

Open Quantum Systems and the Hörmander Condition

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Overview

Open Systems and the Lindblad equation

Decoherence and the Hörmander condition

Quadratic Lindblad case

Gaussian propagation

Summary

Open Systems

Open Systems: System coupled to environment, treated as noise.

- Classical mechanics:
 - Langevin equation
 - Fokker-Planck-Kolmogorov (FPK) equation
- Quantum mechanics:
 - Lindblad equation, quantum analogue of FPK equation
 - Decoherence
 - Thermalisation

The Lindblad Equation

- States: positive normalised trace class operators $\hat{\rho}$ on Hilbert space \mathcal{H} , $\hat{\rho} > 0$, $\text{tr}[\hat{\rho}] = 1$ Expectation values: $\langle \hat{A} \rangle_{\hat{\rho}} = \text{tr}[\hat{A}\hat{\rho}]$.
- Lindblad-Gorini-Kossakowski-Sudarshan equation

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}] + \frac{i}{2} \sum_k 2\hat{L}_k\hat{\rho}\hat{L}_k^* - \hat{L}_k^*\hat{L}_k\hat{\rho} - \hat{\rho}\hat{L}_k^*\hat{L}_k$$

- \hat{H} internal Hamiltonian, \hat{L}_k Lindblad operators, describing coupling to the environment.
- most general form of generator of completely positive trace preserving semigroup. Quantum channel.

Examples:

- $\hat{L} = \sqrt{\sigma} q$, scattering on environmental "dust"-particles
- $\hat{L}_1 = \sqrt{\gamma_-} \hat{a}$, $L_2 = \sqrt{\gamma_+} \hat{a}^*$, where $\hat{a} = \hat{p} - i\hat{q}$ creation operator, coupling to heat bath.

Phase Space Representation

Let ρ, H, L_k be Weyl-symbols of $\hat{\rho}, \hat{H}, \hat{L}_k$, then the Lindblad equation gives

$$\partial_t \rho = X_0 \rho + \operatorname{div} X_0 \rho + \frac{\hbar}{2} \sum_k X_k^2 \rho + O(\hbar^2)$$

where vector fields $X_k, k = 0, 1, \dots, 2K$ are given by

- $X_0 \rho = \{H, \rho\} + \sum_k \operatorname{Im}(\bar{L}_k \{L_k, \rho\})$
- $X_k \rho = \{\operatorname{Re} L_k, \rho\}$ and $X_{k+K} \rho = \{\operatorname{Im} L_k, \rho\}$

Remarks:

- X_0 describes transport, Lindblad parts give dissipation
- X_k^2 terms describe diffusion, due to external noise
- $O(\hbar^2) = 0$ if H quadratic and L_k linear.
- equation in Hörmander "sum of squares form".

Examples

- Let $\hat{\rho} = |\psi\rangle\langle\psi|$
 - if $\psi = \psi_y$ is coherent state centred at y , then
$$\rho(x) = N e^{-\frac{1}{\hbar}|x-y|^2}$$
 - if $\psi = \psi_{y_1} + \psi_{y_2}$ is superposition of two coherent states, then
$$\rho(x) = N e^{-\frac{1}{\hbar}|x-y_1|^2} + N e^{-\frac{1}{\hbar}|x-y_2|^2} + N \cos(\delta y \cdot x/\hbar) e^{-\frac{1}{\hbar}|x-\bar{y}|^2}$$

where $\delta y = \Omega(y_2 - y_1)$ and $\bar{y} = (y_1 + y_2)/2$ with $\Omega = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$

- Let $H = \frac{1}{2}(p^2 + q^2)$ and $L = \sqrt{\sigma} q$, $x = (p, q)$, then

$$\partial_t \rho = -p \partial_q \rho + q \partial_p \rho + \frac{\hbar \sigma}{2} \partial_p^2 \rho$$

- transport and diffusion in momentum. L models impact of random scatterers.

Decoherence

We say $\rho \in S_{\frac{1}{2}}(\mathbb{R}^{2d})$ if for all α there exists C_α

$$|\partial_x^\alpha \rho(x)| \leq \|\rho\|_\infty C_\alpha \hbar^{-\frac{|\alpha|}{2}}.$$

Examples: $\rho(x) = \hbar^{-d} e^{-\frac{1}{\hbar}|x-y|^2} \in S_{\frac{1}{2}}$, $\cos(\delta y \cdot x/\hbar) \notin S_{\frac{1}{2}}$.

