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Constrained separation of variables in Schrödinger equations via incomplete Stäckel matrices.

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Pseudo-Riemannian metric $ds^2 = g_{ij}dx^i dx^j$,

with orthogonal coordinates,

$$g = \begin{bmatrix} H_1^2 & 0 & 0 & \cdots & 0 \\ 0 & H_2^2 & 0 & \cdots & 0 \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & \cdots & H_{N-1}^2 & 0 \\ 0 & \cdots & \cdots & 0 & H_N^2 \end{bmatrix}.$$

Laplace Beltrami

$$\Delta\Psi = \frac{1}{\sqrt{det\ g}}\,\partial_j\left(g^{jk}\sqrt{det\ g}\ \partial_k\Psi\right) \qquad ;\ g_{jk}g^{km} = \delta_j{}^m$$

invariant under general diffeomorphisms.

Staeckel 1891 found separable forms of Hamilton-Jacobi eq.
Method applies also to linear eigenfn probs., e.g. Schroedinger.
Staeckel matrix has entries s_{ij} = function of x_i . e.g. for N=2,

$$\partial_1^2\Psi + f_1(x^1)\partial_1\Psi + [v_1(x^1) - s_{11}(x^1)E - s_{12}(x^1)\lambda_2]\Psi = 0$$
$$\partial_2^2\Psi + f_2(x^2)\partial_2\Psi + [v_2(x^2) - s_{21}(x^2)E - s_{22}(x^2)\lambda_2]\Psi = 0$$

T = inverse of S.

$$L_1\Psi = [T^{11}\partial_1^2 + T^{12}\partial_2^2]\Psi + T^{11}f_1(x^1)\partial_1\Psi + T^{12}f_2(x^2)\partial_2\Psi + [T^{11}v_1(x^1) + T^{12}v_2(x^2)]\Psi = E\Psi$$
$$L_2\Psi = [T^{21}\partial_1^2 + T^{22}\partial_2^2]\Psi + T^{21}f_1(x^1)\partial_1\Psi + T^{22}f_2(x^2)\partial_2\Psi + [T^{21}v_1(x^1) + T^{22}v_2(x^2)]\Psi = \lambda_2\Psi \;.$$

Demand that L_1 operator equates to target Helmholtz operator involving Laplace-Beltrami operator

$$\Delta\Psi = H_1^{-2}\partial_1^2\Psi + H_2^{-2}\partial_2^2\Psi + \frac{\partial_1(H_2/H_1)}{H_1 H_2}\partial_1\Psi + \frac{\partial_2(H_1/H_2)}{H_1 H_2}\partial_2\Psi$$

Equating 1st order terms,
$$f_1(x^1) = \partial_1 \log\frac{H_2}{H_1}$$
$$f_2(x^2) = -\partial_2 \log\frac{H_2}{H_1} \ .$$

For separation of Schroedinger eq., we need R-separation

$$u = \Psi e^{-R(x)} = u_1(x^1)u_2(x^2)$$, implying

$$f_1(x^1) = \partial_1 \log\frac{H_2}{H_1} + 2\partial_1 R$$
$$f_2(x^2) = -\partial_2 \log\frac{H_2}{H_1} + 2\partial_2 R \ .$$

$$\implies \partial_1\partial_2 \log\frac{H_2}{H_1} = 0 \implies H_2/H_1 = \Pi_1(x^1)\Pi_2(x^2)$$

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Extending the identification of L1 with Helmholtz at all orders, we deduce

$$T = \begin{bmatrix} \frac{g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)}{g_1(x^1)g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)-1} & \frac{g_2}{g_1(x^1)g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)-1} \\ T_{21}(\mathbf{x}) & g_1 g_2 T_{21} \end{bmatrix},$$

with $T_{21} = \gamma_3 T_{11}/g_2\Pi_2^2 \quad (\gamma_3 \in \Re)$

For N>2, this identification implies Robertson conditions, studied by Robertson and Eisenhart since 1920s.
This inverse construction of separable eqs. leads to all known integrable Schroedinger equations.

Theorem: With L_j constructed as above, $[L_i,L_j]=0$.
(L_1= Hamiltonian H).

