Point interactions for 3D sub-Laplacians

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joint work with
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Differential operators on graphs and waveguides
Graz, 28 February 2019

Introduction

Motivations

Q: How does "geometry" affect quantum particles on a manifold?

- M $3D$-manifold (*e.g.*, $M = \mathbb{R}^3$)
- geometric structure ($\rightarrow$ *sub-Riemannian geometry*)

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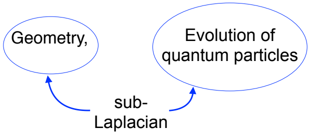
$\rightarrow \Delta$ *"Laplace" operator* (sub-Laplacian)
defined on $C_c^\infty(M) \subset L^2(M)$, $-\Delta \geq 0$, symmetric



Remark (Essential self-adjointness $\longleftrightarrow$ Quantum dynamics in M:)

$H = -\Delta$, $D(H) = C_c^\infty(M)$ is essentially self-adjoint $\overset{\text{(Stone's Theorem)}}{\Longleftrightarrow}$ $\exists!$ solution to

$$\text{(Schrödinger)} \begin{cases} i\partial_t u(p,t) - Hu(p,t) = 0 \\ u(p,0) = u_0(p) \end{cases}, \quad \|u(\cdot,t)\|_{L^2(M)} = \|u_0\|_{L^2(M)}.$$

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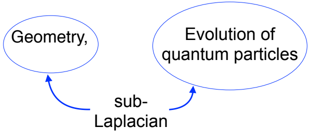

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Question: ?? Point interactions for 3D sub-Laplacians ??

Is the *sub-Laplacian* essentially self-adjoint on $M \setminus \{p\}$, $p \in M$?

Examples

1) Euclidean case. $M = \Omega \subset \mathbb{R}^n$ open;

$$\Delta = \sum_{i=1}^{n} \partial_i^2 = \mathrm{div}(\nabla \cdot\,).$$

- ✓ $\Omega = \mathbb{R}^n \implies H = -\Delta$ is essentially self-adjoint;
- ✗ $\Omega = \mathbb{R}^n \setminus \{0\}$, $n = 1, 2, 3 \implies H = -\Delta$ is *not* essentially self-adjoint (need boundary conditions corresponding to different *dynamics*). [*e.g.*, Albeverio, Gesztesy, Høegh-Krohn, Holden (book)]
- ✓ $\Omega = \mathbb{R}^n \setminus \{0\}$, $n \geq 4 \implies H = -\Delta$ is essentially self-adjoint. [*e.g.*, Albeverio, Gesztesy, Høegh-Krohn, Holden (book)]

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2) The previous results extend to the case where (M, g) is a *complete* Riemannian manifold and $\Delta_{LB} = \mathrm{div}_{\mathrm{vol}_g}(\nabla \cdot \,)$, is the *Laplace-Beltrami* operator (vol_g Riemannian volume). [Gaffney (1951–1954), Colin De Verdière (1982)].

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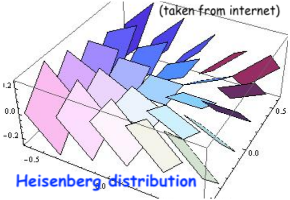
$$= X^2 + Y^2$$

$$X(x,y,z) = \partial_x - \frac{y}{2}\partial_z,\ Y(x,y,z) = \partial_y + \frac{x}{2}\partial_z,$$

where $\mathcal{D} = \mathrm{span}\{X, Y\}$
is the Heisenberg distribution:



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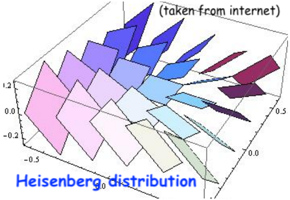

- X and Y are *left invariant vector fields* with respect to the Lie group law

$$(x,y,z) * (x',y',z') = \left(x + x', y + y', z + z' + \frac{1}{2}(xy' - x'y)\right),$$

together with the vertical vector field $Z = \partial_z = [X, Y]$.

