# Bound state problem for the three-body Schrödinger equation with Euclidean invariant decaying potential

The 22nd European Conference on Few-Body Problems in Physics,

Kraków, Poland, September 9–13, 2013

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September 9, 2013

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# The problem (as old as QM...)

$$H \equiv -\sum_{i=1}^{3}(2m_i)^{-1}\Delta_i + \sum_{j>i=1}^{3} V_{ij}(\boldsymbol{r}_{ij}) \equiv T + V$$

- The goal:
  To demonstrate an analytic approach for solving the bound state problem for the three-body Schrödinger equation
- Main result:
  Under certain assumptions on $V_{ij}$: $\boldsymbol{R}^3 \to \boldsymbol{R}$, $\forall\kappa = 0, 1, \ldots,$
  $\exists \boldsymbol{I}_\kappa \subset \boldsymbol{R}^9$: $\sigma(H) = \sum_{\kappa=0}^{\infty} \sigma(H_\kappa)$; $H_\kappa = H_\kappa^0 + \gamma(\nabla_{12} \cdot \nabla_{23})$ in $L^2(\boldsymbol{I}_\kappa)$, $\gamma = m_2^{-1}$,

$$\begin{aligned} H_\kappa^0 &\cong (-\alpha\Delta_{12} + V_{\kappa,1}) \otimes I + I \otimes (-\beta\Delta_{23}) \\ &\cong (-\alpha\Delta_{12}) \otimes I + I \otimes (-\beta\Delta_{23} + V_{\kappa,2}), \quad \alpha = \frac{1}{2}\left(\frac{1}{m_2} + \frac{1}{m_3}\right), \quad \beta = \frac{1}{2}\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \end{aligned}$$

$V_{\kappa,i}$: $[0, \infty) \to \boldsymbol{R}$ $(i = 1, 2)$ is found from $V_\kappa \equiv \sum_{i<j}(\partial^\kappa / \partial r_{ij}^\kappa) V_{ij}$

# Advantage over the center-of-mass representation

$$\text{(1)} \quad \boldsymbol{I} = \left\{(\boldsymbol{t}_1, \boldsymbol{t}_2, \boldsymbol{t}_3) \in \boldsymbol{R}^3 \times \boldsymbol{R}^3 \times \boldsymbol{R}^3 \colon \ \boldsymbol{t}_1 + \boldsymbol{t}_2 = \boldsymbol{t}_3\right\} \cong (\boldsymbol{R}^3; +) \times \boldsymbol{R}^6$$

$$\text{(2)} \quad \boldsymbol{I}_\kappa \cap \boldsymbol{I}_{\kappa'} = \varnothing \quad (\kappa \neq \kappa') \quad \text{disjoint sets}$$

$$\text{(3)} \quad \left\{\cup_{\kappa=0}^{\infty} \boldsymbol{I}_{\kappa+p} = \boldsymbol{I} \colon \ p = 0, 1, \ldots\right\} \quad \text{equivalence class}$$

- Center-of-mass: $\sum_i \nabla_i = 0$, $\nabla_{ij} = (m_j \nabla_i - m_i \nabla_j)/(m_i + m_j)$ on $\boldsymbol{R}^9$ [R. J. Slobodrian, Phys. Rev. C 39, no. 3, 1052 (1989)],

$$H = \underbrace{\left[(-\alpha' \Delta_{12} + V_{12}) + (-\beta' \Delta_{23} + V_{23})\right]}_{\text{Separable}} + \underbrace{\left[\gamma'(\nabla_{12} \cdot \nabla_{23}) + V_{13}\right]}_{\text{Perturbation}} \quad \text{in } L^2(\boldsymbol{R}^6)$$

- The present: $\sum_{i<j} \nabla_{ij} = 0$ on $\boldsymbol{I}_\kappa$,

$$H_\kappa = \underbrace{\left[-\alpha \Delta_{12} - \beta \Delta_{23} + V_\kappa\right]}_{\text{Separable}} + \underbrace{\left[\gamma(\nabla_{12} \cdot \nabla_{23})\right]}_{\text{Perturbation}} \quad \text{in } L^2(\boldsymbol{I}_\kappa)$$

# Outline

1. Similarity for the Hamiltonian
   (a) Translation invariance
   (b) Unitary equivalence
   (c) Nilpotent Lie algebra
2. Coulomb case
   (a) Stability criterion
   (b) Discrete spectrum
3. Summary

Similarity for the Hamiltonian

# Translation invariance

Assumptions:

(A1) $V$ is decaying Euclidean invariant: $V_{ij} \to 0$ as $r_{ij} \to \infty$ and $V_{ij}(\boldsymbol{r}_{ij}) = V_{ij}(r_{ij})$

(A2) $V_{ij} \in C^\infty(\boldsymbol{R}^3)$ and $V_k = 0$ is independent of $\{r_{ij}\}$ for some $k = 1, 2, \ldots$

(A3) $H$ admits self-adjoint extensions: $D(V) \supseteq D(T)$

Note:
(A1)–(A2) are sufficient to reduce the problem formally. (A3) is necessary for the spectral analysis.

