Fixed-Energy-R separation for Schrödinger equation

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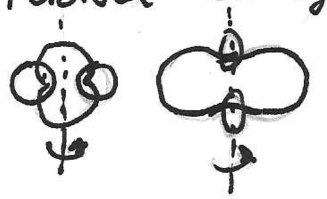
Fixed Energy R - separation of Variables
(FER - separation)

Laplace - Helmholtz _ Schrödinger equations

R sep in Einstein manifolds ⇒ standard sep coord.

FER_sep ⇒ conformal separable coordinates

ex. toroidal bi- cyclidal . . etc. (conf. cyclides)



(Q_n, G) Riemannian manifold $\{(q, p)\}$

$V : Q_n \to \mathbb{R}$, $E \in \mathbb{R}$ $(\mathbb{C})$

$$S\psi = -\frac{\hbar^2}{2}\Delta\psi + (V-E)\psi = 0$$

Δ : Laplace - Beltrami

$$\Delta\psi = g^{ij}\partial^2_{ij}\psi - \Gamma^h \partial_h \psi \quad \left(\Gamma^h = g^{ij}\Gamma^h_{ij}\right)$$

ψ R- solution of S ⟺

$$S\psi = 0$$

$$\psi = R\,\phi \qquad R : Q_n \times ? \to \mathbb{R}$$

"integrating factor"

$S\psi = 0 \iff R\Delta\phi + 2\nabla R \cdot \nabla\phi + R\left(\frac{2}{\hbar^2}E - U\right)\phi = 0$

$\boxed{S'\phi = 0}$

$U = \frac{2}{\hbar^2}V - \frac{\Delta R}{R}$

$S\psi = 0$ is EER-separable $\iff$ $\exists\ (R, E)$:

$S'\phi = 0 \qquad \psi = R\phi$

$\phi = \prod_{i=1}^{n} \phi_i(q^i, c_\alpha) \qquad c_\alpha \in \{$ set of parameters $\}$

+ "completeness" w.r. (c_α)

In S', E is not the eigenvalue.

$S'\phi = 0$ is an eigenvalue problem with null eigenvalue

E eigenvalue $\iff$ (standard) R-separation (K & Miller Moon-Spencer)

$\Updownarrow$

FER-separation for E ~~...~~ fixed

Multiplicative $\Leftrightarrow$ Additive Separation

$$u = \ln \phi \qquad \phi = \Pi_i \phi_i$$

$$S'\phi = 0 \quad \Leftrightarrow \quad g^{ii} u_i u_j + g^{ii} u_{ii} + g^{ij}\left(2\partial_j \ln R - \Gamma_j\right) u_i +$$

$$u_i = \partial_i u \,, \; u_{ii} = \partial^2_{ii} u \qquad + \frac{2}{\hbar^2} E - U = 0 \qquad S'' u = 0$$

$$u = \sum_i w_i(q^i) \qquad E \text{ fixed}$$

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complete additive separable integrability of ℓ-th order PDE (K&M, Benenti ...)

$$\mathcal{H}\left(q^i, u, u_i, u_{ii}, \dots, u_{i^{(\ell)}}, c_\alpha\right) = 0$$

$$\alpha \in \{1, \dots, n\cdot\ell + 1\}$$

(1) $\det \left[\frac{\partial u}{\partial c_\alpha} \middle| \frac{\partial u_i}{\partial c_\alpha} \middle| \cdots \middle| \frac{\partial u_{i^{(\ell)}}}{\partial c_\alpha} \right] \neq 0$

(2.1) $\mathcal{H}\left(u, u_i, \dots, u_{i^{(\ell)}}\right) = c_{n\ell+1}$ Standard Sep.