- The Haar measure (left and right invariant) is the *Lebesgue measure*.

Heisenberg sub-Laplacian

Let $\langle \cdot, \cdot \rangle$ be a metric on $\mathcal{D}$ that makes X, Y orthonormal. Then

- the *sub-Riemannian gradient* ∇_H is

$$\nabla_H \phi := (X\phi)X + (Y\phi)Y, \quad \phi \in C^\infty(M), \qquad \textit{i.e.,}\ \langle \nabla\phi, W \rangle = d\phi(W), \forall W \in \Gamma(D).$$

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Properties:

- Δ_H is invariant under left translations: $\Delta_H(f \circ L_p) = (\Delta_H f) \circ L_p$, where $L_p(q) := p * q,\ p, q \in \mathbb{R}^3$ are *left translations*.

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- [Hördmander (1967)] Δ_H is hypoelliptic

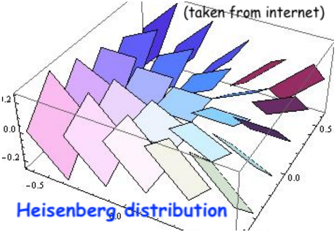
$$f \in C^\infty(\Omega) \quad \text{and} \quad \Delta_h u = f \quad \text{in}\Omega \implies u \in C^\infty(\Omega)$$

- [Folland (1973)] Δ_H is sub-elliptic

$$f \in W^{k,p}(\Omega) \quad \text{and} \quad \Delta_h u = f \quad \text{in}\Omega \implies u \in W^{k,p+1,p}(\Omega)$$

Metric structure and dilations

Metric structure: Thanks to "$[X, Y] = Z$" (Hörmander condition), once $\langle \cdot, \cdot \rangle$ is given, $\mathbb{R}^3$ can be endowed with the *Carnot-Carathéodory distance* d.



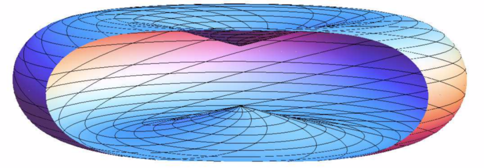


Figure 3: The Heisenberg sub-Riemannian sphere

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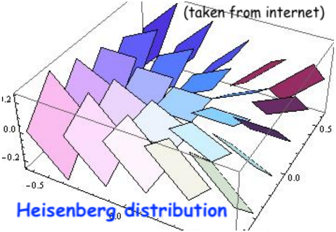

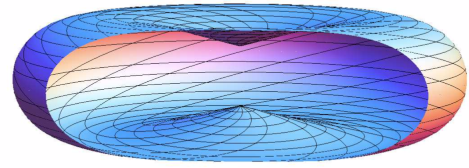

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Dilations: $\lambda > 0, \qquad \delta_\lambda : \mathbb{R}^3 \to \mathbb{R}^3, \qquad \delta_\lambda(x, y, z) = (\lambda x, \lambda y, \lambda^2 z)$

- Laplacian: $\Delta_H(f \circ \delta_\lambda p) = \lambda^2 (\Delta_H f)(\delta_\lambda p)$
- Measure: $\mathcal{L}^3(\delta_\lambda E) = \lambda^4 \mathcal{L}^3(E)$

$\to$ Homogeneous (Hausdorff) dimension $= 4$

Essential self-adjointness of the Heisenberg sub-Laplacian

Results

Question: ?? Point interactions for 3D sub-Laplacians ??

Is the *sub-Laplacian* Δ_H essentially self-adjoint on $\mathbb{R}^3 \setminus \{0\}$?

Two relevant dimensions are involved : the topological one (3) and the Hausdorff one (4).

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Theorem (Srichartz, 1986)

$H = -\Delta_H$, $\mathrm{dom}(H) = C_c^\infty(\mathbb{H}^1)$ *is essentially self-adjoint*

The theorem holds actually for all sub-laplacians with respect to smooth measures.