**Lemma (1)**

Given $H \equiv T + V$ on $\boldsymbol{R}^9$, with $V$ obeying (A1)–(A2). Assume that $\psi \in \mathrm{Ker}(E - H)$, where $\psi \equiv \psi(E; \boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$, with $E \in \sigma(H)$. Then (a) functions $\psi$ are translation invariant, $\psi = \varphi(E; \boldsymbol{r}_{12}, \boldsymbol{r}_{23}, \boldsymbol{r}_{13})$, (b) $\varphi \in \mathrm{Ker}(E - (T_0 + V))$, with $T_0 \equiv -\sum_{i=1}^{3}(2m_i)^{-1}\partial_i^2$, $\partial_1 \equiv \nabla_{12} + \nabla_{13}$, $\partial_2 \equiv \nabla_{23} - \nabla_{12}$, $\partial_3 \equiv -\nabla_{23} - \nabla_{13}$

Similarity for the Hamiltonian

# Translation invariance #2

Note: By Lemma (1) and (A3), $H \equiv T_0 + V$ and $H$: $D(T_0) \to L^2(\boldsymbol{R}^6)$

## Lemma (2)

Define $\boldsymbol{G} \equiv \sum_{i<j} \nabla_{ij}$. There exist domains $D$, $D' \subset D(T_0)$ such that $D = \{\varphi \in D(T_0)\colon\ \boldsymbol{G}\varphi = \boldsymbol{0}\}$, $D \cup D' \subseteq D(T_0)$ and $D \cap D' = \varnothing$.

## Corollary (1)

The operator $T_0 \restriction D$ is represented by the following equivalent forms

$$
\begin{aligned}
T_0 \restriction D &= -\alpha\Delta_{12} - \beta\Delta_{23} + \gamma(\nabla_{12}\cdot\nabla_{23}),\\
&= -\xi\Delta_{23} - \alpha\Delta_{13} + \zeta(\nabla_{13}\cdot\nabla_{23}),\\
&= -\xi\Delta_{12} - \beta\Delta_{13} + \eta(\nabla_{12}\cdot\nabla_{13}).
\end{aligned}
$$

Note: $\boxed{[\boldsymbol{G}, H] \neq \boldsymbol{0} \text{ in } L^2(\boldsymbol{R}^6)}$ (!)

Similarity for the Hamiltonian

# Unitary equivalence: Graph of the additive group on $\boldsymbol{R}^6$

(1) $\boldsymbol{I} \cong (\boldsymbol{R}^3; +) \times \boldsymbol{R}^6 \cong \boldsymbol{R}^9$

(2) $\boldsymbol{G} \equiv \sum_{i<j} \nabla_{ij} = (G_x, G_y, G_z):$ Choose $G_z$

(3) $V_n \equiv G_z^n V;\ \ G_z^n \equiv G_z G_z \ldots G_z\ \ (n = 0, 1, \ldots \text{ times})$

(4) $\boldsymbol{I}_\kappa \equiv \left\{ (\boldsymbol{r}_{12}, \boldsymbol{r}_{23}, \boldsymbol{r}_{13}) \in \boldsymbol{R}^9\colon\ \boldsymbol{r}_{12} + \boldsymbol{r}_{23} = \boldsymbol{r}_{13}, V_{\kappa+1} = 0 \right\}$

(5) $\boldsymbol{I}_\kappa \cong (\boldsymbol{R}^3; +) \times \boldsymbol{J}_\kappa \subseteq (\boldsymbol{R}^3; +) \times \boldsymbol{R}^6 \cong \boldsymbol{I}$

$$\boldsymbol{J}_\kappa \equiv \left\{ (\boldsymbol{t}_1, \boldsymbol{t}_2) \in \boldsymbol{R}^6\colon\ \frac{\partial^{\kappa+1} V_{12}(\boldsymbol{t}_1)}{\partial t_1^{\kappa+1}} + \frac{\partial^{\kappa+1} V_{23}(\boldsymbol{t}_2)}{\partial t_2^{\kappa+1}} + \frac{\partial^{\kappa+1} V_{13}(\boldsymbol{t}_1 + \boldsymbol{t}_2)}{\partial |\boldsymbol{t}_1 + \boldsymbol{t}_2|^{\kappa+1}} = 0 \right\}$$

By (1)–(5): $\left\{ \bigoplus_{\kappa=0}^{\infty} L^2(\boldsymbol{I}_{\kappa+p}) \cong L^2(\boldsymbol{R}^6)\colon\ p = 0, 1, \ldots \right\}$ equivalence class