(2.2) $\mathcal{H}\left(u, u_i, \dots, u_{i^{(\ell)}}\right) = 0 \qquad c_{n\ell+1} = 0$

FE. sep

$$u = \ln \phi \,, \; u_i = \frac{\phi_i'}{\phi} \,, \; u_{ii} = \left(\frac{\phi_i'}{\phi}\right)' \dots$$

completeness $\Leftrightarrow$ $c_\alpha = c_\alpha \left[\phi_0 , \left(\frac{\phi_i'}{\phi}\right)_0 , \dots , \left(\frac{\phi_i'}{\phi}\right)_0^{(\ell)} \right]$

(3)

$u(q^i, c_\alpha)$ is complete separate solution of $\mathcal{H}=0$

$\Leftrightarrow$ $\qquad\qquad\qquad\qquad \mathcal{H} = c_{n+1}$

$$\begin{cases} \partial_i u = u_i \\ \partial_i u_j = \delta_{ij} u_{jj} \\ \vdots \\ \partial_i u_j^{(l)} = \delta_{ij} S_j \end{cases} \qquad S_j = -\frac{1}{\frac{\partial \mathcal{H}}{\partial u_j^{(l)}}}\left(\frac{\partial \mathcal{H}}{\partial q^i} + \frac{\partial \mathcal{H}}{\partial u} u_j + \dots + \frac{\partial \mathcal{H}}{\partial u_j^{(l-1)}} u_j^{(l)}\right)$$

$\Updownarrow \qquad Q \times T : (q^i, u, u_i, \dots, u_i^{(l)})$, T: $nl+1$ dim $\qquad \Updownarrow$

$$D_i = \frac{\partial}{\partial q^i} + u_i \frac{\partial}{\partial u} + u_{ii} \frac{\partial}{\partial u_i} + \dots + S_i \frac{\partial}{\partial u_i^{(l)}} \qquad D_j \mathcal{H} = 0$$

(D_i) generate a connection Δ on $Q \times T$

Δ c.i on $Q \times T$ $\Leftrightarrow$ $[D_i, D_j] = 0$ $\Leftrightarrow$ $D_i S_j \underset{i \neq j}{=} 0$

Standard sep.

Δ c.i. on $\mathcal{H}=0$ $\Leftrightarrow$ $[D_i, D_j]_{|\mathcal{H}=0} = 0$ $\Leftrightarrow$ $D_i S_{j\,|\mathcal{H}=0} \underset{i \neq j}{=} 0$

$l=1$ $\quad \mathcal{H} = c_n (=E)$, $\quad u_i = \frac{\partial u}{\partial q^i} = p_i$, $\quad Q \times T = T^* Q$

$[D_i, D_j] = 0 \equiv$ Levi Civita equations

$[D_i, D_j]_{|\mathcal{H}=0} = 0 \equiv$ L.C. with Lagrangian multipliers

$(\mathcal{H}_k)$ Liouville-integrable system

$\Rightarrow$ $[D_i, D_j] = 0$ $\Leftrightarrow$ (D_i) generate coordinates on $\bigcap_k \{\mathcal{H}_k = c_k\}$ invariant tori

Natural Hamiltonians.

$$\delta' \phi = 0 \iff g^{ij} u_i u_j + g^{ii} u_{ii} + g^{ii}(2\partial_j \ln R - \Gamma_j) u_i + \frac{2}{\hbar^2} E - U = 0$$

$$[D_i, D_j] = 0$$

$$\Updownarrow$$

① $g^{ij} = 0 \quad i \neq j$: orthogonal coordinates

② $2\partial_i \ln R - \Gamma_i = f_i(q^i)$

③ g sep

$\boxed{R\text{-sep.}}$

④ $U = g^{ii} f_i(q^i)$

$\dfrac{g}{\frac{2}{\hbar^2}E - U}$ sep. in (q^i)

$\boxed{\text{FER sep.}}$

$$\Updownarrow$$

$$\begin{cases} g \text{ conf. sep. } (g \text{ conformal to a sep. metric}) \\ \frac{2}{\hbar^2} E - U = g^{ii} f_i(q^i) \end{cases}$$

$\left(\frac{2}{\hbar^2} E - U = 0 \ : \ g \text{ conf. sep} \right)$

Laplace

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③ $\Rightarrow$

$\exists$ n indep. KT (K_i)

$K_n = g$

$[K_i, K_j] = 0$

$d(K_i \, dU) = 0$

$\exists n$ indep. CKT (K_i)

$K_n = g$

$[K_i, K_j] = 2 C_{ij} \odot g$

(conformal involution)