The Staeckel construction results in a complete set of commuting self-adjoint operators, as well as the class of allowable potentials.
Example: with plane polar coords,

$$x^1 = r \quad ; \quad x^2 = \theta \quad ; \quad \Pi_1 = r \quad ; \quad \Pi_2 = 1 \quad .$$

Identify L_1 with Helmholtz , $L_1 \Psi = \Delta \Psi + \Phi(r,\theta)\Psi$,
deduce $R = \frac{-1}{2} \log\ r$ and $\Phi = v_1(r) + r^{-2} v_2(\theta) - \frac{1}{4} r^{-2}$.

r^{-2} potential is familiar from reduction of variables in Kepler prob

$$H = \frac{1}{2}\mu \dot{r}^2 + \frac{1}{2}\mu (r\dot{\phi})^2 + V(r)$$

$$= \frac{1}{2}\mu \dot{r}^2 + \frac{1}{2}\frac{\lambda_3^2}{\mu r^2} + V(r) \quad ; \quad \mu r^2 \dot{\phi} = \lambda_3$$

For quantum hydrogen atom,

$$H' = \partial_r^2 + \frac{2}{r}\partial_r + \frac{1}{r^2}\partial_\theta^2 + \frac{\cot\theta}{r^2}\partial_\theta + \frac{\lambda_3}{r^2\sin^2\theta} + \frac{\alpha}{r}$$

$$L_3\Psi = \partial_\phi^2\Psi = \lambda_3\Psi$$

Question: Analogous to non-classical symmetry reductions, can we generalize the Staeckel construction to find non-regular separation that is valid when some constraint applies ?

Nonclassical Lie symmetry leaves invariant a system of eqs consisting of target PDE plus invariant surface cond (a constraint).

$$\bar{t} = t + \epsilon T(t, x^i, \Psi) + O(\epsilon^2) \quad ; \quad \bar{x}^i = x^i + X^i(t, x^j, \Psi) + O(\epsilon^2)$$

$$\bar{\psi} = \Psi + \epsilon U(t, x^i, \Psi) + O(\epsilon^2)$$

e.g. applied to Schroedinger + ISC

$$\Psi_t = -\Delta\Psi + V(\mathbf{r})\boldsymbol{\Psi};$$

$$T\Psi_t + X^i\Psi_{,i} = U$$

Generalized Staeckel matrix: as above but now one or more columns including $S_{iN}(\mathbf{x})$ can depend on all x_j .

Thm. With only N'th column being non-Staeckel, $[L_i,L_j]=0$ on zero-eigenspace of L_N.

This leads to special (non-regular) separated solutions, compatible with some constraints $L_N=0$.
For N=2, we can prove that no new separable Schrödinger eqs occur (even with magnetic vector potential as well as electrostatic scalar potential).

Schroedinger eq. in Cartesian coords. for charged particle in electromagnetic field in Euclidean space.

$$H\Psi = -\frac{(\hbar)^2}{2}\nabla^2\Psi - \frac{i\hbar}{2}[\mathbf{A}.\nabla + \nabla.\mathbf{A}(\mathbf{x})]\boldsymbol{\Psi} + \mathbf{V}(\mathbf{x})\boldsymbol{\Psi} = \lambda\boldsymbol{\Psi}$$

More generally, extend $\nabla^2\Psi \rightarrow$

$$\Delta\Psi = H_1^{-2}\partial_1^2\Psi + H_2^{-2}\partial_2^2\Psi + \frac{\partial_1(H_2/H_1)}{H_1H_2}\partial_1\Psi + \frac{\partial_2(H_1/H_2)}{H_1H_2}\partial_2\Psi$$

$$\nabla.\mathbf{a} \rightarrow \frac{\partial\bar{\mathbf{a}}^{\mathbf{m}}}{\partial\bar{\mathbf{x}}^{\mathbf{m}}} + \bar{\mathbf{a}}^{\mathbf{m}}\boldsymbol{\Gamma}^{\mathbf{i}}_{\mathbf{im}} = \frac{\mathbf{1}}{\sqrt{\bar{\mathbf{g}}}}\frac{\partial}{\partial\bar{\mathbf{x}}^{\mathbf{i}}}(\bar{\mathbf{a}}^{\mathbf{i}}\sqrt{\bar{\mathbf{g}}}).$$

and extend direct separation to R-separation

$$u = \Psi e^{-R(x)} = u_1(x^1)u_2(x^2)$$

E.g. for N=2 generalized Staeckel construction, with no mag field,

$$T = \begin{bmatrix} \frac{g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)}{g_1(x^1)g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)-1} & \frac{g_2}{g_1(x^1)g_2(x^2)\Pi_1^2(x^1)\Pi_2^2(x^2)-1} \\ T_{21}(\mathbf{x}) & g_1 g_2 T_{21} \end{bmatrix},$$

with T_{21} now <u>general</u>. However, T_{11} and T_{12} are same as in complete Staeckel construction and these determine components of allowable metric and allowable scalar potential.

With N=2, no new Schroedinger eqs can be solved by incomplete Staeckel construction.

Same no-go theorem applies when electromag field is included.

N >2: incomplete Staeckel leads to new examples of separable systems.

New separable solutions may occur for 2D solute transport,

$$\partial_t c + [q^1\partial_1 + q^2\partial_2]c = \Delta c - \mu(\mathbf{x})\mathbf{c}$$

advection dispersion adsorption

but only when g_{ij} is not separated, $g_{11}/g_{12} = H_1^2/H_2^2 \neq g_i(x^1)h_i(x^2)$,

implying $\partial_1(H_2^2 q^2) - \partial_2(H_1^2 q^1) \neq 0.$

It is a non-trivial task even to find examples of this in E^2 .