Similarity for the Hamiltonian

# Nilpotent Lie algebra

**Theorem**

Given the commutation relation $[u, v](\varphi) = w(\varphi)$ on $\boldsymbol{I}_\kappa$ for $\kappa = 0, 1, \ldots$ and $\varphi \in C^1(\boldsymbol{R}^6)$, where $u$, $v$, $w$ denote any quantity from $G_z$, $V_0$, $V_1$, …, $V_\kappa$. Then (1)

$$[G_z, V_n] = V_{n+1}, \quad [V_n, V_m] = 0 \quad \text{for all} \quad n, m = 0, 1, 2, \ldots, \kappa$$

(2) The commutation relations define the Lie algebra $\mathcal{A} = \mathcal{A}(\boldsymbol{I}_\kappa)$, with an operation $\boldsymbol{I}_\kappa \times \boldsymbol{I}_\kappa \to \boldsymbol{I}_\kappa$.

**Corollary (2)**

The Lie algebra $\mathcal{A}(\boldsymbol{I}_\kappa)$ is nilpotent with the nilpotency class $\kappa + 1$.

Similarity for the Hamiltonian

# Nilpotent Lie algebra: Extensions from $C^\infty(\boldsymbol{R}^6)$ to $L^2(\boldsymbol{R}^6)$

1. Rep. of $\mathcal{A}$: $\varrho(e) = G_z$, $\varrho(f_n) = V_n$; $e, f_0, \ldots, f_\kappa$ strictly upper-triangular matrices
2. Matrix Lie group (exponentiation): $\mathcal{L}(\boldsymbol{I}_\kappa) = \{\exp(\mathrm{i}at)\colon\ a \in \mathcal{A}(\boldsymbol{I}_\kappa), t \in \boldsymbol{R}\}$
3. Rep. of $\mathcal{L}$: $\Pi(\exp(\mathrm{i}a)) = \exp(\mathrm{i}\varrho(a))$ on $C^\infty(\boldsymbol{R}^6)$, all $a \in \mathcal{A}$
4. Natural domain of $T_0$ in $L^2(\boldsymbol{I}_s)$ $(s = \kappa, \kappa+1, \ldots)$: $D_{0,s} \subset L^2(\boldsymbol{I}_s)$ densely, $\|T_0\|_{L^2(\boldsymbol{I}_s)} < \infty$
5. Restriction of $T_0 + V_s$, denoted $H_s$, on $D_s = \{\varphi \in D_{0,s}\colon\ \boldsymbol{G}\varphi = \boldsymbol{0}\}$
6. By Theorem, $\boxed{[\boldsymbol{G}, H_s] = \boldsymbol{0} \text{ in } L^2(\boldsymbol{I}_s)}$ (recall Corollary (1)!)
7. For $\varphi \in D_s$, $\Pi$ generates $\{\exp(itV_j)\colon\ j = 0, 1, \ldots, s; t \in \boldsymbol{R}\} \subset \{\exp(itH_j)\colon\ j = 0, 1, \ldots, s; t \in \boldsymbol{R}\} \equiv U_s$, the group of unitary transformations
8. By Corollary (2), $U_s \supset U_s^1 \supset \ldots \supset U_s^s = \{\exp(itH_s)\}$
9. $\boldsymbol{I}_s \to \boldsymbol{I}$ as $s \to \infty$ yields $U_s^s \to \{\exp(itT_0)\} \subset \{\exp(itH)\}$
10. By $\cup_s \boldsymbol{I}_s = \boldsymbol{I}$, $\left\{\bigoplus_{\kappa=0}^{\infty} D_{\kappa+p} \cong D(T_0)\colon\ p = 0, 1, \ldots\right\}$ equivalence class

Coulomb case

# Stability criterion

(1) $H_\kappa = H^0_\kappa + \gamma(\nabla_{12}\cdot\nabla_{23}), \quad H^0_\kappa = T_1 + T_2 + V_\kappa, \quad T_1 = -\alpha\Delta_{12}, \quad T_2 = -\beta\Delta_{23}$

(2) $\inf\sigma(H_\kappa) = \inf\sigma(H^0_\kappa)$ [B. Simon, Helv. Phys. Acta 43, 607 (1970)]

(3) $H^0_\kappa \cong H^0_{\kappa,1}\otimes I + I\otimes T_2 \cong T_1\otimes I + I\otimes H^0_{\kappa,2}, \quad H^0_{\kappa,i} = T_i + V_{\kappa,i} \quad (i=1,2),$

$$V_{\kappa,1}(r_{12}) = \frac{\partial^\kappa}{\partial r_{12}^\kappa}\Big(V_{12}(r_{12}) + \wp^\kappa V_{23}(r_{12}/\wp) + (\wp/c)^\kappa V_{13}(cr_{12}/\wp)\Big) = Z^{eff}_{12}/r_{12}^{\kappa+1},$$

$$V_{\kappa,2}(r_{23}) = \frac{\partial^\kappa}{\partial r_{23}^\kappa}\Big(\wp^{-\kappa} V_{12}(\wp r_{23}) + V_{23}(r_{23}) + c^{-\kappa} V_{13}(cr_{23})\Big) = Z^{eff}_{23}/r_{23}^{\kappa+1}$$

