}\right)^2 - \left(\frac{R_\alpha}{m_\alpha}\right)^2\right]$$

or

$$\cos\gamma_{\alpha\beta} = \frac{m_\alpha}{R_\alpha}\left(sgn(\gamma_{\alpha\beta})\cos\gamma_\beta\frac{r_\beta}{\mu_\beta} - \frac{R_\beta}{M_\gamma}\right)$$

At $(R_\beta, r_\beta, \gamma_\beta) = (0, 0, 0)$:

$$R_\alpha = 0$$

$$R_\beta = 0$$

$\gamma_{\alpha\beta}$ is undefined.

At $(R_\beta, r_\beta, \gamma_\beta) = (A_\beta, a_\beta, \pi)$

$$\begin{aligned} R_\alpha &= m_\alpha \sqrt{\left(\frac{A_\beta}{M_\gamma}\right)^2 + \left(\frac{a_\beta}{\mu_\beta}\right)^2 + 2sgn(\gamma_{\alpha\beta})\frac{a_\beta A_\beta}{\mu_\beta M_\gamma}} \\ &= m_\alpha \left(\frac{A_\beta}{M_\gamma} \pm \frac{a_\beta}{\mu_\beta}\right) \end{aligned}$$

TABLE

Table S1. Energies (in atomic units) of the $\{p,p,\bar{p}\}$ bound state and lowest-lying s-wave resonances for Pn + p calculated in the present work using a simple stabilization method and mass-scaled literature results for Ps^-/Ps + e^- [10]. The $\beta^{-1/2}$ values corresponding to each of the present energies are also given.

Energy / E_h This work	$\beta^{-1/2}$ / a_0	Energy / E_h Literature	
-483.1	0.0009	-481.0	bound state
-132.5	0.00235	-139.6	resonance
-113.4	0.0045	-116.9	resonance
-61.5	0.00365	-64.9	resonance
-53.5	0.00535	-54.8	resonance

FIGURES

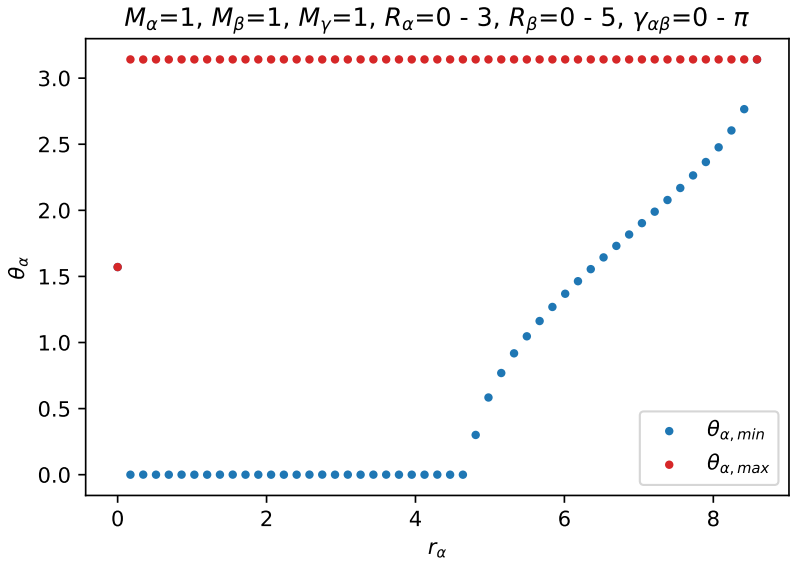

Figure S1. Variation of $\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ with r_α for fixed R_α as described in the text. The masses of particles ABC are set to 1.