Definition

We say a system shows **decoherence in phase space** if for any trace class $\hat{\rho}_0$ the time evolved symbol $\rho_t(x)$ of is in $S_{\frac{1}{2}}$ for any $t \geq T > 0$ uniformly, i.e., for any $T > 0$ and α there exist $C_{T,\alpha} > 0$ such that

$$\sup_{x \in \mathbb{R}^{2n}} |\partial_x^\alpha \rho_t(x)| \leq \|\rho_T\|_\infty C_{T,\alpha} \hbar^{-\frac{|\alpha|}{2}} \quad (1)$$

for all $\hbar \in (0, 1]$ and $t \geq T$.

Hörmander condition

Definition

Suppose X_j , $j = 0, 1, \dots, K$, is a set of vector fields on \mathbb{R}^{2d} , and consider the subspaces $V_k(x) \subset \mathbb{R}^{2d}$, $k = 0, 1, 2, \dots$, spanned by the X_j and iterated commutators,

$$V_0(x) := \text{span}\{X_0(x), X_1(x), \dots, X_K(x)\}$$

$$V_k(x) := \text{span}\{Y(x), [Y, X_j](x), \dots; Y \in V_{k-1}(x), j = 0, 1, 2, \dots, K\}.$$

We say that X_j , $j = 0, 1, \dots, K$, satisfy the **Hörmander condition** if for some r we have $V_r(x) = \mathbb{R}^{2d}$ for all $x \in \mathbb{R}^{2d}$.

Example: $H = \frac{1}{2}p^2 + V(q)$, $L = q$, then

$$X_0 = -p\partial_q + V'(q)\partial_p, \quad X_1 = \partial_p, \quad [X_0, X_1] = \partial_q.$$

So $V_0((0, q)) = \text{span}\{\partial_p\}$, $V_1(x) = \mathbb{R}^{2d}$ for all x .

Hörmander condition: geometric meaning

Let $\phi_k^t(x)$ be flow generated by X_k , then

- $\phi_k^t(x) = tX_k(x) + O(t^2)$
- $\phi_k^{-t} \circ \phi_{k'}^{-t} \circ \phi_k^t \circ \phi_{k'}^t = t^2[X_k, X_{k'}] + O(t^3)$

Can transport in direction of commutators: Hörmander condition gives transport in any direction.

Theorem (Chow '39, Rashevski '38)

Assume the Hörmander condition holds. Then for any x_0, x_1 there exists a C^1 path $x(t)$ with $x_0 = x(0)$ and $x_1 = x(1)$ and controls $u(t) \in L^1([0, 1])$ such that

$$\dot{x}(t) = \sum_k u_k(t) X_k(x(t)) .$$

Hypoellipticity and Hörmander's Theorem

Definition

A linear operator L is called **hypoelliptic** if $Lf \in C^\infty$ implies $f \in C^\infty$.

Theorem (Hörmander 67)

Assume Hörmander's condition holds for the vector fields X_0, X_1, \dots, X_r , then the operator

$$L = X_0 + \sum_{k=1}^r X_k^2$$

is hypoelliptic.

Decoherence and Hörmander's condition

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}] + \frac{i}{2} \sum_k 2\hat{L}_k\hat{\rho}\hat{L}_k^* - \hat{L}_k^*\hat{L}_k\hat{\rho} - \hat{\rho}\hat{L}_k^*\hat{L}_k$$

Theorem (Parsons, Plastow, RS 19)

Suppose $H(x) = \frac{1}{2}x \cdot Qx$ is quadratic and $L_k = l_k \cdot \Omega x$ are linear and the Hamiltonian vector fields of H and $\text{Re } L_k$ and $\text{Im } L_k$ satisfy Hörmander's condition. Then the systems shows decoherence in phase space.

- Decoherence is semiclassical manifestation of hypoellipticity.
- Theorem is direct application of previous results by Kuptsov '72-'83, Lanconelli and Polidoro '94.
- One can as well derive more quantitative estimates, see proof.

