# Scattering states of three-body systems with the Hypersherical Adiabatic method

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## 1 – Three-body: Introduction

☞ **Jacobi coordinates** $\{x_i, y_i, \mu_i\}$ **:**

$$\vec{x}_i = \frac{\vec{r}_j - \vec{r}_k}{\sqrt{2}};\ \vec{y}_i = \sqrt{\tfrac{3}{2}}\left(\frac{\vec{r}_j + \vec{r}_k}{2} - \vec{r}_i\right);\ \mu_i = \hat{x}_i \cdot \hat{y}_i.$$

☞ **Hyperspherical coordinates** $\rho, \Omega_i = \{\theta_i, \mu_i\}$ **:**

$$\rho^2 = \sqrt{\tfrac{1}{3}}(r^2 + s^2 + t^2) = x_i^2 + y_i^2$$

$$\theta_i = \tan^{-1}(y_i/x_i)$$

☞ **Jacobian**

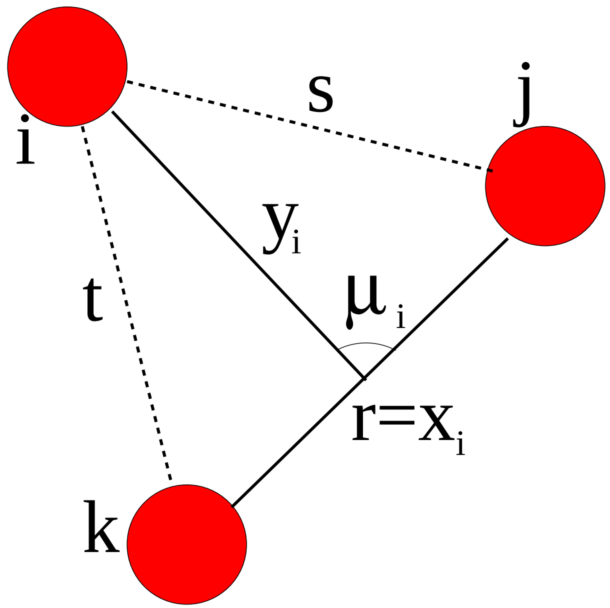
$$\rho^5 \cos^2\theta_i \sin^2\theta_i d\theta_i d\mu_i d\rho$$

☞ **Kinetic energy operator :**

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho} + L^2\frac{1}{\rho^2}\right)$$

☞ **Potential operator :**

$$V = V(s,t,r) = V(\rho,\Omega)$$



# Scattering three-body states ...

## 2 – Basis Expansion:

$$H\Psi = \left[T_\rho + \frac{1}{\rho^2}L^2(\Omega) + V(\rho,\Omega)\right]\Psi = E\Psi$$

HH basis $\{B_k\}$, $\Psi = \sum_k w_k(\rho) B_k(\Omega)$

$L^2 B_k = \lambda_k B_k$

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$\{T_\rho + \lambda_k/\rho^2 - E\}w_k + \sum_{k'} V_{kk'} w_{k'} = 0$

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$V_{kk'}(\rho) = \langle B_k|V|B_{k'}\rangle$

$N_H$ coupled equations

HA basis $\{\Phi_\nu\}$, $\Psi = \sum_\nu u_\nu(\rho)\Phi_\nu(\rho,\Omega)$

$\{\frac{L^2}{\rho^2} + V(\rho,\Omega)\}\Phi_\nu = U_\nu \Phi_\nu$

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$\{T_\rho + U_\nu - E\}u_\nu +$

$\sum_{\nu'} Q_{\nu\nu'} u_{\nu'} + P_{\nu\nu'} \dot{u}_{\nu'} = 0$

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$Q_{\nu\nu'}(\rho) = \langle \Phi_\nu | d^2/d\rho^2 | \Phi_{\nu'}\rangle$

