Schrödinger	Equation

Some known results

A new result

Numerical simulations

Some estimates for the bilinear Schrödinger equation with discrete spectrum

## Thomas Chambrion (joint work with U. Boscain, M. Caponigro and M. Sigalotti)





IHP, 8-11 December 2010

Schrödinger Equation ●○○○	Some known results	A new result 000000	Numerical simulations
Quantum systems	2		

The state of a quantum system evolving in a space  $(\Omega, \mu)$  can be represented by its *wave function*  $\psi$ . Under suitable hypotheses, the dynamics for  $\psi$  is given by the Schrödinger equation :

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

$$\begin{split} \Omega &: \text{finite dimensional manifold, for instance a bounded domain of } & \mathbf{R}^{\mathbf{d}}, \text{ or } \mathbf{R}^{\mathbf{d}}, \text{ or } SO(3), ... \\ \psi &\in L^2(\Omega, \mathbf{C}) : \text{ wave function (state of the system)} \\ & V : \Omega \to \mathbf{R} : \text{physical potential} \end{split}$$

Schrödinger Equation	Some known results	A new result	Numerical simulations
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Quantum syste	mc		

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Schrödinger Equation	Some known results	A new result	Numerical simulations
0000			
Quantum system	c		

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 $\Omega$ : finite dimensional manifold, for instance a bounded domain of  $\mathbf{R}^{\mathbf{d}}$ , or  $\mathbf{R}^{\mathbf{d}}$ , or SO(3),... $\psi \in L^{2}(\Omega, \mathbf{C})$ : wave function (state of the system)  $V: \Omega \rightarrow \mathbf{R}$ : physical potential  $W: \Omega \rightarrow \mathbf{R}$ : control potential

The well-posedness is far from obvious. It may require to add boundary conditions ( $\psi_{|\partial\Omega} = 0$  if  $\Omega$  is a bounded subspace of  $\mathbf{R}^{\mathbf{d}}$ ) and hypotheses on V and W.

Schrödinger Equation	Some known results	A new result	Numerical simulations
○●○○	0000000	000000	
Abstract form			

$$\frac{d\psi}{dt} = A(\psi) + uB(\psi), \qquad u \in U \qquad (A, B, U)$$

- *H* complex Hilbert space;
- $U \subset \mathbf{R}$ ;

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Schrödinger Equation	Some known results	A new result	Numerical simulations
○●○○	0000000	000000	
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- every eigenspace of A is finite-dimensional;
- $\phi_n \in D(B)$  for every  $n \in \mathbf{N}$ ;

• for every u in U, A + uB has a unique self-adjoint extension. Under these assumptions

 $\forall u \in U, \exists \ e^{t(A+uB)} : H \rightarrow H$  group of unitary transformations

Schrödinger Equation	Some known results	A new result	Numerical simulations
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Definition of sol	utions		

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

We choose piecewise constant controls

#### Definition

We call  $\Upsilon^{u}_{T}(\psi_{0}) = e^{t_{k}(A+u_{k}B)} \circ \cdots \circ e^{t_{1}(A+u_{1}B)}(\psi_{0})$  the solution of the system starting from  $\psi_{0}$  associated to the piecewise constant control  $u_{1}\chi_{[0,t_{1}]} + u_{2}\chi_{[t_{1},t_{1}+t_{2}]} + \cdots$ .

If B is bounded, it is possible to extend this definition for controls u that are only measurable bounded or locally integrable.

Schrödinger Equation ○○○●	Some known results	A new result 000000	Numerical simulations
Controllability			

#### Exact controllability

 $\psi_a$ ,  $\psi_b$  given. Is it possible to find a control  $u : [0, T] \to U$  such that  $\Upsilon^u_T(\psi_a) = \psi_b$ ?

#### Approximate controllability

 $\epsilon > 0$ ,  $\psi_a$ ,  $\psi_b$  given. Is it possible to find a control  $u : [0, T] \rightarrow U$  such that  $\|\Upsilon^u_T(\psi_a) - \psi_b\| < \epsilon$ ?

#### Simultaneous approximate controllability

 $\epsilon > 0, \ \psi_a^1, \psi_a^2, \dots, \psi_a^p, \ \psi_b^1, \dots, \psi_b^p$  given. Is it possible to find a control  $u : [0, T] \to U$  such that  $\|\Upsilon_T^u(\psi_a^j) - \psi_b^j\| < \epsilon$  for every j?

Some known results

A new result

Numerical simulations

## A negative result

## Theorem (Ball-Marsden-Slemrod, 1982 and Turinici, 2000)

If  $\psi \mapsto W\psi$  is bounded, then the reachable set from any point (with  $L^{1+r}$  controls) of the control system :

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

has dense complement in the unit sphere.

