Regularity of propagators of the bilinear Schrödinger equation

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Structure of the talk

1. Bilinear quantum systems
   - A bit of physics and a 30 years old topological obstruction
2. Measure as controls
   - Generalizing the notion of admissible controls, in order to prove compacity of the attainable set (Banach)
3. Higher norms
   - Exploiting the Hilbert structure, and a bit of Lie brackets
4. Example
   - Two of my favorite examples
5. Conclusion
   - Achievements and some open questions

Physical context

A quantum system evolving in Ω, a finite dimensional Riemannian manifold, is described by its *wave function* ψ in the unit sphere of $L^2(\Omega, \mathbf{C})$. The system is in the subset ω with probability $\int_\omega |\psi|^2 \mathrm{d}\mu$. The time evolution is given by the Schrödinger equation

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x,t) = (-\Delta + V(x))\psi(x,t)$$

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When submitted to an external field (*e.g.*, a laser) with time variable intensity, ψ satisfies

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (-\Delta + V(x))\psi(x,t) + u(t)W(x)\psi(x,t)$$

Abstract framework

$$\frac{d\psi}{dt} = A\psi + u(t)B\psi$$

- H : infinite dimensional, separable, complex Hilbert space, Hilbert product $\langle \cdot, \cdot \rangle$.
- $A : D(A) \to H$ skew-adjoint ;
- $B : D(B) \to H$ skew-symmetric such that $A + uB$ is skew-adjoint for every u in $\mathbf{R}$;

Solution with piecewise constant controls

If $u : [0, T] \to \mathbf{R}$ is piecewise constant, $u = \sum_{j=1}^{n} u_j \mathbf{1}_{]t_j, t_j+\tau_j[}$
$\Upsilon^u_{t,0}\psi_0 = e^{(t-t_l)(A+u_l B)} \circ e^{\tau_{l-1}(A+u_{l-1}B)} \circ \dots \circ e^{\tau_1(A+u_1 B)}\psi_0$

Method to prove exact controllability

$$x' = (A + uB)x, \qquad x \in H$$

- Find a suitable (Banach, Hilbert,...) subspace G of H ;
- Prove that the input-output mapping $\Upsilon_t : \mathcal{U} \to H$ is differentiable (in a suitable sense) ;
- Prove that $\mathrm{d}\Upsilon_t : \mathcal{U} \to G$ is a bijection ;
- Apply some inverse/implicit function theorem.

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Method applied by Beauchard, Coron, Laurent to give the first positive results of controllability of the bilinear Schrödinger equation (2005–2010).

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All of these steps are difficult. The choice of G is *very* difficult.

A topological obstruction (result)

Proposition (Ball-Marsden-Slemrod 1982 and Turinici 2001)

Assume that A generates a strongly continuous semi-group of bounded operators in H and $B : H \to H$ is bounded. Then, for every t, $u \mapsto \Upsilon^u_{t,0}$ admits a unique continuous extension to $L^1(\mathbf{R}, \mathbf{R})$ and, for every ψ in H,

$$\bigcup_{\alpha>0} \bigcup_{r>1} \bigcup_{T\geq 0} \bigcup_{u\in L^r(\mathbf{R},\mathbf{R})} \{\alpha \Upsilon^u_{t,0}\psi | 0 \leq t \leq T\}$$

is meager hence has empty interior in H.

A topological obstruction (method of proof)

- Well-posedness with L^1 controls
  - classical result ;
  - Banach fixed point theorem
- Continuity of the end-point mapping
  - If $(u_n)_n \rightharpoonup u$ in L^q then $\Upsilon^{u_n}_{t,0}\psi \to \Upsilon^{u}_{t,0}\psi$.
- For α, T, $r > 1$, K fixed, $\bigcup_{\|u\|_{L^r} \leq K} \{\alpha \Upsilon^{u}_{t,0}\psi | 0 \leq t \leq T\}$ is relatively compact and has empty interior.
  - The balls of L^r are weakly relatively compact.
- Baire theorem : a countable union of relatively compact sets has empty interior.

Aim of the talk

The result (with basically the same proof) is true for $r = 1$.

