Decoherence timescales and the Hörmander Condition

Roman Schubert
Bristol
Joint work with Tom Plastow

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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
  - short time behaviour: Hypoellipticity and Decoherence
  - long time behavior: Hypocoercivity and Thermalisation

Main question: Assume noise is coupled only to some degrees of freedom, how is the effect of the noise transported through the system?

Density operators

General states in Quantum Mechanics are given by density operators $\hat{\rho}$: trace class, positive, self-adjoint and normalised $\operatorname{tr}\hat{\rho} = 1$.

- $\hat{A}$ observable, expectation value $\langle \hat{A} \rangle_{\hat{\rho}} = \operatorname{tr}[\hat{A}\hat{\rho}]$
- pure state: if $\operatorname{tr}[\hat{\rho}^2] = 1$ then $\hat{\rho} = |\psi\rangle\langle\psi|$ for some $|\psi\rangle$
- In general $\hat{\rho} = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n|$ with $\lambda_n \geq 0$ and $\sum \lambda_n = 1$.
- If $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and $|\psi\rangle \in \mathcal{H}$, then reduced state for A,

  $$\hat{\rho}_A := \operatorname{tr}_B[|\psi\rangle\langle\psi|] ,$$

  is typically not pure.
- Schrödinger equation gives von Neumann equation:

  $$\mathrm{i}\hbar\partial_t \hat{\rho} = [\hat{H}, \hat{\rho}] .$$

The Lindblad Equation I

- 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:

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

The Lindblad Equation II

- If $\hat{L}_k^* = \hat{L}_k$ for all k, then

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

- dual equation for observables $\hat{A}$

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

  Generalisation of Heisenberg equation
- write semigroups as $V(t) = e^{t\mathcal{L}}$ and $V^\dagger(t) = e^{t\mathcal{L}^\dagger}$, so that $\hat{\rho}(t) = e^{t\mathcal{L}}\hat{\rho}_0$ and $\hat{A}(t) = e^{t\mathcal{L}^\dagger}\hat{A}_0$.
- Consider evolution on Banach space of trace class operators $\mathcal{B}_1(\mathcal{H})$ and on Hilbert space of Hilbert Schmidt operators $\mathcal{B}_2(\mathcal{H})$.

Phase Space Representation

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

$$\partial_t \rho = X_0 \rho + \operatorname{div} X_0\, \rho + \frac{\hbar}{2} \sum_k X_k^2 \rho + O(\|\rho\|_{C^3} \hbar^2)$$

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

- $X_0 \rho = \{H, \rho\} + \sum_k \operatorname{Im}(\bar{L}_k \{L_k, \rho\})$
- $X_k^2 \rho = \{\operatorname{Re} L_k, \rho\}$ 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 $|\psi\rangle = |z\rangle$ is coherent state centred at $z = (p, q)$, then $\rho(x) = N\mathrm{e}^{-\frac{1}{\hbar}|x-z|^2}$
  - if $|\psi\rangle = |z_1\rangle + |z_2\rangle$ is superposition of two coherent states, then

$$\rho(x) = N\mathrm{e}^{-\frac{1}{\hbar}|x-z_1|^2} + N\mathrm{e}^{-\frac{1}{\hbar}|x-z_2|^2} + N\cos\left(\delta z \cdot x/\hbar\right)\mathrm{e}^{-\frac{1}{\hbar}|x-\bar{z}|^2}$$

where $\delta z = \Omega(z_1 - z_1)$ and $\bar{z} = (z_1 + z_2)/2$ with $\Omega = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$

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

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

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

Example

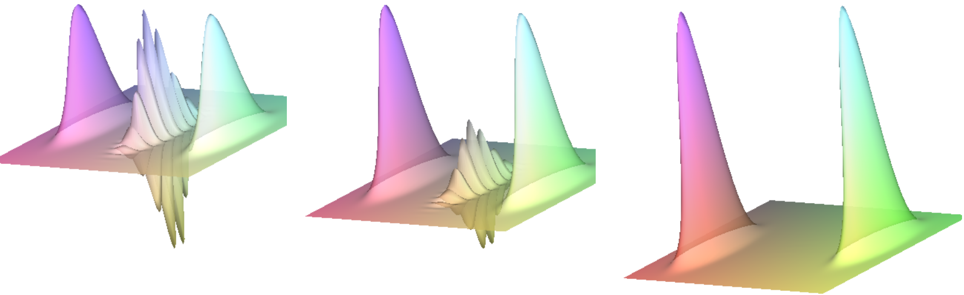

Figure: Cat state Wigner function, free evolution and $L = \hat{q}$. Times $(t = 0, 0.01, 0.1)$, $\hbar = 1/50$. $\mathrm{e}^{t\mathcal{L}}(|z\rangle\langle z'|) \to 0$ if $z \neq z'$.

Decoherence

We say $\rho \in S_{\frac{1}{2}}$ if for all α there exists C_α

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

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

Definition

We say a system defined by the Lindblad equation shows **decoherence in phase space** *if for any $T > 0$ and ρ_0 the time evolved symbol $\rho_t(x)$ is in $S_{\frac{1}{2}}$ for any $t \geq T > 0$ uniformly, i.e., for any α there exist $C_{T,\alpha} > 0$ such that*

$$\sup_{x \in \mathbb{R}^{2n}} |\partial_x^\alpha \rho_t(x)| \leq \|\rho_0\|_\infty C_{T,\alpha} \hbar^{-\frac{|\alpha|}{2}} \tag{1}$$

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

Hörmander condition (Special case)

Definition

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

$$V_0(x) := \mathrm{span}\{X_1(x), \cdots, X_K(x)\}$$
$$V_k(x) := \mathrm{span}\{Y(x), [Y, X_0](x), ;\ Y \in V_{k-1}(x), j = 0, 1, 2, \cdots, K\}\ .$$

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

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 $V_0(x) = \mathrm{span}\{\partial_p\}$, $V_1(x) = \mathbb{R}^2$ 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 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 $Lf \in \mathbb{C}^\infty$ implies $f \in C^\infty$.*

Theorem (Hörmander 67)

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

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

is hypoelliptic.