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Answer: YES!

Theorem (Adami, Boscain, F., Prandi(2019 - submitted))

$\mathring{H} = -\Delta_H, \quad \text{dom}(\mathring{H}) = C_c^\infty(\mathbb{R}^3 \setminus \{0\})$ *is essentially self adjoint.*

Elements of the proof

1) Essential self-adjointness criterion:
$\mathring{H} = -\Delta_H$, $\mathrm{dom}(\mathring{H}) = C_c^\infty(\mathbb{R}^3 \setminus \{0\})$ is ≥ 0 symmetric:
$\mathring{H}$ ess a.a. $\iff$ $\ker(\mathring{H}^* + i) = \{0\}$.

Lemma (ABFP - Pavlov's type)

$\mathring{H}$ is ess. s.-a. $\iff$ there are no L^2-solutions of

$$(H+i)\theta = \sum_{|\alpha|\in\mathbb{N}} c_\alpha D^\alpha \delta_0 \text{ in the sense of distributions,} \qquad (*)$$

where $c_\alpha \in \mathbb{R}$, and $H = -\Delta_H$, $\mathrm{dom}(H) = C_c^\infty(\mathbb{H}^1)$ is the (essentially self-adjoint) sub-Laplacian on $\mathbb{R}^3$.

2) Non commutative Fourier transform helps in ...

Elements of the proof

...solving $(*)$!

$(-\Delta_H + i)\theta = \sum_{|\alpha|\in\mathbb{N}} c_\alpha D^\alpha \delta_0$ in the sense of distributions.

- Euclidean idea: Let us focus on the distributional equation $(-\Delta + i)\theta = \delta_0$ $(**)$. By Fourier transform we get

$$(**) \iff (|\lambda|^2 + i)\hat{\theta}(\lambda) = 1 \iff \hat{\theta}(\lambda) = \frac{1}{|\lambda|^2 + i}$$

$$\implies \|\theta\|_2^2 = \|\hat{\theta}\|_2^2 = \int_{\mathbb{R}^n} \frac{1}{||\lambda|^2 + i|^2}\, d\lambda \sim \int_0^\infty \frac{\rho^{n-1}}{|\rho^2 + i|^2} d\rho \overset{\rho\to\infty}{\sim} \int \rho^{n-5}$$

$$\implies \|\theta\|_2^2 < \infty \iff n - 5 < -1 \iff n < 4.$$

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- By non-commutative Fourier tr. in $\mathbb{H}^1$: $\|\theta\|^2_{L^2(\mathbb{H}^1)} \geq \|\tilde{\theta}\|^2_{L^2(\tilde{\mathbb{H}}^1)} \gtrsim \displaystyle\int_1^{+\infty} \frac{d\lambda}{|\lambda|} = +\infty$.

  Hence, there are no L^2 solutions of $(*)$, meaning that $\mathring{H}$ is essentially self-adjoint.

$\square$

General 3D sub-Laplacians

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A sub-Riemannian manifold is $(M, \mathcal{X})$ where M is a smooth n-dimensional manifold and $\mathcal{X} = \{X_1, \dots, X_m\}$ is a family of smooth vector fields on M satisfying the *Hörmander condition:* for any $p \in M$

$$\exists s(p) \in \mathbb{N} : \mathrm{span}\{X_1(p), \dots, X_m(p), [X_i, X_j](p), \dots, [X_{i_1}, [X_{i_2}, \dots [X_{i_{s-1}}, X_{i_s}]](p)\} = T_p\mathbb{R}^n,$$

For $p \in M$, we let

$$\mathcal{D}_p = \mathrm{span}\{X_1(p), \dots, X_m(p)\}, \qquad n_1(p) = \dim(\mathcal{D}_p) \text{ rank at } p.$$

Examples:

• *Heisenberg group* : $M = \mathbb{R}^3 \ni (x, y, z) = p$, $\mathcal{X} = \{X_1, X_2\}$, $X_1 = \partial_x$, $X_2 = \partial_y + x\partial_z$.
Hörmander condition: $[X_1, X_2] = \partial_z$. rank $n_1 \equiv 2 < n = 3$.