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Naive approach (hand waving, part 1/2)

Trying to copy-past the proof of Ball-Marsden-Slemrod

- $e^{t(A+\frac{1}{t}B)} \to e^B$ as $t \to 0$ (for all the quantum systems in the physic books).
- Let us choose : $\Upsilon^{\delta_1}_{t,0} = \begin{cases} e^{tA} & \text{if } t<1 \\ e^{(t-1)A} \circ e^B \circ e^A & \text{if } t>1 \end{cases}$

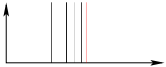
We “define” propagators by concatenations of

- constant controls : $e^{t(A+uB)}$
- Dirac masses e^{aB}

$$\Upsilon^u_{t,0} = e^{(t-t_n)(A+u_nB)} \circ e^{a_nB} \circ e^{(t_n-t_n)(A+u_{n-1}B)} \circ e^{a_{n-1}B} \circ \cdots \circ e^{(t_2-t_1)(A+u_1B)}$$

How can we define the propagator at time t if $u(t)$ “ $=$” δ_t ?

Naive approach (hand waving, part 2/2)



- $u_n = \delta_{\frac{1}{2}-\frac{1}{n}} (\rightarrow u = \delta_{\frac{1}{2}} ?)$
- $\Upsilon^{u_n}_{\frac{1}{2},0} \rightarrow e^{B} e^{\frac{1}{2}A}$

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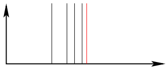

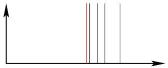

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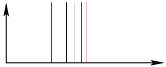

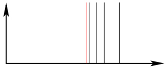

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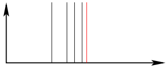

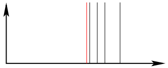

Two bad solutions :

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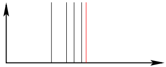

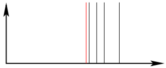

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Two bad solutions :

- one can chose a topology such that at most one of the above sequences converges (but one needs to be able to extract a convergent subsequence) FAIL !
- one can lose the continuity of the propagator (loss of the relative compactness) FAIL !

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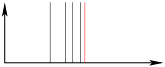

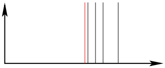

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The naive approach does not allow to define propagators associated with measures.

Radon Measures

Definition

A Radon measure on $\mathbf{R}$ is any locally finite and inner continuous measure on the σ algebra of the Borel sets.

- topological dual of the set of continuous functions with compact support ;
- examples : Lebesgue measure, Dirac masses,...
- for every locally integrable $f : \mathbf{R} \to \mathbf{R}$, $\mu(X) := \int_X f(x)\mathrm{d}x$ is a Radon measure.

Radon measures as derivative of BV functions

If μ is a Radon measure, then $t \mapsto \mu((0,t])$ has bounded variations.

Bounded variation functions

- BV functions are the difference between two non-decreasing functions.
- (equivalent definition) TV is finite

$$TV(u) = \sup_{n \in \mathbf{N}} \sup_{a_1 \leq a_2 \leq \cdots \leq a_n} \sum_{j=1}^{n-1} |u(a_{j+1}) - u(a_j)|$$

Helly's selection theorem

Let $(u_n)_n : [0, T] \to \mathbf{R}$ be a sequence of BV functions **uniformly bounded** and with **uniformly bounded TV** by K. Then there exists a subsequence $(u_{n_k})_k$ that converges pointwise to u, BV with TV lower than K.

A theorem by Kato

Assume

- $\mathcal{A}(t)$ is maximal dissipative with domain $D = D(\mathcal{A}(0))$;
- $t \mapsto \mathcal{A}(t)$ has bounded variations from $\mathbf{R}$ to $L(D, H)$;
- $\sup_{t \in \mathbf{R}} \|(1 - \mathcal{A}(t))^{-1}\|_{L(H,D)} < +\infty$

$x' = \mathcal{A}(t)x$, Propagators for BV generators (Kato, 1953)

There exists a unique contraction propagator X such that $X_{t,s}$ is strongly left differentiable in t (with derivative $\mathcal{A}(t+0)$) and right differentiable in s (with derivative $-\mathcal{A}(s-0)$).

Interaction framework

Assumptions :

Construction :

- Physicists trick : $x' = (A + uB)x$, define $y(t) = e^{-(\int_0^t u(s)ds)B}x$
  x is a strong solution $\Rightarrow$ $y' = e^{-(\int_0^t u(s)ds)B} A e^{(\int_0^t u(s)ds)B} y$.

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- For v BV, $Y^v_{t,0}$ propagator associated with $t \mapsto e^{-v(t)B} A e^{v(t)B}$.
- If u is L^1_{loc}, $\Upsilon^u_{t,0} = e^{(\int_0^t u(s)ds)B} Y^{t \mapsto \int_0^t u}_{t,0}$. If u is Radon, consider $t \mapsto u((0,t])$ (for instance)

Continuity result and differential equation

Continuity result

If $(v_n)_n$ has **uniformly bounded TV** and **converges pointwise** to v BV, then $e^{v_n(t)B} Y^{v_n}_{t,0}\psi$ converges to $e^{v(t)B} Y^{v}_{t,0}\psi$ for every ψ in H.