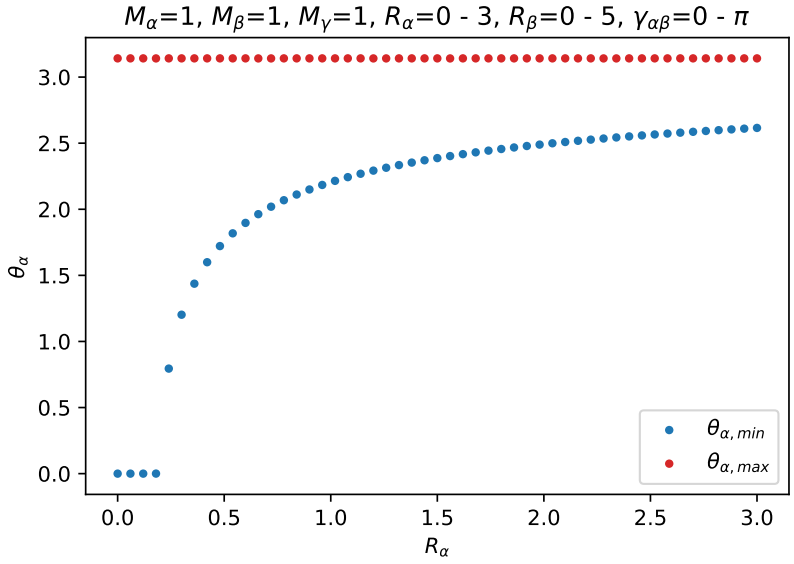

Figure S2. Variation of $\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ with R_α for large fixed r_α as described in the text. The masses of particles ABC are set to 1.

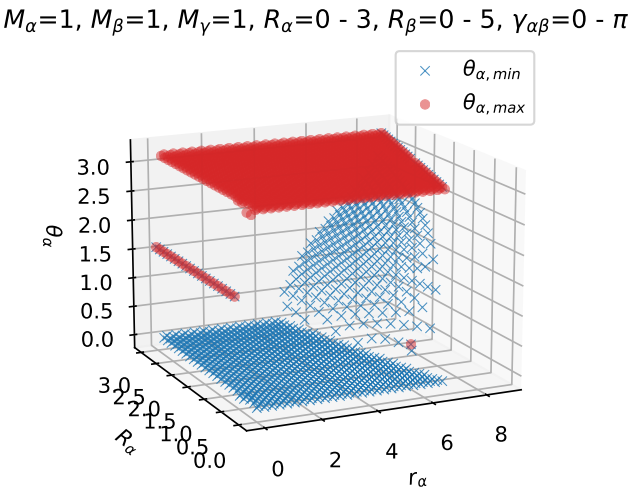

Figure S3. Preliminary 3d plot of the variation of $\theta_{\alpha,min}$ and $\theta_{\alpha,max}$ with R_α and r_α as described in the text. The masses of particles ABC are set to 1.

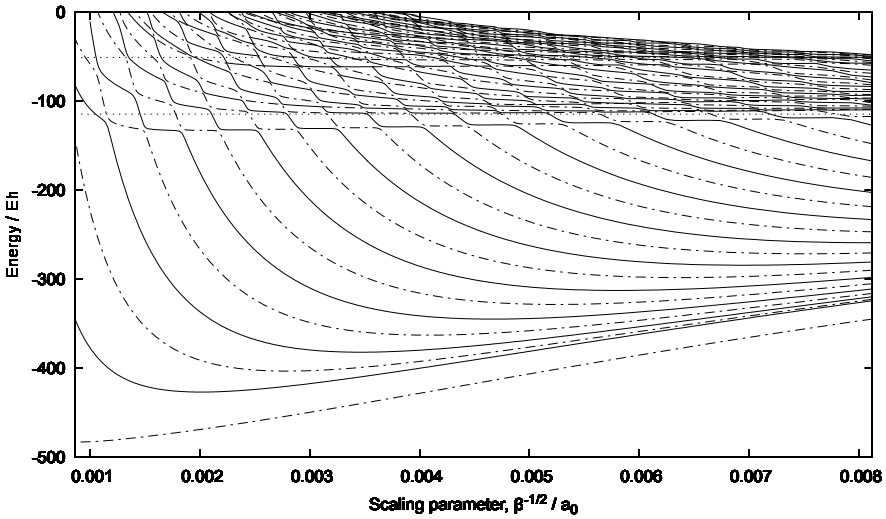

Figure S4. Stabilization diagram for the $\{\mathrm{p,p,\bar{p}}\}$ system. The horizontal dotted lines represent the protonium $n = 2$ ($-114.7\ E_\mathrm{h}$) and $n = 3$ ($-51.0\ E_\mathrm{h}$) states.