Ingredients in proof I

- Let $\sum_k \bar{l}_k l_k^T = M + iN$, M, N real, $F = \Omega Q$ and $A = F + N\Omega$.
- Characteristic function $\chi(t, \xi) := \frac{1}{(2\pi\hbar)^d} \int e^{-\frac{i}{\hbar} x \cdot \xi} \rho(t, x) dx$ is given by

$$\chi(t, \xi) = \chi_0(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi},$$

where $R_t = e^{tA}$ and $D_t = \int_0^t R_s M R_s^T ds$.

- **Decoherence equivalent to $D_t > 0$ for $t > 0$.**

Hörmander condition: $V_r = \mathbb{R}^{2d}$ for some $r \leq 2d$ where

$$V_0 = \text{span}\{\text{Re } l_k, \text{Im } l_k\}, \quad V_r = V_0 + FV_0 + \dots + F^r V_0.$$

orthogonal decomposition: $\mathbb{R}^{2d} = W_0 \oplus W_1 \oplus \dots \oplus W_r$ with $W_0 = V_0$ and $V_k = V_{k-1} \oplus W_k$.

Ingredients in proof II, short time approximation

$$A = \begin{pmatrix} A_{00} & A_{01} & \cdots & & \\ F_{10} & F_{11} & & & \\ 0 & F_{21} & & & \\ \vdots & & \ddots & & \\ 0 & 0 & F_{r,r-1} & F_{r,r} & \end{pmatrix}, F^\# := \begin{pmatrix} 0 & 0 & 0 & \cdots & \\ F_{10} & 0 & 0 & & \\ 0 & F_{21} & 0 & & \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & F_{k,k-1} & 0 \end{pmatrix}$$

Lemma

Let $\xi \in W_j$, then with $R_t^\# = e^{tF^\#}$

$$\begin{aligned} \xi \cdot D_t \xi &= \sum_k \int_0^t |\xi \cdot R_s^\# l_k|^2 ds + O(t^{2j+2}) \\ &= \frac{t^{2j+1}}{(2j+1)(j!)^2} \sum_k |\xi \cdot F^j l_k|^2 + O(t^{2j+2}). \end{aligned}$$

Decoherence timescales

Theorem (Parsons, Plastow, RS 19)

Suppose that the characteristic function of $\hat{\rho}_0$ satisfies

$$|\chi_0(\xi)| \leq \frac{1}{\sqrt{\det G}} e^{-\frac{1}{4\hbar}(\xi - \Omega\xi_0) \cdot G^{-1}(\xi - \Omega\xi_0)},$$

where G is symmetric and strictly positive. If $\xi_j \in W_j$ then

$$\|\hat{\rho}_t\|_{HS} \leq e^{-\frac{1}{2\hbar}[d_j(\xi_0)t^{2j+1} + O(t^{2j+2})]}(\sqrt{\det G} + O(t))$$

where $d_j(\xi_0) = \frac{1}{(2j+1)(j!)^2} \sum_{k=1}^K |L_k(F^j \xi_0)|^2$ and $F = \Omega H''$ is the Hamiltonian map of H .

Dilations and Carnot Groups

Short time approximation defined by F^\sharp gives rise to

$$L^\sharp = X_0^\sharp + \frac{\hbar}{2} \sum_{k \geq 1} X_k^2, \text{ where } X_0^\sharp = -(F^\sharp x) \cdot \nabla.$$

- Dilations: $\delta_\lambda(\xi) = \lambda^{2j+1}$ for $\xi \in W_j$, then $\delta_{1/\lambda} \circ L^\sharp \circ \delta_\lambda = \lambda^2 L^\sharp$, so $\partial_t - L^\sharp$ invariant under $(t, x) \mapsto (\lambda^2 t, \delta_\lambda(x))$. Gives geometric explanation of different time scales of decoherence.
- F^\sharp nilpotent: gives rise to nilpotent Lie group with Lie Algebra given by X_0^\sharp, X_1, \dots , graded and with dilation, hence a Carnot group (Lanconelli Polidoro '92).
- Underlying geometry of Decoherence is sub-Riemannian Geometry described by distribution of Hörmander vector fields.