• *Martinet space*: $M = \mathbb{R}^3$, $X_1 = \partial_x$, $X_2 = \partial_y + \frac{x^2}{2}\partial_z$.

$$\Longrightarrow \ [X_1, X_2](x, y, z) = x\partial_z, \quad [X_1, [X_1, X_2]](x, y, z) = \partial_z$$

$$\Longrightarrow \ n(x, y, z) = \begin{cases} (2,3) & \text{if } x \neq 0 \\ (2,2,3) & \text{if } x = 0 \end{cases},$$

There is a singular region $\mathcal{Z} = \{x = 0\}$ in which commutators of length 2 are not sufficient to generate the whole tangent space. The others are called contact points.

sub-Riemannian manifolds: sub-Laplacian

- the *sub-Riemannian gradient* ∇_H is

$$\nabla_H \phi := \sum_{i=1}^{m} (X_i \phi) X_i, \quad \phi \in C^\infty(M),$$

- given ω measure on M, the *sub-Laplacian* is the operator on $L^2_\omega(M)$ defined by

$$\Delta_\omega = \mathrm{div}_\omega(\nabla_H \cdot\ ) = \sum_{i=1}^{m} X_i^* X_i = \sum_{i=1}^{m} X_i^2 + \mathrm{div}_\omega(X_i) X_i.$$

Sub-Laplacians are hypoelliptic and sub-elliptic:

$$f \in W^{k,p}(\Omega) \quad \text{and} \quad \Delta_h u = f \quad \text{in}\Omega \implies u \in W^{k,p+\frac{2}{s},p}(\Omega)$$

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✓ (M, d) complete and ω smooth $\implies$ $H = -\Delta_\omega$ is essentially self-adjoint [Strichartz (86)].

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Let $H = -\Delta_\omega$, where ω is a smooth measure and $\mathrm{dom}(H) = C_c^\infty(\mathbb{R}^3 \setminus \{p\})$, *where p is a contact point. Then H is essentially self adjoint.*

Based on sub-elliptic estimates and local normal forms for $\mathcal{D}$ around contact points.

A comment on Hardy inequality

A quite standard way to obtain essential self-adjointness is to combine *Hardy inequalities* with *Agmon type estimates* to prove that $\ker(\mathring{H}^* + i) = \{0\}$.

Q: Can we find a Hardy inequality of the following type ?

$$?? \quad \int_{\mathbb{H}^1} |\nabla_H u|^2 \, dq \geq C_H \int_{\mathbb{H}^1} \frac{u^2}{\delta_0^2} \, dq, \quad \text{for } u \in C_c^\infty(\mathbb{H}^1 \setminus \{0\}), \quad \text{with } C_H \geq 1 \quad ??$$

- [Lehrbäck (2017)]: $\exists C_H > 0$;
- [Garofalo, Lanconelli (1990)]: in $\mathbb{H}^n$ the following inequality is sharp

$$\int_{\mathbb{H}^n} |\nabla_H u|^2 \, dq \geq \left(\frac{Q-2}{2}\right)^2 \int_{\mathbb{H}^n} \frac{u^2}{(K/|\nabla_H K|)^2} \, dq, \quad \text{for } u \in C_c^\infty(\mathbb{H}^n \setminus \{0\})$$

where $K(x,y,z) = \left((|x|^2 + |y|^2)^2 + 16z^2\right)^{\frac{1}{4}}$ is the Korány norm.

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- [Yang (2012)]: *FALSE* proof of $C_H = \left(\frac{Q-2}{2}\right)^2 = 1$.
- We can actually prove that $C_H < 1$ (by approximating K^{-1}).