$P_{\nu\nu'}(\rho) = \langle \Phi_\nu | d/d\rho | \Phi_{\nu'}\rangle$

$N_A$ coupled equations

$\Phi_\nu(\rho;\Omega) = \sum_k^M C_k^{(\nu)}(\rho) B_k(\Omega)$

unitarity case $M=N_A=N_H$

## 3 – Bound state calculations: HH

$$V_G(r) = A \exp\left[-(r\,d)^2\right]$$

A= -66.327 MeV, d=0.64041 fm$^{-1}$

$\hbar^2/m$ = 41.47 MeV fm$^2$

E$_{2b} = -2.22448$ MeV, a$_s$ = 5.4208 fm

$$\Psi = \sum_{kn} A_{nk} L_n(\rho) B_k(\Omega)$$

$$\sum_{kn} (H_{knk'n'} - E) A_{kn} = 0$$

Three-nucleon binding energies [MeV]

HH expansion

| N$_H$ | E$_0$ | E$_1$ |
|---|---|---|
| 10 | -22.0874 | -2.0348 |
| 20 | -22.0874 | -2.3036 |
| 30 | -22.0874 | -2.3474 |
| 40 | -22.0874 | -2.3582 |
| 50 | -22.0874 | -2.3615 |
| 60 | -22.0874 | -2.3626 |
| 70 | -22.0874 | -2.3630 |
| 80 | -22.0874 | -2.3632 |

## 4 – Bound state calculations: HH vs HA

| | M=10 | | M=20 | | M=40 | | M=80 | |
|---|---|---|---|---|---|---|---|---|
| N | HH | HA | HH | HA | HH | HA | HH | HA |
| 1 | - | -2.0085 | - | -2.2823 | - | -2.3423 | - | -2.3484 |
| 10 | -2.0348 | -2.0348 | -2.0348 | -2.3036 | -2.0348 | -2.3581 | -2.0348 | -2.3632 |
| 20 | | | -2.3036 | -2.3036 | -2.3036 | -2.3582 | -2.3036 | -2.3632 |
| 40 | | | | | -2.3582 | -2.3582 | -2.3582 | -2.3632 |
| 60 | | | | | | | -2.3626 | -2.3632 |
| 80 | | | | | | | -2.3632 | -2.3632 |

N= number of coupled equations

## 5 – Asymptotic functions

☞ **dimer-monomer asymptotic function:**

$$\Phi^{(\pm)} = \sum_i \mathcal{N}\mathcal{R}(y_i)\frac{e^{\pm\imath k y_i}}{y_i}\Phi_{2b}(x_i)P_0(\mu_i)\ \eta = \sqrt{2m_y E/\hbar^2}$$

☞ **normalization :**

$$\langle\Phi^+|\mathcal{H}-E|\Phi^-\rangle - \langle\Phi^-|\mathcal{H}-E|\Phi^+\rangle = 1/2$$