Weak solution

If $D(A) \subset D(B)$, u is Radon, ψ in $D(A)$, considering $v(t) = u((0,t])$, for every f in $C^1_c([0,T],H)$:

$$\int_0^T \langle f'(t), \Upsilon^u_t \psi \rangle dt = \int_0^T \langle f(t), A\Upsilon^u_t \psi \rangle dt + \int_0^T \langle f(t), B\Upsilon^u_t \psi \rangle du$$

"Generalized" propagator

$$t \mapsto e^{v(t)B} Y^v_{t,0}, \qquad (Y^v_{t,0}\psi)' = e^{-v(t)B} A e^{v(t)B} Y^v_{t,0}\psi$$

- If u is L^1, $v : t \mapsto \int_0^t u(s)\mathrm{d}s$ is BV, continuous, and $v' = u$.
- $\|u\|_{L^1} = TV(v)$

Warning !

I did not call $\mathbf{Y}^v : t \mapsto e^{v(t)B} Y^v_{t,0}$ a propagator

- Because $\mathbf{Y}^v_{0,0} \neq \mathrm{Id}$ if $v(0)B \neq 0$;
- Because $t \mapsto \mathbf{Y}^v_{t,0}\psi$ may be not continuous ;
- Because it is not clear how to relate it with $x' = (A + u(t)B)x$.

Special case : B bounded

Even if $B : H \to H$ is bounded, it is not clear that the two assumptions are satisfied :

- B and $-B$ generate continuous semi-groups of contractions leaving $D(A)$ invariant ;
- $t \mapsto e^{tB} A e^{-tB} \in L(D(A), H)$ is locally Lipschitz-continuous.

Duhamel's formula (for u L^1 and ψ in $D(A)$) :

$$\Upsilon^u_{t,s}\psi = e^{(t-s)A}\psi + \sum_{n=1}^{p} \int_{s\leq s_1 \leq \ldots \leq s_p \leq t} e^{(t-s_p)A} B e^{(s_{p-1}-s_{p-2})A} \ldots B$$

$$e^{(s_1-s)A}\Upsilon^u_{s_1,s}\psi u(s_1)\ldots u(s_p) ds_1..ds_p$$

- Pass to the limit as $p \to \infty$ with u Radon ($v(t) = v((0,t])$).
- Correct by the discontinuity term : $e^{(v(t)-v(t^+))B}\Upsilon^{t\mapsto u((0,t])}_{t,0}$

What we have done up to this point

- Under some strong Lipschitz condition ($t \mapsto e^{tB}Ae^{-tB} \in L(D(A), B)$ Lip.), we can consider the propagator Y^v of $y' = e^{v(t)B}Ae^{-v(t)B}y$ for v with BV.

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- From any sequence $(v_n)_n$ of uniformly bounded (L^∞ and TV) BV functions, one can extract a convergent subsequence.

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- From any sequence $(v_n)_n$ of uniformly bounded (L^∞ and TV) BV functions, one can extract a convergent subsequence.
- This gives an extension of Ball-Marsden-Slemrod.
- No need for other assumptions if B is bounded.

Structure of the talk

Some problems with the previous result

- In quantum control, we usually work in some domain $D(|A|^s)$.
- As long as s is an integer, it may be (more or less) easy to check the assumptions.
- When s is not integer, basic calculus is not enough.

Basic idea

- check the assumptions in H ("easy")
- find uniform bound in $D(|A|^r)$
- use interpolation for $D(|A|^s)$ with $0 < s < r$.

Weak-coupling

Weak-coupling : definition

A couple (A, B) of skew-adjoint operators is k-weakly-coupled if

- A has is invertible with bounded inverse from H to $D(A)$;
- e^{tB} maps $D(|A|^{\frac{k}{2}})$ to itself;
- there exists $c, c' \geq 0$ such that $B - c$ and $-B - c'$ generate contraction semi-groups on $D|A|^{\frac{k}{2}})$.

$$c_k(A, B) := \sup_{t \in \mathbf{R}} \frac{\log \left\| e^{tB} \right\|_{L(D(|A|^{\frac{k}{2}}), D(|A|^{\frac{k}{2}}))}}{|t|}$$

Weak-coupling

Expression in terms of commutators

- If $A + uB$ is skew-adjoint with domain $D(A)$ for every u and
- $D(|A+uB|^{\frac{k}{2}}) = D(|A|^{\frac{k}{2}})$ for $k \geq 1$ and
- $\exists C / \ |\langle [|A|^k, B]\psi, \psi\rangle| \leq C|\langle |A|^k \psi, \psi\rangle|$

Then (A, B) is k-weakly-coupled.