With distinct ~~common~~ eigenvalues and eigenvectors

(q^i) orthogonal coordinates

conformally separable for $\frac{g}{\frac{2}{\hbar^2}E-U}$ and

$\frac{g}{\frac{2}{\hbar^2}E'-U}$, $E \neq E' \Rightarrow (q^i)$ separable for g

— • —

$$S_{ij}(g^{kk}) = \partial^2_{ij} \log g^{kk} - \partial_i \log g^{jj} \partial_j \log g^{kk} - \partial_j \log g^{ii} \partial_i \log g^{kk}$$

$$LC_{ij} \equiv g^{ii} g^{jj} \partial^2_{ij} g^{kk} - g^{ii} \partial_i g^{jj} \partial_j g^{kk} - g^{jj} \partial_j g^{ii} \partial_i g^{kk} = 0$$

$k = 1..n$

$i, j \neq$

— • —

3 g separable

$$S_{ij}(g^{kk}) = 0$$

$i, j, k = 1-n, \quad i, j \neq$

g conformally sep.

$$\frac{S_{ij}(g^{kk})}{g^{kk}} = \frac{S_{ij}(g^{hh})}{g^{hh}}$$

— • —

Equivalence classes of CKT

$$K \simeq K + f g \qquad f : Q \to \mathbb{R}$$

g Conf. sep. $\Rightarrow$ $\partial_i \Gamma_j = \partial_j \Gamma_i$ $\Rightarrow$ (2) integrable always

(g sep $\Uparrow$)

— o —

R by (2) gives possibility to fulfill Robertson condition $\partial_i \Gamma_j = 0_{i \neq j}$

— o — o —

In orthogonal conformal separable coordinates:

$$R_{ij} = \frac{3}{2} \partial_i \Gamma_j - \frac{n-2}{4} \frac{L c_{ij}(g^{kk})}{g^{kk} g^{ii} g^{jj}} \qquad (i \neq j)$$

Separation of Laplace–Schrödinger both standard and Fixed-Energy, always requires Robertson condition: $\partial_i \Gamma_j = 0$ $i \neq j$

$\Rightarrow$ in Einstein manifolds, separation of Laplace–Schrödinger (standard and fixed-energy) in orthogonal coordinates occurs in standard separable coordinates (Stäckel) only.

— o —

$$\frac{\Delta R}{R} = \frac{1}{4} g^{ii} \left[\partial_i \Gamma_i - \frac{1}{2} \Gamma_i^2 + \theta_i(q^i) \right] \qquad \text{in conf. sep. coord.}$$

(3) $\Leftrightarrow$ $\frac{2}{\hbar^2}(E - V) + \frac{\Delta R}{R} = g^{ii} f_i(q^i)$

$$\overset{\shortparallel}{\left(\frac{2}{\hbar^2} E - U\right)}$$

(6)

Separated equations

$$K^{ii}_{j} = \varphi^{i}_{(j)}$$

$$K^{ii}_{n} = \varphi^{i}_{(n)} = g^{ii} \quad \text{or} \quad \frac{g^{ii}}{\frac{2}{\hbar^2}E - U}$$

Sep. Conf. separable

— o —

$$\varphi^{i}_{(j)}\left(u_{ii} + u_i^2 - \xi_i u_i + f_i\right) = c_j \qquad \varphi^{i}_{(j)}\left(u_{ii} + u_i^2 - \xi_i u_i\right) = c_j$$

$$g^{ii}\left(\quad \text{———} \quad \right) = E \qquad \frac{g^{ii}}{\frac{2}{\hbar^2}E - U}\left(\quad \text{———} \quad \right) = 1$$

$\xi_i = 0 \Rightarrow$ canonical form of sep. eq.