## 6 – Scattering wavefunction:

$$\Psi = \Psi_c + \Psi_a = \Psi_c + \Phi^+ + \mathcal{L}\Phi^-$$

HH basis $\Psi_c = \sum_k w_k(\rho) B_k(\Omega)$

$$H_{kk'} = \langle B_k | H - E | B_{k'} \rangle$$

$$t_k^{\pm}(\rho) = \langle B_k | H - E | \Phi^{(\pm)} \rangle$$

$N_H$+1 coupled equations

HA basis $\Psi_c = \sum_\nu u_\nu(\rho) \Phi_\nu(\rho, \Omega)$

$$H_{\nu\nu'} = \langle \Phi_\nu | H - E | \Phi_{\nu'} \rangle$$

$$y_\nu^{\pm}(\rho) = \langle \phi_\nu | H - E | \Phi^{\pm} \rangle$$

$N_A$+1 coupled equations

$$\Phi_\nu(\rho; \Omega) = \sum_k^M C_k^{(\nu)}(\rho) B_k(\Omega)$$

unitarity case M=$N_A$

$$[\mathcal{L}, E] = \mathcal{L} + C\langle \Psi^* | H - E | \Psi \rangle$$

## 7 – Scattering Calculations

| $N_A \backslash M$ | 20 | 40 | 60 | 80 | 100 | 120 |
|---|---|---|---|---|---|---|
| 1 | -78.349 | -73.251 | -73.220 | -73.114 | -72.968 | -72.954 |
| 5 | -75.982 | -72.345 | -72.211 | -72.171 | -72.121 | -72.172 |
| 10 | -75.027 | -72.032 | -71.877 | -71.850 | -71.829 | -71.844 |
| 20 | -73.846 | -71.787 | -71.627 | -71.604 | -71.597 | -71.597 |
| 40 | | -71.668 | -71.529 | -71.509 | -71.503 | -71.501 |
| 60 | | | -71.504 | -71.491 | -71.486 | -71.484 |
| 80 | | | | -71.483 | -71.481 | -71.479 |
| 100 | | | | | -71.478 | -71.476 |
| 120 | | | | | | -71.476 |
| HH | -73.846 | -71.668 | -71.504 | -71.483 | -71.478 | -71.476 |

MT-III : $V(r) = A_1 \exp[-r\, d_1]/r - A_2 \exp[-r\, d_2]/r$

${}^4\delta_{3/2}$ at $E_{c.m.} = 2$ MeV

## 8 – Hyperspherical adiabatic approach II:

$$\Psi = \sum_k w_k(\rho) B_k(\Omega) = \sum_\nu u_\nu(\rho)\Phi_\nu(\rho,\Omega)$$

$$\Phi_\nu(\rho,\Omega) = \sum_n C_n^{(\nu)} B_n \Rightarrow w_k = \sum_\nu u_\nu C_k^{(\nu)}$$

bound states HA $\ll$ HH

continuum states HA $\sim$ HH

$$y_\nu^\pm = \langle \Phi_\nu | H - E | \Phi^\pm \rangle_\Omega$$

$$\sum_\nu [(T_\rho + U_\lambda(\rho) - E)\delta_{\lambda,\nu} + Q_{\lambda,\nu}(\rho) + P_{\lambda,\nu}\tfrac{d}{d\rho}] u_\nu(\rho) = 0 \;\; (\lambda = 1, 2, \ldots)$$

- boundary conditions for $\{u_\nu\}$
- need of calculating U, Q, P as accurately as possible at large $\rho$

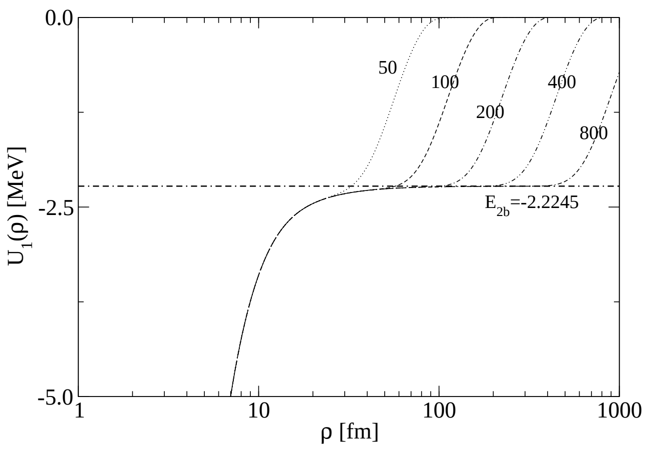
## 9 – lowest adiabatic potential

$$\Psi = u(\rho)\Phi(\rho;\Omega)/\rho^{5/2}$$

$$\Phi:\ \left\{\frac{L^2}{\rho^2} + V(\rho,\Omega) - U(\rho)\right\}\Phi = 0$$

$$u:\ \left\{-\frac{\hbar^2}{2m}\left[\frac{d^2}{d\rho^2} - \frac{15}{4\rho^2}\right] + Q(\rho) + U(\rho) - E\right\}u = 0$$