Gaussian states I

Let $\hat{\rho}$ be a quantum state (pure or mixed) with Gaussian Wignerfunction,

$$\rho(x) = \frac{\sqrt{\det G}}{(\pi\hbar)^n} e^{-\frac{1}{\hbar}(x-X)G(x-X)},$$

- $x = (q, p), X = (Q, P) \in \mathbb{R}^n \oplus \mathbb{R}^n$
- G is symmetric and satisfies the uncertainty relation $G^{-1} + i\Omega > 0$ with $\Omega = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$
- X expectation values of $\hat{x} = (\hat{q}, \hat{p})$, G^{-1} corresponding covariance matrix.
- $\hat{\rho}$ pure if G symplectic.

Propagation of Gaussian states in closed systems

Let \hat{H} be Weyl-quantisation of $H(x)$, then $e^{-\frac{i}{\hbar}t\hat{H}}\hat{\rho}e^{\frac{i}{\hbar}t\hat{H}}$ has Wignerfunction

$$\rho(t, x) = \frac{\sqrt{\det G_t}}{(\pi\hbar)^n} e^{-\frac{1}{\hbar}(x-X_t)G_t(x-X_t)} + R_t$$

and

- $\dot{X}_t = \Omega \nabla H(X_t)$ classical flow
- $\dot{G}_t = H''(X_t)\Omega G_t - G_t\Omega H''(X_t)$ linearised flow
- $\|R_t\|_{L^1} = O_t(\sqrt{\hbar}/\lambda_{\min}(G))$ where $\lambda_{\min}(G)$ is the smallest eigenvalue of G

Hepp '74, Heller '75, Littlejohn, Hagedorn Simple propagation scheme. Very versatile tool in applications.

Main proof idea: Taylor expand H around centre X_t of wave packet.

Non-Hermitian propagation of Gaussian states

Let $\hat{H} - i\hat{\Gamma}$ be Weyl-quantisation of $H(x) - i\Gamma(x)$, H, Γ real, then $e^{-\frac{i}{\hbar}t(\hat{H}-i\hat{\Gamma})}\hat{\rho}e^{\frac{i}{\hbar}t(\hat{H}+i\hat{\Gamma})}$ has Wignerfunction

$$\rho(t, x) = e^{-\frac{\alpha(t)}{\hbar}} \frac{\sqrt{\det G_t}}{(\pi\hbar)^n} e^{-\frac{1}{\hbar}(x-X_t)G_t(x-X_t)} + R_t$$

and

- $\dot{X}_t = \Omega \nabla H(X_t) - G_t^{-1} \nabla \Gamma(X_t)$ Hamiltonian + gradient
- $\dot{G}_t = H'' \Omega G_t - G_t \Omega H'' + \Gamma'' - G_t \Omega^T \Gamma'' \Omega G_t$
- $\dot{\alpha} = 2\Gamma(X_t) + \frac{\hbar}{2} \text{tr}[\Omega^T \Gamma'' \Omega G_t]$
- Graefe and RS '11; Burns, Lupercio and Urube '13
- evolution of centre X_t and variance G_t coupled!

The Lindblad Equation

- Time evolution of density operator $\hat{\rho}$, Lindblad-GKS equation ('76)

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}] + \frac{i}{2} \sum_k 2\hat{L}_k\hat{\rho}\hat{L}_k^* - \hat{L}_k^*\hat{L}_k\hat{\rho} - \hat{\rho}\hat{L}_k^*\hat{L}_k$$

- \hat{H} internal Hamiltonian, \hat{L}_k Lindblad operators, describing coupling to the environment.
- most general form of generator of completely positive trace preserving semigroup.

Examples:

- $\hat{L} = \sqrt{\sigma} \hat{q}$, scattering on environmental "dust"-particles
- $\hat{L}_1 = \sqrt{\gamma_-} \hat{a}$, $\hat{L}_2 = \sqrt{\gamma_+} \hat{a}^*$, where $\hat{a} = \hat{p} - i\hat{q}$ annihilation operator, coupling to heat bath.