All the systems encountered in physics books are k-weakly-coupled for every $k > 0$.

Weak-coupling= limited growth of the higher norms

Assume

- (A, B) is k-weakly-coupled ;
- B is A-bounded ;

Then

- $\| |A|^{\frac{k}{2}} \Upsilon^u_{t,0} \psi \| \leq e^{c_k \int_0^t |u(d)| ds} \| |A|^{\frac{k}{2}} \psi \|$;
- $\exists m > 0$ s.t. for u with BV
  $\| |A|^{1+\frac{k}{2}} \Upsilon^u_{t,0} \psi \| \leq m e^{m TV(u)} e^{c_k \int_0^t |u(d)| ds} \| |A|^{1+\frac{k}{2}} \psi \|$

By interpolation, extension of the construction of generalized propagators (done in H) to $D(|A|^s)$ with $s < \frac{k}{2}$.

Applications

Good Galerkin Approximations

- Assumptions : (A, B) k-weakly-coupled ; A has discrete spectrum and B is A bounded.
- Conclusion : For every $\varepsilon, K > 0$ and every $s < k/2$, there exists $N > 0$ such that

$$\|u\|_{L^1} < K \Rightarrow \|X^{u,(N)}_{t,0}\phi_1 - \Upsilon^u_{t,0}\phi_1\|_s < \varepsilon \quad \forall t > 0$$

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Equivalence

- Assumptions : as above + Lispchitz assumption (or B bounded) ;
- Conclusion : for every $a \neq b$ and $s < k/2$, the closure attainable set of $x' = (A + uB)x$ in $D(|A|^s)$ is the same if the admissible controls are the Radon measures $v(t) = u((0, t])$ or the piecewise constant functions with value in $\{a, b\}$.

Structure of the talk

1. Bilinear quantum systems
   - A bit of physics and a 30 years old topological obstruction
2. Measure as controls
   - Generalizing the notion of admissible controls, in order to prove compacity of the attainable set (Banach)
3. Higher norms
   - Exploiting the Hilbert structure, and a bit of Lie brackets
4. Example
   - Two of my favorite examples
5. Conclusion
   - Achievements and some open questions

Square potential well

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta \psi + u(t) x \psi \qquad x \in (0, \pi)$$

$H = L^2((0,\pi), \mathbf{C})$, $A = -\mathrm{i}\Delta$ with eigenvalues $(\mathrm{i}n^2)_{n\in\mathbf{N}}$,
$B : \psi \mapsto \mathrm{i}x\psi$ bounded in H.

- Example studied by Beauchard, Coron, Nersesyan, Mirahimi, Laurent, Morancey from 2003.
- One of the very few examples for which the attainable set with L^2 controls from the first eigenstate is known : $D(|A|^{\frac{3}{2}}) \cap S$.

Square potential well

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\Delta\psi + u(t)x\psi \qquad x \in (0,\pi)$$

Regularity

- B bounded from $D(|A|^s)$ to $D(|A|^s)$ with $s < 5/4$.
- $e^B\phi_1 \notin D(|A|^{\frac{5}{4}})$

Estimates of the attainable set

The attainable set from ϕ_1 with Radon controls $(v(t) = u(0,t]))$ is contained in $D(|A|^s)$ for every $s < 5/4$ and not contained in $D(|A|^{\frac{5}{4}})$.

Notice that $1 + \frac{5}{4} > \frac{3}{2}$: use periodic controls for approach in H^3_0.

Quantum harmonic oscillator

$$\mathrm{i}\frac{\partial\psi}{\partial t} = \underbrace{(-\Delta + x^2 + \eta e^{-\pi x^2})\psi}_{\mathrm{i}A\psi} + u(t)\underbrace{x\psi}_{\mathrm{i}B\psi}, \quad x \in \mathbf{R}$$

- B is not bounded ;

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- B is not bounded, (A, B) does not satisfy the Lispschitz condition in this set.

Take home message

Defining propagators for Radon controls is possible but not easy.

- Naive approach fails.
- "Generalized propagators" to keep continuity properties.
- Lipschitz assumptions sometimes difficult to check.

Weak-coupling may be useful

- Commutators bounded with respect to the drift.
- A priori higher norms estimates.
- Use interpolation to conclude.

The negative result of Ball-Marsden-Slemrod is true with $r = 1$.

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Thank you.