— o — o —

From sep. eq. $\quad u = \ln \frac{\psi}{R}$

$\Rightarrow$ Symmetry operators

$$H_j \psi = \Delta_j \psi - \frac{1}{R} \Delta_j R\, \psi$$

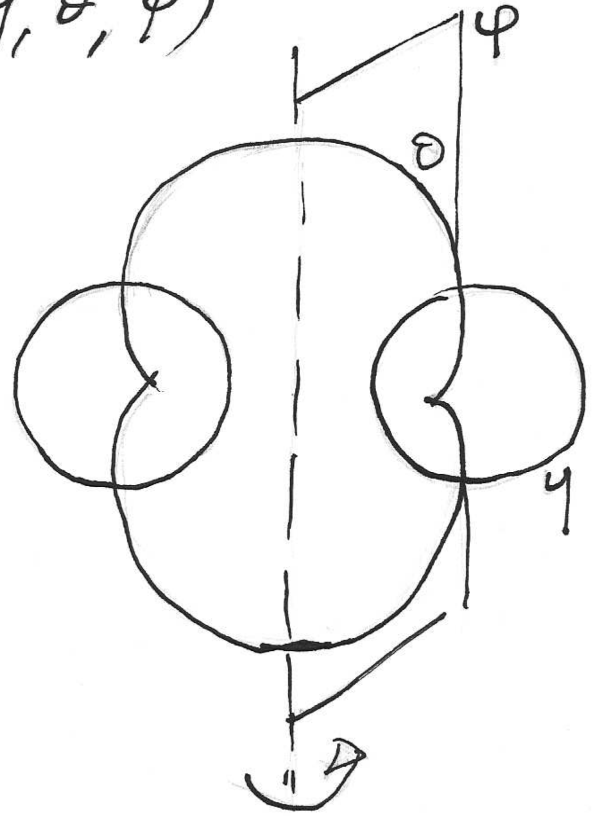
$$\Delta_j = \varphi^{i}_{(j)} \left(\partial^2_{ii} - \Gamma_i \partial_i \right)$$

$$[H_j, H_j] = 0 \qquad H_n = \frac{\Delta \psi}{\frac{2}{\hbar^2}E - U} - \frac{\Delta R}{R}\psi$$

$$H_n^{\psi} = 1 \sim S\psi = 0$$

Toroidal Coordinates $\mathbb{E}_3$

$(q^i) = (\eta, \theta, \varphi)$



$$g^{11} = g^{22} = \left(\frac{\operatorname{ch}\eta - \cos\theta}{a}\right)^2$$

$$g^{33} = \frac{g^{11}}{\operatorname{sh}^2\eta}$$

$$\Delta\psi - V\psi = 0$$

FER- sep $\Leftrightarrow$

$$\frac{\Delta R}{R} - \frac{2}{\hbar^2}V = (\operatorname{ch}\eta - \cos\theta)^2\left[f_1(\eta) + f_2(\theta) + \frac{1}{\operatorname{sh}^2\eta}f_3(\varphi)\right]$$

$$R = (\operatorname{ch}\eta - \cos\theta)^{\frac{1}{2}} \qquad \text{Noncanonical}$$

$$R = \left(\frac{\operatorname{ch}\eta - \cos\theta}{\operatorname{sh}\eta}\right)^{\frac{1}{2}} \qquad \text{canonical}$$

— o —

$$g^{ii} = \sigma\,\bar{g}^{ii} \qquad \sigma = (\operatorname{ch}\eta - \cos\theta)^2\left[f_1 + f_2 + \frac{1}{\operatorname{sh}^2\eta}f_3\right] \qquad \bar{g} \text{ Stäckel metric}$$

CKT: g

$$\partial_\theta \otimes \partial_\theta \qquad\qquad\qquad\qquad \partial_\varphi \otimes \partial_\varphi$$

$$\begin{bmatrix} \frac{x^2z^2}{a^2} & \frac{xyz^2}{a^2} & -\frac{(x^2+y^2-z^2-a^2)zx}{2a^2} \\ \cdot & \frac{z^2y^2}{a^2} & -\frac{(x^2+y^2-z^2-a^2)zy}{2a^2} \\ \cdot & \cdot & \frac{(x^2+y^2-z^2-a^2)^2}{4a^2} \end{bmatrix} \begin{bmatrix} y^2 & -xy & 0 \\ -xy & x^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Stächel matrix:

$$
S = \begin{pmatrix} f_1 & -1 & -\frac{1}{\operatorname{sh}^2 y} \\ f_2 & 1 & 0 \\ f_3 & 0 & 1 \end{pmatrix}
$$

— o —

Sep equations

$$
\begin{cases}
\dfrac{d^2\phi_1}{dy^2} + \left\{\coth y \dfrac{d\phi_1}{dy}\right\} + \left(\cancel{\#} - c_2 - c_3 \operatorname{sh}^{-2} y + f_1\right)\phi_1 = 0 \\[2ex]
\dfrac{d^2\phi_2}{d\theta^2} + \left(c_2 + f_2\right)\phi_2 = 0 \\[2ex]
\dfrac{d^2\phi_3}{d\varphi^2} + \left(c_3 + f_3\right)\phi_3 = 0
\end{cases}
$$