Although the parabolic solute transport eq resembles the hyperbolic Schroedinger eq with magnetic field, incomplete Staeckel construction now allows extra freedom because the first-order terms are real.

Since we may replace x^1 by a function of x^1 and we may multiply a column of S by a scalar function, to investigate admissible separable equations, assume canonical form

$$S = \begin{pmatrix} 1 & 1 \\ 1 & f(u,v) \end{pmatrix}. \qquad T=S^{-1}$$

$$g_{11} = T^{-1}_{11} = 1 - \frac{1}{f} \; ; \quad g_{22} = T^{-1}_{12} = 1 - f$$

Condition of zero Gauss curvature is

$$0 = f_{uu} + 2f^{-3} f_v^2 - f^{-2} f_{vv} - \frac{(f+1)f_u^2}{2f(f-1)} + \frac{(f+1)f_v^2}{2f^3(f-1)}$$

Note: conformal maps don't change g11/g22 - not interesting

Example in E².

$$ds^2 = dx^2 + dy^2 = \frac{f(u,v)-1}{f(u,v)}du^2 + (1 - f(u,v))dv^2,$$

$$f(u,v) = -\frac{1}{4}\left(u + v + \sqrt{(u+v)^2 - 4}\right)^2.$$

Here $x = (u+v)\cos(\phi - u), \quad y = (u+v)\sin(\phi - u),$

$$\phi = \frac{1}{2}\left(u + v + \sqrt{(u+v)^2 - 4}\right) - 2\arctan\left(\frac{u + v + \sqrt{(u+v)^2 - 4}}{2}\right),$$

and $|u + v| \geq 2.$

After separating t variable from solute eq, Helmholtz eigenval eq is

$$\left(\Delta_2 - \frac{f}{f-1}\left(\frac{1}{2}\frac{f_u}{f}\partial_u - U(u)\right) + \frac{1}{f-1}\left(\frac{-1}{2}\frac{f_v}{f}\partial_v - V(v)\right)\right)\Psi = E\Psi.$$

The separation equations are

$$(\partial_{uu} + U(u) - E)\Psi^{(1)}(u) = 0,$$
$$(\partial_{vv} + V(v) - E)\Psi^{(2)}(v) = 0,$$
$$\text{with } \Psi = \Psi^{(1)}(u)\Psi^{(2)}(v).$$

Taking simplest case U=V=0, direct separation is possible with R=0.

$$\Psi = \int_0^\infty A(\omega)e^{-\omega^2 t} cos(\omega[u+\delta(\omega)])cos(\omega[v+\varepsilon(\omega)])d\omega$$

$$(H_1)^2 q^1 = -(H_2)^2 q^2 = 1/\sqrt{(u+v)^2 - 4} = [r^2 - 4]^{-0.5}.$$

Squared magnitude of velocity is

$$(q^1)^2 \mathbf{e}_1.\mathbf{e}_1 + (q^2)^2 \mathbf{e}_2.\mathbf{e}_2 = H_1^2 (q^1)^2 + H_2^2 (q^2)^2 = \frac{1}{r^2 - 4}$$

This is not a realistic fluid velocity but it gives the only known example of separation in 2D by incomplete Staeckel matrix.

$$\Psi = \int_0^\infty A(\omega) e^{-\omega^2 t} cos(\omega[u + \delta(\omega)]) cos(\omega[v + \varepsilon(\omega)]) d\omega$$

For orthogonal coords (u,v),

$$(y_u, y_v) = h(u,v)(-x_v, x_u)$$

Exact differential dy implies

$$h(x_{uu} + x_{vv}) + h_u x_u + h_v x_v = 0.$$

$$ds^2 = dx^2 + dy^2 = \frac{1 - f(u,v)}{-f} du^2 + (1 - f) dv^2$$

implies $$x_u^2 + h^2 x_v^2 = 1 - f^{-1}$$

$$h^2 x_u^2 + x_v^2 = 1 - f \quad .$$

Eliminating f implies h^2 is positive root of quadratic

$$h^4(x_u^2 x_v^2) + h^2(x_v^4 + x_u^4 - [x_u^2 + x_v^2]) + x_u^2 x_v^2 - [x_u^2 + x_v^2].$$

Hamilton-Jacobi equation

$$\mathcal{H} \equiv \sum_{i=1}^{N} H_i^{-2} u,_i^2 + V(\mathbf{x}) = E.$$

Theorem: If a natural Hamiltonian H admits maximal nonregular separation on the submanifold $L^n=0$ in a given orthogonal coordinate system,
then the system is separable with a side condition and can be constructed with a generalized Staeckel matrix.