 Schrödinger Equation
 Some known results
 A new result
 Numerical simulations

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 Non controllability of the harmonic oscillator (I)
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$$\boldsymbol{\Omega}=\boldsymbol{\mathsf{R}}$$

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}x^2\psi - u(t)x\psi$$

#### Theorem (Mirrahimi-Rouchon, 2004)

The quantum harmonic oscillator is not controllable.

(see also Illner-Lange-Teismann 2005 and Bloch-Brockett-Rangan 2006)



The Galerkin approximation of order n is controllable (in U(n)) :

$$A = -\frac{i}{2} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 2n+1 \end{pmatrix}$$
$$B = -i \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 \\ 1 & 0 & \sqrt{2} & \ddots & \cdots & 0 \\ 1 & 0 & \sqrt{2} & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 & \sqrt{n+1} \\ 0 & \cdots & \cdots & 0 & \sqrt{n+1} & 0 \end{pmatrix}$$

Schrödinger Equation	Some known results 000●000	A new result 000000	Numerical simulations
Exact controllat	pility for the pote	ential well	

$$\Omega=(-1/2,1/2)$$

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} - u(t)x\psi$$

### Theorem (Beauchard, 2005)

The system is exactly controllable in the intersection of the unit sphere of  $L^2$  with  $H^7_{(0)}.$ 

Theorem (Boscain-Chambrion-Mason-Sigalotti, 2009)

If  $(\lambda_{n+1} - \lambda_n)_{n \in \mathbb{N}}$  is Q-linearly independent and if B is connected w.r.t. A, then for every  $\delta > 0$   $(A, B, (0, \delta))$  is approximately controllable on the unit sphere.

- The family  $(\lambda_{n+1} \lambda_n)_{n \in \mathbb{N}}$  is Q-linearly independent if for every  $N \in \mathbb{N}$  and  $(q_1, \ldots, q_N) \in \mathbb{Q}^N \setminus \{0\}$  one has  $\sum_{n=1}^N q_n(\lambda_{n+1} \lambda_n) \neq 0.$
- B is connected w.r.t. A if for every  $\{j, k\}$  in  $\mathbb{N}^2$ ,  $\exists p \in \mathbb{N}$ ,  $\exists j = l_1, l_2, \dots, l_p = k$  such that  $b_{l_i, l_{i+1}} \neq 0$ , for  $1 \le i \le p$ .

Schrödinger Equation	Some known results ○○○○○●○	A new result 000000	Numerical simulations
Lvapounov techni	aues		

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

## $\Omega$ is a bounded domain of $R^d,$ with smooth boundary.

## Theorem (Nersesyan, 2009)

• 
$$b_{1,j} 
eq 0$$
 for every  $j \geq 1$  and

• 
$$|\lambda_1 - \lambda_j| \neq |\lambda_k - \lambda_l|$$
 for every  $j > 1$ ,  $\{1, j\} \neq \{k, l\}$ 

then the control system is approximately controllable on the unit sphere of  $L^2$  for  $H^s$  norms.

Schrödinger Equation	Some known results ○○○○○○●	A new result 000000	Numerical simulations
Fixed point theore	-m		

$$\Omega = (0,1)$$

$$i\frac{\partial\psi}{\partial t}(x,t) = \underbrace{-\Delta\psi(x,t)}_{A\psi} + u(t)\underbrace{W(x)\psi(x,t)}_{B\psi}$$

#### Theorem (Beauchard-Laurent, 2009)

If there exists C > 0 such that for every  $j \in \mathbf{N}$ ,

$$|b_{1,j}| > \frac{C}{j^3}$$

then the system is exactly controllable in the intersection of the unit sphere with  $H^3_{(0)}$ .

Schrödinger Equation	Some known results	A new result ●00000	Numerical simulations
A new result (sim	ple statement)		

### Definition

 $S \subset \mathbb{N}^2$  is a non resonant chain of connectedness of (A, B) if

• for every  $j \leq k$  in N, there exists a sequence  $(s_1^1, s_2^1), \ldots, (s_1^p, s_2^p)$  in  $S \cap \{1, \ldots, k\}$  such that  $s_1^1 = j, s_2^p = k, s_2^l = s_1^{l+1}$ ;

• 
$$b_{s_1,s_2} 
eq 0$$
 for every  $(s_1,s_2) \in S$ 

• for every 
$$(j, k)$$
 in  $\mathbb{N}^2$ ,  $(s_1, s_2) \in S$ ,  
 $\{s_1, s_2\} \neq \{j, k\} \Rightarrow |\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_j - \lambda_k|$  or  $b_{j,k} = 0$ 

#### Theorem (Boscain-Caponigro-Chambrion-Sigalotti)

If A has simple spectrum and (A, B) admits a non resonant chain of connectedness, then, for every  $\delta > 0$ , (A, B) is approximately simultaneously controllable by means of controls in  $[0, \delta]$ .