$$Q(\rho) = \langle\Phi|T_\rho|\Phi\rangle_\Omega$$



## 10 – Asymptotic Equation

$$\left\{ \frac{L^2}{\rho^2} + V(\rho,\Omega) - U_\nu(\rho) \right\} \Phi_\nu = 0$$

$$\rho \gg x_0 \Rightarrow \left\{ -\frac{\hbar^2}{2m\rho^2}\frac{d^2}{d\theta^2} + V_{12}(r_{12}) - \lambda_\nu(\rho) \right\} \phi_\nu(\rho,\theta) = V_{12}(r_{12}) A f(\rho,\theta)$$

$$0 \le \theta \le \pi/2,\ \phi_\nu(\rho,0) = \phi_\nu(\rho,\pi/2) = 0$$

$$\Phi_\nu = \sum_{i=1,3}^{3} \Phi_\nu^{(i)} = \sum_{i=1}^{3} \frac{\phi_\nu(\theta_i,\rho)}{\cos\theta_i \sin\theta_i}.$$

$$U_\nu = \lambda_\nu - 4\frac{\hbar^2}{2m\rho^2}$$

$$\lambda_\nu < 0 \quad f(\rho,\theta) = -2\frac{e^{k(\pi/2-\theta)} - e^{-k(\pi/2-\theta)}}{k} \frac{e^{k\pi/6} - e^{-k\pi/6}}{\sin(\pi/3)}$$

$$\lambda_\nu > 0 \quad f(\rho,\theta) = -\frac{8\sin(k\pi/6)}{\sqrt{3}} \sin[k(\pi/2-\theta)]/k$$

E. Nielsen, D. V. Fedorov, A. S. Jensen and E. Garrido, *Physics Reports* **347** (2001) 373–459 .

# 11 – asymptotic equation: numerical results 1

Helium trimer, LM2M2 potential

$U(\rho)$ [K]

| M$\backslash\rho$ | 150 | 200 | 250 | 300 | 1500 | $\infty$ |
|---|---|---|---|---|---|---|
| 100 | -0.388 [-3] | 0.042 [-3] | 0.058 [-3] | 0.041 [-3] | 1.166 [-6] | |
| 200 | -3.213 [-3] | -0.431 [-3] | -0.142 [-3] | -0.051 [-3] | 5.626 [-7] | |
| 400 | -6.896 [-3] | -3.732 [-3] | -1.443 [-3] | -0.597 [-3] | 3.395 [-7] | |
| 800 | -7.008 [-3] | -4.518 [-3] | -3.263 [-3] | -2.540 [-3] | 2.656 [-8] | |
| as eq. | -7.008 [-3] | -4.518 [-3] | -3.277 [-3] | -2.623 [-3] | -1.342 [-3] | -1.300 [-3] |

$$[n] = 10^n$$

## 12 – asymptotic equation: numerical results 2

Helium trimer, LM2M2 potential

$Q(\rho)$ [K]

| M$\backslash\rho$ | 150 | 200 | 250 | 300 | 1500 |
|---|---|---|---|---|---|
| 100 | 4.925 [-5] | 2.323 [-6] | 4.622 [-8] | 2.469 [-8] | 1.254 [-13] |
| 200 | 2.450 [-5] | 8.892 [-5] | 5.650 [-7] | 4.337 [-6] | 2.088 [-12] |
| 400 | 8.254 [-5] | 2.831 [-5] | 1.056 [-3] | 4.909 [-6] | 1.164 [-10] |
| 800 | 1.067 [-4] | 7.305 [-5] | 5.899 [-5] | 2.898 [-5] | 1.674 [-9] |
| as. eq. | 1.067 [-4] | 7.354 [-5] | 6.182 [-5] | 5.707 [-5] | 3.425 [-6] |

$$[n] = 10^n$$

## 13 – asymptotic equation at large $\rho$

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{d^2}{d\rho^2}-\frac{15}{4\rho^2}\right]+Q(\rho)+U(\rho)-E\right\}u=0$$