— o —

OSep geod HJ	$S_{ij}(g^{kk})=0$	#	#
Sep Helmholtz	$S_{ij}(g^{kk})=0$	$\partial_i\Gamma_j=0$ (1)	#
OSep natural HJ	$S_{ij}(g^{kk})=0$	#	$S_{ij}(V)=0$
Sep Schröd.	$S_{ij}(g^{kk})=0$	$\partial_i\Gamma_j=0$ (1)	$S_{ij}(V)=0$
OSep null geod HJ	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	#	#
Sep Laplace	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	$\partial_i\Gamma_j=0$ (2)	#
OFEsep nn geod HJ	$\Rightarrow S_{ij}(g^{kk})=0$	#	$\frac{S_{ij}(E)}{E}=\frac{S_{ij}(g^{kk})}{g^{kk}}=0$
FEsep Helm ($E\neq 0$)	$\Rightarrow S_{ij}(g^{kk})=0$	$\partial_i\Gamma_j=0$ (1)	$\frac{S_{ij}(E)}{E}=\frac{S_{ij}(g^{kk})}{g^{kk}}=0$
FEsep natural HJ	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	#	$\frac{S_{ij}(E-V)}{E-V}=\frac{S_{ij}(g^{kk})}{g^{kk}}$
FEsep Schröd	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	$\partial_i\Gamma_j=0$ (2)	$\frac{S_{ij}(E-V)}{E-V}=\frac{S_{ij}(g^{kk})}{g^{kk}}$
Rsep Helmholtz	$S_{ij}(g^{kk})=0$	$\partial_i\ln R=\frac{1}{2}\Gamma_i$	$S_{ij}(\frac{\Delta R}{R})=0$
Rsep Schröd	$S_{ij}(g^{kk})=0$	$\partial_i\ln R=\frac{1}{2}\Gamma_i$	$S_{ij}(V-\frac{\Delta R}{R})=0$
Rsep Laplace	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	$\partial_i\ln R=\frac{1}{2}\Gamma_i$	$\frac{S_{ij}(\frac{\Delta R}{R})}{R^{-1}\Delta R}=\frac{S_{ij}(g^{kk})}{g^{kk}}$
FERsep Helm	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	$\partial_i\ln R=\frac{1}{2}\Gamma_i$	$\frac{S_{ij}(E+\frac{\Delta R}{R})}{E+R^{-1}\Delta R}=\frac{S_{ij}(g^{kk})}{g^{kk}}$
FERsep Schr	$\frac{S_{ij}(g^{kk})}{g^{kk}}=\frac{S_{ij}(g^{hh})}{g^{hh}}$	$\partial_i\ln R=\frac{1}{2}\Gamma_i$	$\frac{S_{ij}(E-V+\frac{\Delta R}{R})}{E-V+\frac{\Delta R}{R}}=\frac{S_{ij}(g^{kk})}{g^{kk}}$

$\Gamma_i=\partial_i(\log\frac{g_{ii}}{\sqrt{g}})$ with $g=\det(g_{ij})$. $\frac{\Delta R}{R}$ can be written as $g^{ii}(\partial_i\Gamma_i-\frac{1}{2}\Gamma_i^2)$

(1) it is equivalent to $R_{ij}=0$ (2) it is equivalent to $R_{ij}=\frac{n-2}{4}\frac{S_{ij}(g^{kk})}{g^{kk}}$

Indeed, in conf sep coords we have $R_{ij}=\frac{3}{2}\partial_i\Gamma_j-\frac{n-2}{4}\frac{S_{ij}(g^{kk})}{g^{kk}}$. Hence no proper conformal sep coords on an Einstein manifold satisfy condition (2) (while all sep coords satisfy (1)). Thus, in Einstein manifolds Sep of Laplace, FEsep of Helmholtz, FEsep of Schr occur in all (orthogonal) separable coordinates only (if $V\neq 0$, V must be a Stäckel factor).

+ Dirac Equation!