Schrödinger 0000	r Equation	Some known res	sults	A new result ○●○○○○	Numerical simulations
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### Idea of the geometric proof

Up to a time reparametrization,  $e^{t(A+uB)} = e^{tu(\frac{1}{u}A+B)}$  the control system is

$$\dot{X} = \mathcal{P}uAX + BX, \qquad \mathcal{P}u > \frac{1}{\delta}.$$

Schrödinger Equation	Some known results	A new result	Numerical simulations

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Idea of the means	trie proof		

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This time-reparametrization exchanges time and  $L^1$  norm. After the change of variable  $Y = e^{-\int \mathcal{P} uA} X$ , one finds

$$\dot{Y} = e^{-\int \mathcal{P} u A} B e^{\int \mathcal{P} u A} Y$$

For every k,  $|\langle \phi_k, Y \rangle| = |\langle \phi_k, X \rangle|$ 

Schrödinger Equation	Some known results	A new result ○●○○○○	Numerical simulations
Idea of the geome	tric proof		

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For every k,  $|\langle \phi_k, Y \rangle| = |\langle \phi_k, X \rangle|$ Galerkin approximation :

$$\dot{Y} = \left[e^{i(\lambda_j - \lambda_k)\int \mathcal{P}^u}b_{j,k}\right]_{j,k}Y.$$

Schrödinger Equation	Some known results	A new result ○○●○○○	Numerical simulations
Tracking			

Non-resonant chain of connectedness : for every (j, k) in  $\mathbb{N}^2$ ,  $(s_1, s_2) \in S$ ,  $\{s_1, s_2\} \neq \{j, k\} \Rightarrow |\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_j - \lambda_k|$  or  $b_{j,k} = 0$ .

Schrödinger Equation	Some known results 0000000	A new result ○○●○○○	Numerical simulations
Tracking			

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Non-resonant chain of connectedness : for every (j, k) in  $\mathbb{N}^2$ ,  $(s_1, s_2) \in S$ ,  $\{s_1, s_2\} \neq \{j, k\} \Rightarrow |\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_j - \lambda_k|$  or  $b_{j,k} = 0$ . For every  $\epsilon > 0$ , for every  $\theta \in \mathbb{R}$ , there exists a piecewise constant control u such that the system can track (in projection), up to  $\epsilon$ , the finite dimensional system :

$$\dot{Y} = \rho \begin{pmatrix} 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & e^{i\theta}b_{j,k} & 0 & \vdots \\ \vdots & & 0 & \cdots & 0 \\ 0 & e^{-i\theta}b_{k,j} & 0 & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix} Y$$

Schrödinger Equation	Some known results 0000000	A new result ○○●○○○	Numerical simulations
Tracking			

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$$\rho \ge \prod_{k=2}^{\infty} \cos\left(\frac{\pi}{2k}\right) \approx 0.4298156$$

Non-simple spect	rum		
Schrödinger Equation	Some known results	A new result ○○○●○○	Numerical simulations

The result extends to the case where A has finitely degenerated eigenvalues if  $(A, B, \Phi)$  satisfies the extra condition

#### Hypothesis

$$j \neq k$$
 and  $\lambda_j = \lambda_k \Rightarrow b_{j,k} = 0.$ 

This is just a particular choice of the Hilbert basis  $\Phi$ .

Schrödinger Equation	Some known results 0000000	A new result	Numerical simulations
The result (non si	mple spectrum)		

Theorem (Boscain-Caponigro-Chambrion-Sigalotti)

If  $(A, B, \Phi)$  admits a non resonant chain of connectedness, then the control system is approximately simultaneously controllable on the sphere.

Example :

$$A = i \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} \qquad \qquad B = i \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Schrödinger Equation	Some known results 0000000	A new result	Numerical simulations
The result (non si	mple spectrum)		

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Slightly weaker hypotheses as for the finite result of controllability on the sphere for finite dimensional systems, obtained in 2000 by Turinici.

