Which notion of energy for bilinear quantum systems

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Bilinear quantum systems

- A quantum system evolving on a manifold Ω.
- The state is described by the *wave function*, a point in some Hilbert space H (usually $L^2(\Omega, \mathbf{C})$).
- Every physical quantity is associated with a linear operator on H.
- Dynamics given by the Schrödinger equation

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

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which can be rewritten as $\frac{d}{dt}\psi = A\psi + u(t)B\psi$
A and B are skew-adjoint operators (not necessarily bounded).

Abstract form

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

- A skew-adjoint with domain $D(A)$, with eigenvalues $(\mathrm{i}\lambda_n)_{n\in\mathbf{N}}$
- for every u in $\mathbf{R}$, $A + uB$ skew-adjoint (not necessarily on $D(A)$)
- solutions are well defined for piecewise constant functions

Control of bilinear quantum systems

- Practically finished for finite dimensional H;
- Very badly understood for infinite dimensional H;
- Only one example in infinite dimension for which the attainable set is knwon (Beauchard,Coron, Laurent)
- All the other results deal with approximate controllability

Energy of quantum systems

Energy of a the system in state ψ

$$E(\psi) = \langle |A|\psi, \psi\rangle := \|\psi\|_{1/2}.$$

Energy growth

$$\frac{\mathrm{d}E(\psi)}{dt} = ??\langle\rangle$$

Question

Is it possible to compute (bound...) the change of energy knowing only the “size” of u?

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- Optimization methods
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Recent (spectacular) advances for infinite dimensional bilinear systems:
Beauchard ’05 ’10, Mirrahimi ’08, Boscain ’09 ’11, Nersessyan ’09, ...
but these difficult results are hardly applicable in practice.

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Finite dimensional approximations are necessary.

The underlying Hilbert space is very often infinite dimensional.

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How can we ensure that the finite dimensional approximations of a bilinear quantum systems actually reflect the behavior of the original infinite dimensional system?

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- There exists $k(< 1/2)$ such that $\|B\psi\| \leq d\||A|^k\psi\|$ for ψ in $D(A)$;
- There exists $C > 0$ s. t. $|\Im\langle A\psi, B\psi\rangle| \leq C|\langle A\psi, \psi\rangle|$ for ψ in $D(A)$.

- B can be bounded or unbounded (dominated by some A^k, $k \in \mathbf{N}$).
- All the systems with discrete spectrum we have encountered in the physics literature are weakly-coupled. (Do you have a counter-example?)

Growth of energy

$$\frac{d}{dt}|\langle A\psi(t),\psi(t)\rangle| \leq 2|u(t)||\Im\langle A\psi(t),B\psi(t)\rangle| \leq 2C|u(t)||\langle A\psi(t),\psi(t)\rangle|$$

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Energy growth

If (A,B) is weakly-coupled, then, for every control u, for every time t,

$$|\langle A\psi(t),\psi(t)\rangle| \leq e^{2C\int_0^t |u(s)|\mathrm{d}s}|\langle A\psi(0),\psi(0)\rangle|.$$

The bound on the energy is uniform with respect to u and t, as long as the L^1 norm of u is in some ball of $L^1(\mathbf{R},\mathbf{R})$.

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No large tails

$$\|B(1-\pi_N)\psi(t)\| \leq \frac{de^{C\int_0^t |u(s)|\mathrm{d}s}|\langle A\psi(0),\psi(0)\rangle|}{{\lambda_N}^{1/2-k}}.$$

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$$B = \begin{pmatrix} b_{1,1} & \cdots & b_{1,N} & b_{1,N+1} & \cdots \\ \vdots & & \vdots & & \\ b_{N,1} & \cdots & b_{N,N} & b_{N,N+1} & \cdots \\ b_{N+1,1} & & \vdots & b_{N+1,N+1} & \cdots \\ \vdots & & \vdots & & \end{pmatrix}$$

$$B^{(N)} = \left(\begin{array}{cccc|cc} b_{1,1} & \cdots & & b_{1,N} & 0 & \cdots \\ \vdots & & & \vdots & \vdots & \\ b_{N,1} & \cdots & & b_{N,N} & 0 & \cdots \\ \hline 0 & \cdots & \cdots & 0 & 0 & \cdots \\ \vdots & & & & \vdots & \end{array}\right)$$

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$$\frac{d}{dt}\pi_N\psi(t) = A^{(N)}\pi_N\psi(t) + u(t)B^{(N)}\pi_N\psi(t) + u(t)\pi_N B(1-\pi_N)\psi(t)$$

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If (A,B) is weakly-coupled, then, for every $\varepsilon, K > 0$, there exists N such that

$$\|u\|_{L^1} < K \implies \|\psi(t) - X^{(N)}(t,0)\pi_N\psi(0)\| < \varepsilon.$$

Examples

General explicit formula (can be improved in most of the examples)

$$\sqrt{\lambda_{N+1}} > \frac{Kde^{CK}|\langle A\psi(0), \psi(0)\rangle|}{\varepsilon}$$

Rotation of a planar molecule

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta\psi(\theta, t) + u(t)\cos\theta\ \psi(\theta, t) \quad \theta \in SO(2)$$

For $\psi(0) =$ ground state, $K = 3$ and $\varepsilon = 10^{-4}$, $N = 14$.

Harmonic oscillator

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (-\Delta + x^2)\psi(x, t) + u(t)\ x.\psi(x, t) \quad x \in \mathbf{R}$$

For $\psi(0) =$ ground state, $K = 3$ and $\varepsilon = 10^{-4}$, $N = 420$.

Application: RWA is valid for infinite dimensonal spaces

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- $\lambda_j - \lambda_k \neq \lambda_2 - \lambda_1$ if $(j,k) \neq (1,2)$;
- $b_{1,2} \neq 0$.

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Assume that $(1, 2)$ non degenerate transition of (A, B) and $u(t) = \cos(|\lambda_2 - \lambda_1|t)$. Define $u_n = u/n$ and $T^* = \pi/2$.

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If $\psi_n(0) = \phi_1$, then $|\langle \psi_n(nT^*), \phi_2 \rangle|$ tends to one as n tends to infinity.

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This is not the best way to justify infinite dimensional RWA!

Much more general proofs are availabe.

Conclusion

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• Approximation procedure with an error bound depending only upon the L^1 norm of the control.
• Valid for most (all?) of the physical systems with discrete spectrum.
• May be used for numerical or theoretical investigations.

Future works

• Generalization to systems with mixed spectrum (done for bounded B).
• Generalization to open systems.
• What is the smallest time needed to steer a system to given target?