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We proved Essential self-adjointness of 3D pointed sub-Laplacians (around regular points) with respect to a smooth measure.

* Can this be extended to topological dimension $n \geq 4$?
* No Hardy inequality for the CC distance with constant $1 \to$ what's the best constant?

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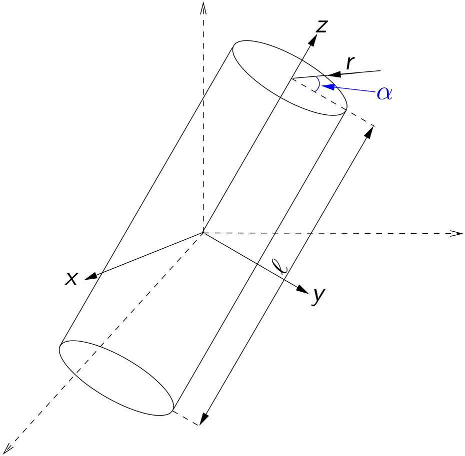
Thank you for your attention!

Rotations of a thin molecule

We apply our result to the Schrödinger evolution on $SO(3)$ of a thin molecule rotating around its center of mass, described as follows. Consider a rod-shaped molecule of mass $m > 0$, radius $r > 0$, and length $\ell > 0$



The classical Hamiltonian is

$$H = \frac{1}{2}\left(I\omega_x^2 + I\omega_y^2 + I_z\omega_z^2\right)$$
$$= \frac{1}{2}\left(\frac{L_x^2}{I} + \frac{L_y^2}{I} + \frac{L_z^2}{I_z}\right).$$

where $(\omega_x, \omega_y, \omega_z)$ is the angular velocity,

$$I_x = I_y = I := m\frac{3r^2 + \ell^2}{12}, \quad I_z = m\frac{r^2}{2}.$$

are the momenta of inertia, and $L_x = I\omega_x$, $L_y = I\omega_y$, $L_z = I_z\omega_z$ are the corresponding angular momenta

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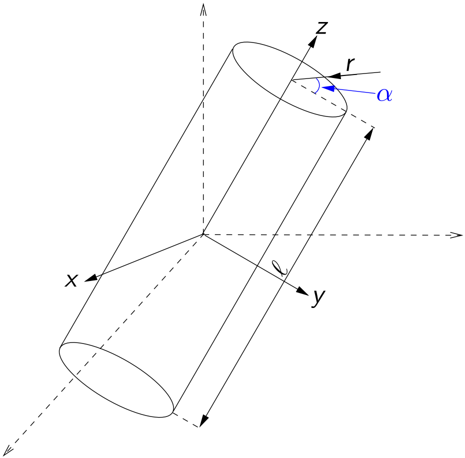

Letting $r \to 0$, we have that $I_z \to 0$, and the classical Hamiltonian reads

$$H_{\text{thin}} = \frac{1}{2I}\left(L_x^2 + L_y^2\right).$$

The corresponding Schrödinger equation is $i\hbar\frac{d\psi}{dt} = \hat{H}_{\text{thin}}\psi$, where

$$\hat{H}_{\text{thin}} = \frac{1}{2I}\left(\hat{L}_x^2 + \hat{L}_y^2\right).$$

Here, $\hat{L}_x$, $\hat{L}_y$, (and $\hat{L}_z$) are the three angular momentum operators :
$\hat{L}_x = iF_x,\ \hat{L}_y = iF_y,\ \hat{L}_z = iF_z$, for v.f. on $SO(3)$ such that $[F_x, F_y] = F_z$. Hence $(SO(3), \{F_x, F_y\})$ is a sR manifold whose corresponding sub-Laplacianis

$$\Delta_{dh} = F_x^2 + F_y^2 = -2I\hat{H}_{\text{thin}}.$$

$\Longrightarrow$ *a point interaction at* $(\alpha_0, \beta_0, \gamma_0)$ *does not affect the evolution of a thin molecule.*