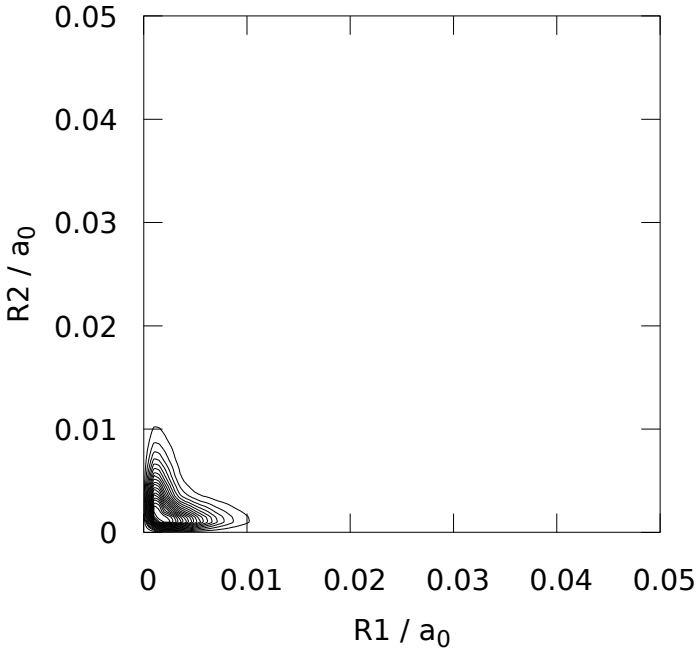

Figure S5. Radial density plot for the lowest energy state (the true bound state) of $\{p,p,\bar{p}\}$. In this and the subsequent plots, the contours are given for 5% to 95% of the maximum density in steps of 10%

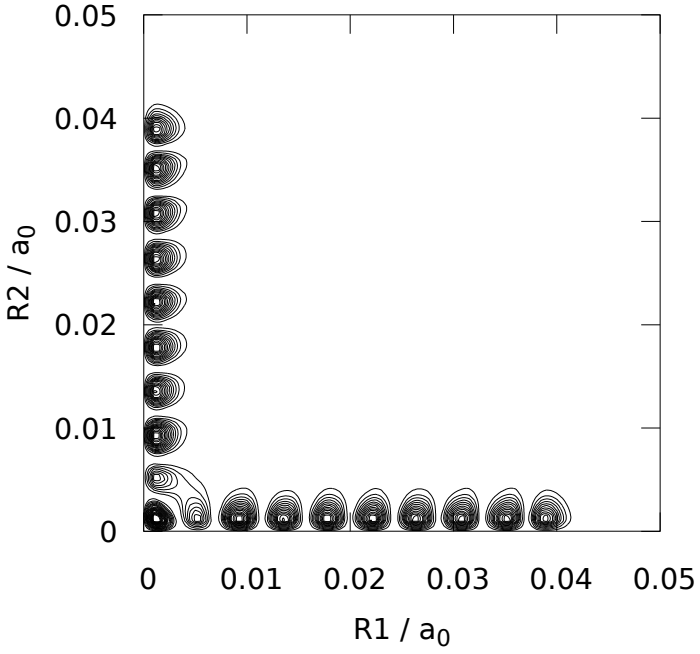

Figure S6. Radial density plot for the 10th lowest energy state (an ordinary scattering state) of $\{p,p,\bar{p}\}$.

