Hölder estimates for Schrödinger semigroups on finite dimensional RCD spaces from probability theory

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- Consider the Schrödinger operator $H_V = -\Delta + V$ in $L^2(\mathbb{R}^{3m})$, where $V : \mathbb{R}^{3m} \to \mathbb{R}$ is of the form

$$V = \sum_{i,j=1}^{m} V_i \circ \pi_j + \sum_{1 \le i < j \le m} V_{ij} \circ (\pi_i - \pi_j), \quad \pi_j : \mathbb{R}^{3m} \to \mathbb{R}^3,$$

- Kato has shown (in 1957!) that for $\alpha \in (0,1]$ the eigenfunctions of H_V are globally α-Hölder continuous, if $V_j, V_{ij} \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $q \ge 2$ with $0 < \alpha < 2 - 3/q$. The proof uses the Fourier transform.

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Let $X = (X, \mathfrak{d}, \mathfrak{m})$ be a metric measure measure (mms).

- X comes equipped with a natural functional $\mathscr{E}$ in $L^2(X)$, the Cheeger energy, which is canonically induced by

$$f \mapsto \int_X |\nabla f|(x)^2 \mathfrak{m}(dx) := \int_X \left(\limsup_{y \to x} \frac{|f(x) - f(y)|}{\mathfrak{d}(x,y)} \right)^2 \mathfrak{m}(dx).$$

- X is called infinitesimally Hilbertian or Riemannian, if $\mathscr{E}$ is a quadratic form. Then $\mathscr{E}$ is a local Dirichlet form in $L^2(X)$ and we denote the induced self-adjoint operator with $H \geq 0$ (Laplacian).

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- One has $e^{-tH}: L^q(X) \to C(X)$, and there is a unique cont. map $(t,x,y) \mapsto p(t,x,y)$ s.t. $e^{-tH}f(x) = \int_X p(t,x,y)f(y)m(dy)$ for all x.
- There is a unique (nonexplosive) diffusion $\mathfrak{P} = (\mathfrak{P}^x)_{x\in X}$ on X s.t. the transition density of $\mathfrak{P}^x$ is given by $(t,y) \mapsto p(t,x,y)$ for *all* x

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- A central smoothing result (Ambrosio/Gigli/Savare, Bakry/Émery, Sturm):

$$\left| e^{-tH} f(x) - e^{-tH} f(y) \right| \leq F_K(t) \mathfrak{d}(x,y) \left\| f \right\|_\infty ,$$

where

$$F_K(t) := \begin{cases} \sqrt{\frac{2}{t}}, & \text{if } K = 0 \\ 2\sqrt{\frac{K}{e^{2Kt}-1}}, & \text{if } K \neq 0. \end{cases}$$

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- After some thinking: given $\alpha \in [0,1]$ say that $V : X \to \mathbb{R}$ is in the <u>α-Kato class $\mathcal{K}^{\alpha}(X)$</u>, if

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For $V \in \mathcal{K}(X)$ the form $\mathscr{E}(f) + \int V|f|^2 d\mathfrak{m}$ induces a self-adjoint semibounded operator H_V in $L^2(X)$ (Schrödinger operator) and its semigroup $(e^{-tH_V})_{t\geq 0}$ in $L^2(X)$ (Schrödinger semigroup), is given by the Feynman-Kac formula

$$e^{-tH_V}\Psi(x) = \int e^{-\int_0^t V(\omega(s))ds}\Psi(\omega(t))\mathfrak{P}^x(d\omega).$$

The RHS makes sense for all $\Psi \in L^q(X)$, $q \in [1, \infty]$.

Theorem

Let X be an $\mathrm{RCD}(K, N)$ space for some $K \in \mathbb{R}$, $N \in \mathbb{N}$, and let $\alpha \in [0, 1]$. Then for all $V \in \mathcal{K}^\alpha(X)$ and all $t > 0$ one has $e^{-tH_V} : L^\infty(X) \to C^{0,\alpha}(X)$, with completely explicit constants $C = C(K, \alpha, t, V)$.

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On the geometry of Kato's result:

Corollary

Let $X, \widetilde{X}$ be Riemannian manifolds with Ricci curvature $\geq K$ and let $\alpha \in [0,1]$. Let $\pi_j, \pi_{ij} : \widetilde{X} \to X$ be a finite collection of nice Riemannian submersions and let $V_j, V_{ij} \in L^q_{1/\mathfrak{m}}(X) + L^\infty(X)$ for some $q > \dim(X)/(2-\alpha)$. Then with

$$V := \sum_{ij} V_i \circ \pi_j + \sum_{ij} V_{ij} \circ \pi_{ij} : \widetilde{X} \longrightarrow \mathbb{R}$$

one has $e^{-tH_V} : L^\infty(\widetilde{X}) \to C^{0,\alpha}(\widetilde{X})$.

For molecules: $X = \mathbb{R}^3$, $\widetilde{X} = \mathbb{R}^{3m}$, $\pi_{ij} = \pi_i - \pi_j$,
$V_j(\mathbf{x}) = -Z_i/|\mathbf{x} - \mathbf{R}_i|$, $V_{ij} = e/|\mathbf{x}|$, $\alpha \in (0,1)$.

Sktech of proof of Theorem: By Duhamel

$$\left\| e^{-tH_V}\Phi \right\|_{C^{0,\alpha}} \leq \left\| e^{-tH}\Phi \right\|_{C^{0,\alpha}} + \int_0^t \left\| e^{-\frac{s}{2}H} \right\|_{L^\infty \to C^{0,\alpha}} \left\| e^{-\frac{s}{2}H} \circ V \right\|_{L^\infty \to L^\infty} \left\| e^{-(t-s)H_V}\Phi \right\|_{L^\infty} ds.$$

Recall

$$\left\| e^{-tH}\Phi \right\|_{C^{0,\alpha}} \leq 2^{1-\alpha} F_K(t)^\alpha \left\| \Phi \right\|_{L^\infty}, \quad \left\| e^{-\frac{s}{2}H} \right\|_{L^\infty \to C^{0,\alpha}} \leq 2^{1-\alpha} F_K(s/2)^\alpha$$

and by Feynman-Kac and Khashminskii

$$\left\| e^{-(t-s)H_V}\Phi \right\|_{L^\infty} \leq \sup_{x\in X} \int e^{\int_0^t |V(\omega(s))| ds} \mathfrak{P}^x(d\omega) \left\| \Phi \right\|_{L^\infty} < \infty.$$

Finally, since $F_K(s)^\alpha \sim s^{-\alpha/2}$ near $s = 0$,

$$\int_0^t \left\| e^{-\frac{s}{2}H} \right\|_{L^\infty \to C^{0,\alpha}} \left\| e^{-\frac{s}{2}H} \circ V \right\|_{L^\infty \to L^\infty} ds$$
$$\leq 2^{2-\alpha} \sup_x \int_0^{t/2} F_K(s)^\alpha \int_X p(s,x,y)|V(y)|\mathfrak{m}(dy) ds < \infty.$$

- Do not use coupling of $\mathfrak{P}$ and FK to estimate $e^{-tH_V}\Phi(x) - e^{-tH_V}\Phi(y)$ for unbounded V's!
- Similar global Hölder-estimates for magnetic Schrödinger semigroups (G.-Fürst). Feynman-Kac-Itô formula on RCD spaces?
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Thank you very much for your attention!