Lindblad evolution of Gaussian states

Let ρ, H, L_k be Weyl-symbols of $\hat{\rho}, \hat{H}, \hat{L}_k$, then a Gaussian state evolves as

$$\rho(t, x) = \frac{\sqrt{\det G_t}}{(\pi \hbar)^n} e^{-\frac{1}{\hbar}(x-X_t)G_t(x-X_t)} + R_t$$

where

- $\dot{X}_t = \Omega \nabla H(X_t) + \Omega \sum_k \text{Im}(L_k \nabla \bar{L}_k)(X_t)$
- $\dot{G}_t = \Lambda \Omega G_t - G_t \Omega \Lambda^T - 2G_t \Omega^T D \Omega G_t$
- here $\Lambda = H'' + \sum_k \text{Im}(L_k \bar{L}_k'' + \nabla L_k \nabla \bar{L}_k^T)$ and $D = \sum_k \text{Re}(\nabla L_k \nabla \bar{L}_k^T)$
- $\|R_t\|_{L^1} = O_t(\sqrt{\hbar}/\lambda_{\min}(G))$ where $\lambda_{\min}(G)$ is the smallest eigenvalue of G

Generalisation of previous results by Brodier and Ozorio de Almeida '10.

Gradient flow in Lindblad equation

Often there exist a $W(x)$ with $\Omega \sum_k \text{Im}(L_k \nabla \bar{L}_k)(x) = -\nabla W(x)$

$$\dot{X}_t = \Omega \nabla H(X_t) - \nabla W(X_t)$$

holomorphic/anti-holomorphic Lindblads

- Let $a = p - iq$ and $a^* = p + iq$
- holomorphic: $\frac{\partial L}{\partial a^*} = 0$, then $2\Omega \text{Im}(L \nabla \bar{L})(x) = -\nabla |L(x)|^2$.
- anti-holomorphic: $\frac{\partial L}{\partial a} = 0$, then $2\Omega \text{Im}(L \nabla \bar{L})(x) = \nabla |L(x)|^2$.
- So if all L_k are either holomorphic or anti-holomorphic, then

$$W(x) = \frac{1}{2} \sum_{hol} |L_k(x)|^2 - \frac{1}{2} \sum_{anti-hol} |L_k(x)|^2 .$$

- Gradient dynamics, but not coupled to G .

Gaussian states II: superposition of coherent states

- Let $\hat{\rho} = |\psi\rangle\langle\psi|$
 - if $\psi = \psi_y$ is coherent state centred at y : $\rho(x) = Ne^{-\frac{1}{\hbar}|x-y|^2}$
 - if $\psi = \psi_{y_1} + \psi_{y_2}$ is superposition of two coherent states, then

$$\rho(x) = Ne^{-\frac{1}{\hbar}|x-y_1|^2} + Ne^{-\frac{1}{\hbar}|x-y_2|^2} + N \cos(\xi \cdot x/\hbar) e^{-\frac{1}{\hbar}|x-\bar{y}|^2}$$

where $\xi = \Omega(y_2 - y_1)$ and $\bar{y} = (y_1 + y_2)/2$.

- Get coherent states on phase space:

$$\rho_{cross}(x) = Ne^{\frac{i}{\hbar}\xi \cdot x} e^{-\frac{1}{\hbar}(x-y) \cdot G(x-y)}$$

- **Decoherence: rapid suppression of interference effects from superpositions, due to noise from environment.**
- Expect $\rho_{cross} \rightarrow 0$ as $t > 0$ if $\xi \neq 0$.

Example

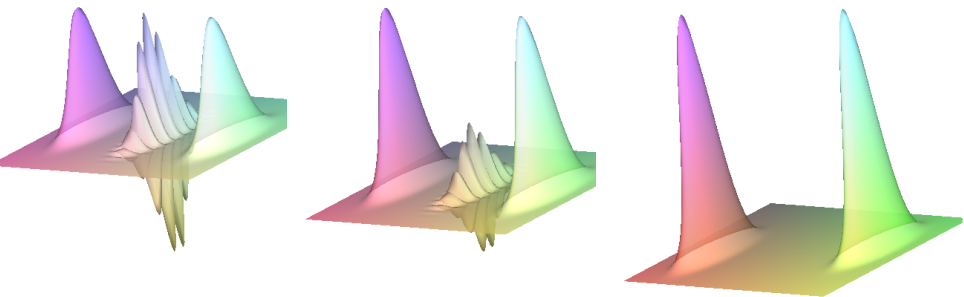


Figure: Cat state Wigner function, evolving with Harmonic oscillator $\omega = 1$ and $L = a$. Times ($t = 0, 0.01, 0.1$), $\hbar = 1/50$.