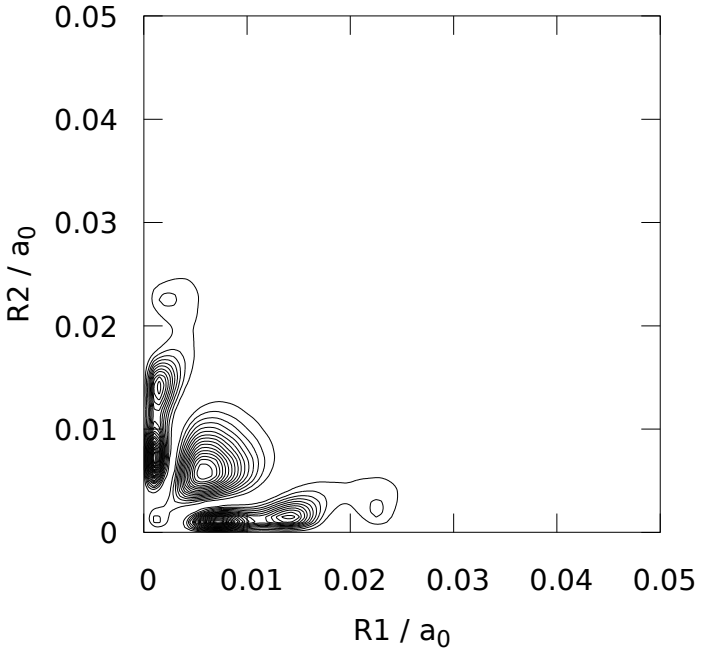

Figure S7. Radial density plot for the 11th lowest energy state (the lowest resonance) of $\{p,p,\bar{p}\}$.

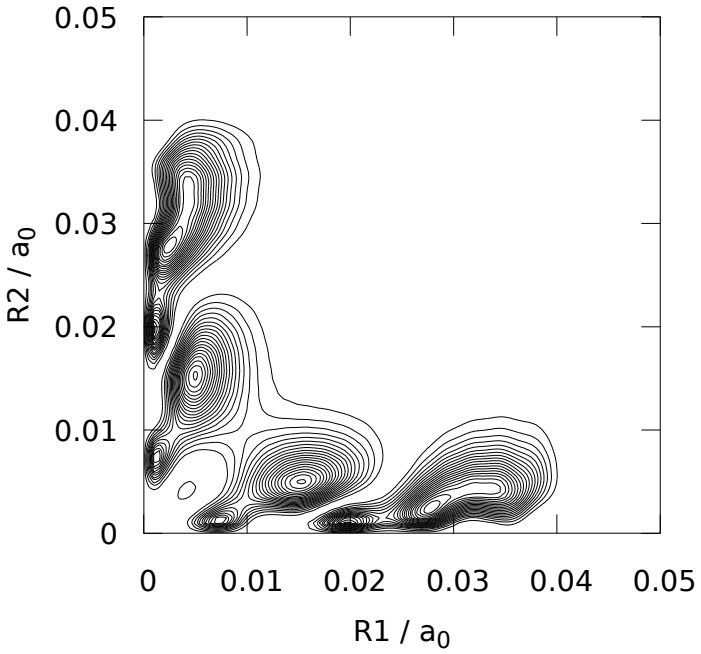

Figure S8. Radial density plot for the 12th lowest energy state (the second lowest resonance) of $\{p,p,\bar{p}\}$.

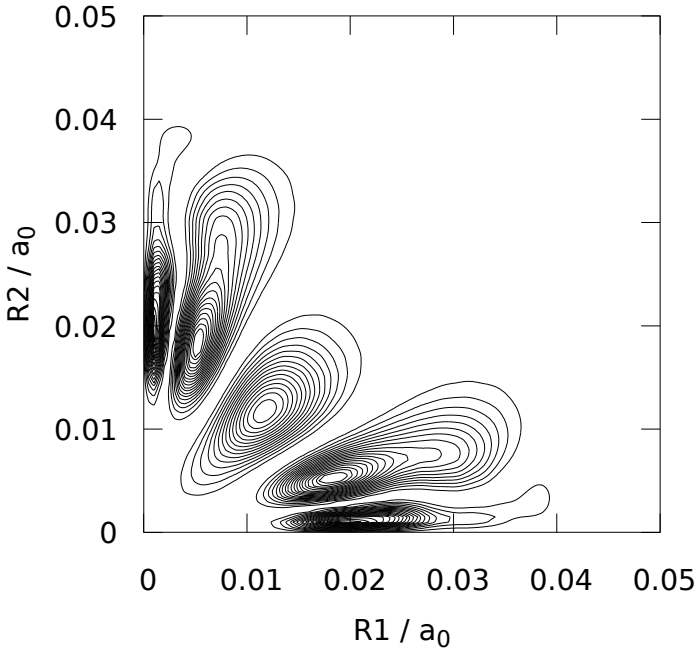

Figure S9. Radial density plot for the 20th lowest energy state (the third lowest resonance) of $\{p,p,\bar{p}\}$.