(4) Stability criterion (recall $\boldsymbol{J}_{\kappa+p}$):

$$(\partial^{\kappa+p+1}/\partial r_{12}^{\kappa+p+1})\Big(V_{12}(r_{12}) + \wp^{\kappa+p+1} V_{23}(r_{12}/\wp) + (\wp/c)^{\kappa+p+1} V_{13}(cr_{12}/\wp)\Big) = 0$$

Eg: For $V_{ij} = Z_{ij} r_{ij}^{-1}$, (4) yields $Z_{12} + \wp^k Z_{23} + (\wp/c)^k Z_{13} = 0$ (hence $V$ fulfills (A2)), $k = \kappa + p + 2$; the latter together with (3) determine multipliers $\wp$ and $c$

Coulomb case

# Discrete spectrum

1. $\kappa = 0$ (potential $A_0/r$, $A_0 < 0$):

$$\sigma_{\text{disc}}(H_0^0) = \left\{ -\frac{1}{4}\left(\frac{Z_1(Z_2+Z_3)}{n_1\sqrt{\alpha}} + \frac{Z_{23}}{n_2\sqrt{\beta}}\right)^2 \colon 1/2 \le \frac{n_1}{n_2}\sqrt{\frac{\alpha}{\beta}} \le 1, \right.$$
$$\left. n_i = l_i + 1, l_i + 2, \ldots; l_i = 0, 1, \ldots; i = 1, 2 \right\}$$

Eg: $E_0(\text{He}) = -2.914048$ (ground st.), $E_0(\text{Ps}^-) = -1/4$ (threshold)

2. $\kappa = 1$ (potential $A_1/r^2$, $A_1 > 0$):

$$\sigma_{\text{disc}}(H_1^0) = \inf_{D_k(\wp)\neq\varnothing} \left\{ \chi B_1 < 0 \colon \chi \equiv \chi(i) = \begin{cases} \alpha, & i = 1 \\ \beta, & i = 2 \end{cases}; B_1 = B_1(i) \right.$$
$$\left. = -\left(\frac{2}{r_0}\right)^2 \left(\frac{\Gamma(n_i+\nu_i)}{\Gamma(n_i-\nu_i)}\right)^{1/\nu_i}; \nu_i^2 = A_1^2 + (l_i + 1/2)^2; 1/2 < \nu_i < n_i \right\}$$

Eg: $E_1(\text{He}) = \varnothing$, $E_1(\text{Ps}^-) = -0.515488/r_0^2$; by [A. Martin et al, Phys. Rev. A 46, 3697 (1992)], ground st. of $\text{Ps}^- \approx -0.261995$. Then $E_0 + E_1 = -0.261995$ yields $r_0 \approx 6.56$ (eg $r_0 = 4$ in [A. P. Mills et al, New. Dir. Ant. Chem. Phys. (2002)])

Coulomb case

# Summary

Main conclusion:

Imposed under (A1)–(A3), for $H = T + V$ in $L^2(\boldsymbol{R}^9)$, there exists a subspace $L^2(\boldsymbol{I}_\kappa)$ such that $H$ projected onto it admits SO(3)–invariance ($H_\kappa = H_\kappa^0$+Hughes–Eckart).

1. Geometry of $\boldsymbol{I}$ is advantageous over Jacobi coordinates, perimetric coordinates, center-of-mass representation because it leaves $V$ unchanged and allows one to simplify $T$ on certain domains
2. By partitioning $\boldsymbol{I}$ into disjoint subsets $\boldsymbol{I}_\kappa$, one obtains the equivalence relation between $L^2(\boldsymbol{R}^6)$ and the decomposition $\oplus L^2(\boldsymbol{I}_\kappa)$ eventually implying that the spectrum of $H$ is the sum of the spectra of $H_\kappa$
3. In the Coulomb case, the spectrum of $H_\kappa^0$ is found by solving the radial Schrödinger equation in $L^2([0,\infty);dr)$ with the potential of the form $A_\kappa r^{-\kappa-1}$, where $A_\kappa < 0$ for $\kappa = 0,2,\ldots$, and $A_\kappa > 0$ for $\kappa = 1,3,\ldots$

$$L_{\kappa,l} = -d^2/dr^2 + l(l+1)/r^2 + A_\kappa/r^{\kappa+1} \quad (l = 0,1,\ldots; A_\kappa \in \boldsymbol{R})$$