Lindblad equation as non-Hermitian Schrödinger equation

Goal: Write the Lindblad equation for Hilbert Schmidt operators $\hat{\rho}$ as Schrödinger equation for $\rho(x)$ with (possibly) non-Hermitian Hamiltonian.

- recall $\langle \hat{\rho}, \hat{\sigma} \rangle = \text{tr}[\hat{\rho}^* \hat{\sigma}] = \frac{1}{(2\pi\hbar)^n} \int \bar{\rho}(x) \sigma(x) dx$
- key identities: $\hat{A} \hat{\rho} = \widehat{A \sharp \rho}$ and $\hat{\rho} \hat{A} = \widehat{\rho \sharp A}$ with

$$A \sharp B = A e^{\frac{i\hbar}{2} \overleftarrow{\nabla} \Omega \overrightarrow{\nabla}} B$$

- $A \sharp \rho(x) = \hat{A}^{(-)} \rho$ and $\rho \sharp A = \hat{A}^{(+)} \rho$ with

$$\hat{A}^{(\pm)} = A(x \pm 2\Omega \hat{\xi}) \quad \hat{\xi} = \frac{\hbar}{i} \nabla_x$$

Weyl quantisation on doubled phase space of
 $A^{(\pm)}(x, \xi) = A(x \pm \frac{1}{2} \Omega \xi)$.

Lindblad equation on doubled phase space

$$i\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}] + \frac{i}{2} \sum_k 2\hat{L}_k\hat{\rho}\hat{L}_k^* - \hat{L}_k^*\hat{L}_k\hat{\rho} - \hat{\rho}\hat{L}_k^*\hat{L}_k$$

then translates into

$$i\hbar\partial_t\rho = \hat{K}\rho$$

with $K = K^{(0)} + \hbar K^{(1)} + \dots$ and

$$K^{(0)} = H^{(+)} - H^{(-)} + \sum_k \text{Im} (\bar{L}_k^{(-)} L_k^{(+)}) - \frac{i}{2} \sum_k |L_k^{(+)} - L_k^{(-)}|^2$$

$$K^{(1)} = \frac{1}{2} \sum_k \{\bar{L}_k, L_k\}^{(+)} + \{\bar{L}_k, L_k\}^{(-)}$$

$\text{Im} K^{(0)} \leq 0$ for $\xi > 0$ responsible for decoherence.

Example

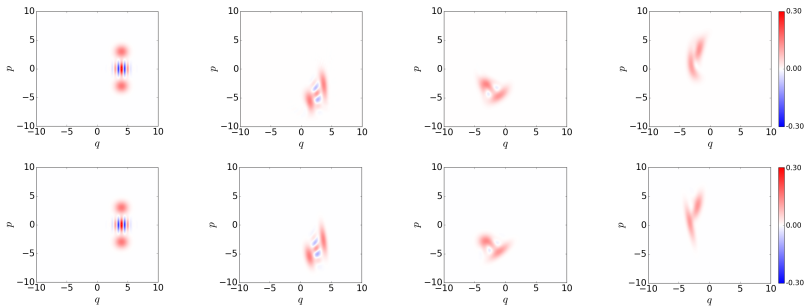


Figure: The quantum (top) and semiclassical (bottom) dynamics of an initial cat state in an anharmonic potential with $\beta = 0.1$ and damping at a rate $\gamma = 0.3$. Times $t = 0, 0.5, 1.5, 2.5$ are shown from left to right.

Summary and Outlook

- Open quantum systems described by Lindblad equation, which gives rise to phase-space evolution of "sum of squares" type

$$\partial_t \rho = \mathcal{X}_0 \rho + \frac{\hbar}{2} \sum_{k \geq 1} \mathcal{X}_k^2 \rho .$$

- Decoherence: rapid suppression of interference effects due to smoothing by noise.
- Decoherence is semiclassical manifestation of hypoellipticity, expect Hörmander condition to give sufficient condition for decoherence. We demonstrated this for special class of Hamiltonian and Lindblad operators.
- Decoherence is connected to sub-Riemannian geometry.
- Future directions: More general operators, e.g., quadratic Lindblad's, local modelling by Carnot groups, sub-Riemannian heat-kernel estimates.