Decoherence and Hörmander's condition

Theorem (Plastow, RS 23)

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 $\operatorname{Re} L_k$ and $\operatorname{Im} L_k$ satisfy Hörmander's condition. Then the systems shows decoherence in phase space.

Furthermore, if $z - z' \in V_j^{\Omega}$, then

$$\| |z\rangle\langle z'| \|_{HS} = \mathrm{e}^{-\frac{1}{2\hbar}t^{2j+1}(d_j(z-z')+O(t))}(1 + O(t))$$

where $d_j(z - z') = \frac{1}{(2j+1)(j!)^2} \sum_k |L_k(F^j(z - z'))|^2$.

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

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

where $R_t = \mathrm{e}^{tA}$ and $D_t = \int_0^t R_s M R_s^T\,\mathrm{d}s$.

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

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

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

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

Ingredients in proof II, nilpotentisation

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

Lemma

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

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

Examples

Collisional Decoherence: $H = \frac{1}{2}p^2,\ L = q,\ V_0 = \langle \partial_p \rangle,\ V_1 = \mathbb{R}^2$

$$\|\mathrm{e}^{t\mathcal{L}}(|z\rangle\langle z'|)\|_{HS} \sim \begin{cases} \mathrm{e}^{-\frac{t}{2\hbar}|q-q'|^2} & q \neq q' \\ \mathrm{e}^{-\frac{t^3}{6\hbar}|p-p'|^2} & q = q' \end{cases}$$

Coupled oscillators: $H = \sum_k \omega_k a_k a_k^* + \sum_{k \neq l} \delta_{k,l}(a_k a_l^* + a_l a_l^*)$, couple k'th oscillator to thermal bath $L_1 \sim a_k,\ L_2 \sim a_k^*$.

- Linear chain with noise coupled to first oscillator: Decoherence in k'th oscillator $\sim \exp(-\frac{t^{2k+1}}{2(2k+1)(k!)^2\hbar}\delta^{2k}|z_k - z_k'|^2)$
- Linear chain of 3 oscillators, noise coupled to 2'nd one. Hörmander condition not fulfilled, states anti-symmetric under exchange of oscillator 1 and 3 protected from decoherence.

Dilations and Carnot Groups

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

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

- 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 $X_0^\sharp, X_1, \cdots$, graded and with dilation, hence a Carnot group (Lanconnelli Polidoro '92).
- Underlying geometry of Decoherence is sub-Riemannian Geometry described by distribution of Hörmander vector fields.

Beyond quadratic case: Gaussian propagation

Consider $\langle z|\hat{\rho}_t|z'\rangle = \mathrm{tr}\left[\hat{\rho}_t(|z\rangle\langle z'|)\right]$:

- Weyl symbol of $|z\rangle\langle z'|$ is Gaussian.
- FBI transform of ρ_t, $\bar{z} = \frac{1}{2}(z+z')$ $\delta z = z_2 - z_1$:

$$\langle z|\hat{\rho}_t|z'\rangle = \int_{\mathbb{R}^{2d}} \rho_t(x) \frac{1}{(\pi\hbar)^d} \mathrm{e}^{-\frac{1}{\hbar}|x-\bar{z}|^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\delta z\cdot\Omega x}\, \mathrm{d}x$$

- $\langle z|\hat{\rho}_t|z'\rangle = \mathrm{tr}[\hat{\rho}_0 \mathrm{e}^{t\mathcal{L}^\dagger}(|z\rangle\langle z'|)]$ and so

$$|\langle z|\hat{\rho}_t|z'\rangle| \leq \|\hat{\rho}_0\|_{HS} \|\mathrm{e}^{t\mathcal{L}^\dagger}(|z\rangle\langle z'|)\|_{HS}$$

- Use estimates on Gaussian propagation to prove decoherence for general states.

Lindblad equation as non-Hermitian Schrödinger equation (Graefe, Longstaff, Plastow, RS 2018)

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

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

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

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

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

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

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

then translates into

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

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

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

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

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

Decoherence

Decoherence related to $\int_0^t \sum_k \left| L_k(x + \frac{1}{2}\Omega\xi) - L_k(x - \frac{1}{2}\Omega\xi) \right|^2 \mathrm{d}s$, where $x(s), \xi(s)$ satisfy mixed Hamiltonian/gradient equation from Graefe, RS 2011.

- Tayler expansion around $t = 0$ reveals iterated Poissonbrackets related to commutators and Hörmander condition.
- Hamiltonian K and semiclassical approximation for wavepackets simplify for small y (formally $\delta y \sim \sqrt{\hbar}$):

$$H(x + \frac{1}{2}\Omega\xi) - H(x - \frac{1}{2}\Omega\xi) = H'(x) \cdot \Omega\xi + O(\xi^3)$$

- Simplified Hamiltonian for small y:

$$K(\xi, x) \approx X_0(x) \cdot \xi - \frac{\mathrm{i}}{2} \sum_k |X_k(x) \cdot \xi|^2$$

where $X_0 = \Omega H' + \Omega \sum_k \mathrm{Im}(L_k^* L_k')$ and $X_k = \Omega L_k'$.

Summary and Outlook

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

$$\partial_t \rho = X_0 \rho + \frac{\hbar}{2} \sum_{k \geq 1} X_k^2 \rho \ .$$

- 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: extend to non-quadratic case by using non-Hermitian propagation on doubled phase space.