$$\lim_{\rho\to\infty} u = ?(Q,U \Rightarrow u)$$

$$\rho\approx\infty \to Q,U\sim\rho^{-2} \qquad Q+U+\frac{\hbar^2}{2m}\frac{15}{4\rho^2}\sim E_{2b}+o(\rho^{-3})$$

$$\Rightarrow \left\{\frac{\hbar^2}{2m}\frac{d^2}{d\rho^2}+E-E_{2b}+o(\rho^{-3})\right\}u=0$$

$$u\sim A\sin k\rho+B\cos k\rho \qquad E=E_{2b}+\hbar^2k^2/2m$$

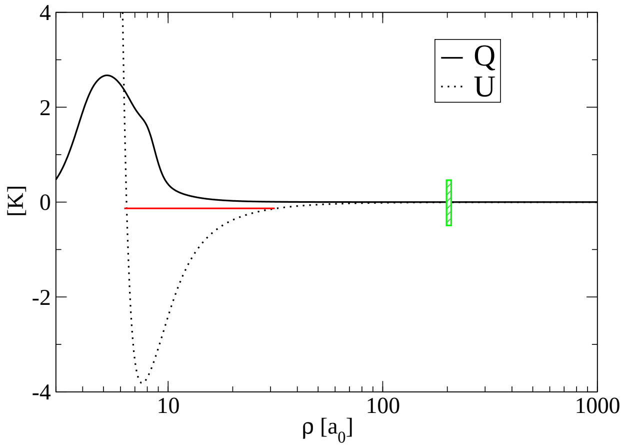
$$u\sim A\rho+B \qquad E=E_{2b}$$

$$\Phi^{\pm}\approx\frac{\exp\left[\pm\imath k\rho\right]}{\rho^{5/2}}\Phi_1(\rho,\Omega)$$

# 14 – asymptotic equation at large $\rho$

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{d^2}{d\rho^2}-\frac{15}{4\rho^2}\right]+Q(\rho)+U(\rho)-E\right\}u=0$$

Helium trimer (LM2M2 potential)




| | HH | HH+as. eq. | Kolganova *et al* |
|---|---|---|---|
| $E_0$ [mK] | 105.98 | 105.98 | 125.9 |
| $E_1$ [mK] | 2.069 | 2.114 | 2.28 |
| $a_s$ [Å] | - | 122.43 | 118.7 |

## 15 – Conclusions

- ☞ investigated hyperspherical adiabatic (HA) basis to describe continuum states
- ☞ established a useful parallelism with the HH basis
- ☞ convergence for continuum observables not as good as in bound states
- ☞ studied the hyperradial system of equations
- ☞ its solution is numerically engaging
- ☞ ... more work to be done

# Scattering three-body states ...

## 16 – large $\rho$ analysis

$$\left\{-\frac{\hbar^2}{2m\rho^2}\frac{d^2}{d\theta^2}+V(r)-\lambda\right\}u=0$$

$$w=\sqrt{2}\rho\left(\frac{\pi}{2}-\theta\right)\quad r=\sqrt{2}\rho\cos\theta$$

$$\left\{-\frac{\hbar^2}{m}\frac{d^2}{dw^2}+V(r)-\lambda\right\}u=0$$

$$r\approx w-\frac{w^3}{12\rho^2}\Rightarrow V(r)\approx V(w)+\frac{w^3}{12\rho^2}\dot{V}(w)=V+\Delta V$$

zeroth-order : $g(w),\lambda=E_{2b}$

first-order : $\lambda=\langle g|\Delta V|g\rangle, Q=\langle g|T_\rho|g\rangle$

$$\lambda\sim E_{2b}+\frac{\hbar^2}{2m}\left(\frac{1}{2}-d\right)+o(\rho^{-4})$$

$$Q\sim\frac{\hbar^2}{2m\rho^2}\left(d-\frac{1}{4}\right)+o(\rho^{-3})$$

$$\lambda+Q\sim\frac{\hbar^2}{2m}\frac{1}{4}$$

$$d=\langle\dot{g}|w^2|\dot{g}\rangle_w$$