Schrödinger	Equation

Some known results

A new result

Numerical simulations

## Estimates

### Theorem (Boscain-Caponigro-Chambrion-Sigalotti)

If  $(A, B, \Phi)$  admits a non resonant chain of connectedness containing (1, 2), then, for every  $\delta > 0$ , for every  $\epsilon > 0$ , there exist a piecewise constant control  $u : [0, T] \rightarrow [0, \delta]$  such that

$$\|\Upsilon^u_T(\phi_1) - \phi_2\| < \epsilon \text{ and } \|u\|_{L^1} \leq \frac{5\pi}{4|\langle \phi_1, B\phi_2\rangle|}$$

Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
The planar molec	ule		

Let us consider a 2D-planar molecule submitted to a laser

$$irac{\partial\psi}{\partial t}( heta,t)=-rac{1}{2}\partial_{ heta}^{2}\psi( heta,t)+u(t)\cos( heta)\psi( heta,t)\qquad heta\in\mathsf{R}/2\pi$$

- The parity of  $\psi$  cannot change  $\Rightarrow$  no global controllability
- We just look at the even part
- We try to steer the system from the first even eigenstate to the second even eigenstate

Some known results

A new result

Numerical simulations

# Galerkin approximation

$$A = i \begin{pmatrix} 0 & 0 & \dots & \\ 0 & 1 & 0 & \ddots \\ \vdots & \ddots & 4 & \ddots \\ \vdots & \ddots & 9 \end{pmatrix} B = i \begin{pmatrix} 0 & 1/\sqrt{2} & 0 & \dots \\ 1/\sqrt{2} & 0 & 1/2 & \ddots \\ 0 & 1/2 & 0 & 1/2 \\ \vdots & \ddots & 1/2 & 0 \end{pmatrix}$$

 $\{(k, k \pm 1); k \in N\}$  is a non-resonant chain of connectedness.

Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
Moduli of the firs	t coordinates for	0 < t < 20	



Some known results

A new result

Numerical simulations

## First coordinates for $0 \le t \le 20$



Some known results

A new result

Numerical simulations

# Second coordinate for $0 \le t \le 420$



Some known results

A new result

Numerical simulations

# Simultaneous control ( $0 \le t \le 420$ )



Schrödinger Equation	Some known results 0000000	A new result 000000	Numerical simulation
		10 ( 0 / 1	< 100

#### Moduli of coordinates 1, 2, 3, 8, 10 for $0 \le t \le 420$



Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
Concluding remark	ks		

• A sufficient criterion for simultaneous approximate controllability

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Schrödinger Equation	Some known results 0000000	A new result 000000	Numerical simulations
Concluding remar	ks		

- A sufficient criterion for simultaneous approximate controllability
  - valid on **R**<sup>n</sup> or finite dimensional manifolds;

Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
Concluding remar	ks		

- A sufficient criterion for simultaneous approximate controllability
  - valid on **R**<sup>n</sup> or finite dimensional manifolds;
  - for bounded or unbounded potentials;

Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
Concluding rer	narks		

- A sufficient criterion for simultaneous approximate controllability
  - valid on **R**<sup>n</sup> or finite dimensional manifolds;
  - for bounded or unbounded potentials;
  - and arbitrarly small controls.

Schrödinger Equation	<b>Some known results</b> 0000000	A new result 000000	Numerical simulations
Concluding rema	rks		

- A sufficient criterion for simultaneous approximate controllability
  - valid on **R**<sup>n</sup> or finite dimensional manifolds;
  - for bounded or unbounded potentials;
  - and arbitrarly small controls.
- It provides

Schrödinger	Equation	

# Concluding remarks

- A sufficient criterion for simultaneous approximate controllability
  - valid on  $\mathbf{R}^n$  or finite dimensional manifolds;
  - for bounded or unbounded potentials;
  - and arbitrarly small controls.
- It provides
  - an explicit construction of the control (effective numerical computations);

Schrödinger	Equation

A new result

# Concluding remarks

- A sufficient criterion for simultaneous approximate controllability
  - valid on  $\mathbf{R}^n$  or finite dimensional manifolds;
  - for bounded or unbounded potentials;
  - and arbitrarly small controls.
- It provides
  - an explicit construction of the control (effective numerical computations);
  - easily computable estimates of the  $L^1$  norm of the control.

Schrödinger Equation	Some known results	A new result 000000	Numerical simulations
Future works			

## • Simultaneous approximate controllability in higher norms

Schrödinger Equation	Some known results	A new result	Numerical simulations
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Future works			

- Simultaneous approximate controllability in higher norms
- Time estimates

Schrödinger Equation	Some known results	A new result 000000
Future works		

- Simultaneous approximate controllability in higher norms
- Time estimates
- Implementation in the real life?