Bilinear control of Schrödinger PDEs

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Abstract

This article is an introduction to modern issues about controllability of Schrödinger PDEs with bilinear controls. This model is pertinent for a quantum particle, controlled by an electric field. We review recent developments in the field, with discrimination between exact and approximate controllability, in finite or infinite time. We also underline the variety of mathematical tools used by various teams in the last decade. The results are illustrated on several classical examples.

1 Introduction

A quantum particle, in a space with dimension N ($N = 1, 2, 3$), in a potential $V = V(x)$ and an electric field $u = u(t)$ is represented by a wave function $\psi : (t, x) \in \mathbb{R} \times \Omega \to \mathbb{C}$ on the $L^2(\Omega, \mathbb{C})$-sphere $\mathcal{S}$

$$\int_\Omega |\psi(t,x)|^2 dx = 1, \quad \forall t \in \mathbb{R},$$

where $\Omega \subset \mathbb{R}^N$ is a possibly unbouded open domain. In first approximation, the time evolution of the wave function is given by the Schrödinger equation,

$$\begin{cases} i\partial_t \psi(t,x) = (-\Delta + V)\psi(t,x) - u(t)\mu(x)\psi(t,x), & t \in (0,+\infty), x \in \Omega, \\ \psi(t,x) = 0, \quad x \in \partial\Omega \end{cases} \tag{1.1}$$

where μ is the dipolar moment of the particle and $\hbar = 1$ here. Sometimes, this equation is considered in the more abstract framework

$$i\frac{d}{dt}\psi = (H_0 + u(t)H_1)\psi \tag{1.2}$$

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where ψ lives on the unit sphere of a separable Hilbert space $\mathcal{H}$, and the Hamiltonians H_0, H_1 are Hermitian operators on $\mathcal{H}$. A natural question, with many practical applications, is the existence of a control u that steers the wave function ψ from a given initial state ψ_0, to a prescribed target ψ_f.

The goal of this survey is to present well established results concerning exact and approximate controllability for the bilinear control system (1.1), with applications to relevant examples. The main difficulties are the infinite dimension of $\mathcal{H}$ and the nonlinearity of the control system.

2 Preliminary results

When the Hilbert space $\mathcal{H}$ has finite dimension n, then controllability of equation (1.2) is well understood [17]. If, for example, the Lie algebra spanned by H_0 and H_1 coincides with $u(n)$, the set of skew-Hermitian matrices, then system (1.2) is globally controllable: for any initial and final states $\psi_0, \psi_f \in \mathcal{H}$ of length one, exist $T > 0$ and a bounded open-loop control $[0, T] \ni t \mapsto u(t)$ steering ψ from $\psi(0) = \psi_0$ to $\psi(T) = \psi_f$.

In infinite dimension, this idea served to intuit a negative controllability result in [26], but the above characterization cannot be generalized because iterated Lie brackets of unbounded operators are not necessarily well defined. For example, the quantum harmonic oscillator

$$i\partial_t\psi(t,x) = -\partial_x^2\psi(t,x) + x^2\psi(t,x) - u(t)x\psi(t,x), \quad x \in \mathbb{R}, \tag{2.1}$$

is not controllable (in any reasonable sense) [26] even if all its Galerkin approximations are controllable [20]. Thus much care is required in the use of Galerkin approximations to prove controllability in infinite dimension. This motivates the search of different methods to study exact controllability of bilinear PDEs of form (1.1).

In infinite dimension, the norms need to be specified. In this article, we use Sobolev-norms. For $s \in \mathbb{N}$, the Sobolev space $H^s(\Omega)$ is the space of functions $\psi : \Omega \to \mathbb{C}$ with square integrable derivatives $d^k\psi$ for $k = 0, ..., s$ (derivatives are well defined in the distribution sense). $H^s(\Omega)$ is endowed with the norm $\|\psi\|_{H^s} := \left(\sum_{k=0}^s \|d^k\psi\|^2_{L^2(\Omega)}\right)^{1/2}$. We also use the space $H^1_0(\Omega)$ which contains functions $\psi \in H^1(\Omega)$ that vanish on the boudary $\partial\Omega$ (in the trace sense) [21].

The first control result of the litterature states the noncontrollability of system (1.1) in $(H^2 \cap H^1_0)(\Omega) \cap \mathcal{S}$ with controls $u \in L^2((0,T), \mathbb{R})$ [31, 2]. More precisely, by applying $L^2(0,T)$-controls u, the reachable wave functions $\psi(T)$ form a subset of $(H^2 \cap H^1_0)(\Omega) \cap \mathcal{S}$ with empty interior. This statement does not give obstructions for system (1.1) to be controllable in different functional spaces as we will see below, but it indicates that controllability issues are much more subtle in infinite dimension than in finite dimension.

3 Local exact controllability

3.1 In 1D and with discrete spectrum

This section is devoted to the 1D PDE

$$\begin{cases} i\partial_t\psi(t,x) = -\partial_x^2\psi(t,x) - u(t)\mu(x)\psi(t,x), & x \in (0,1), t \in (0,T), \\ \psi(t,0) = \psi(t,1) = 0. \end{cases} \tag{3.1}$$

We call 'ground state' the solution of the free system ($u = 0$) built with the first eigenvalue and eigenvector of $-\partial_x^2$: $\psi_1(t,x) = \sqrt{2}\sin(\pi x)e^{-i\pi^2 t}$. Under appropriate assumptions on the dipolar moment μ, then system (3.1) is controllable around the ground state, locally in $H^3_{(0)}(0,1)\cap\mathcal{S}$, with controls in $L^2((0,T),\mathbb{R})$, as stated below.

Theorem 1 *Assume* $\mu \in H^3((0,1),\mathbb{R})$ *and*

$$\left|\int_0^1 \mu(x)\sin(\pi x)\sin(k\pi x)dx\right| \geqslant \frac{c}{k^3}, \forall k \in \mathbb{N}^* \tag{3.2}$$

for some constant $c > 0$. *Then, for every* $T > 0$, *there exists* $\delta > 0$ *such that for every* $\psi_0, \psi_f \in \mathcal{S}\cap H^3_{(0)}((0,1),\mathbb{C})$ *with* $\|\psi_0 - \psi_1(0)\|_{H^3} + \|\psi_f - \psi_1(T)\|_{H^3} < \delta$, *there exists* $u \in L^2((0,T),\mathbb{R})$ *such that the solution of (3.1) with initial condition* $\psi(0,x) = \psi_0(x)$ *satisfies* $\psi(T) = \psi_f$.

Here, $H^3_{(0)}(0,1) := \{\psi \in H^3((0,1),\mathbb{C}); \psi = \psi'' = 0 \text{ at } x = 0,1\}$. We refer to [8, 7] for proof and generalizations to nonlinear PDEs. The proof relies on the linearization principle, by applying the classical inverse mapping theorem to the end-point map. Controllability of the linearized system around the ground state is a consequence of assumption (3.2) and classical results about trigonometric moment problems. A subtle smoothing effect allows to prove C^1-regularity of the end-point map.

The assumption (3.2) holds for generic $\mu \in H^3((0,1),\mathbb{R})$ and plays a key role for local exact controllability to hold in *small* time T. In [10], local exact controllability is proved under the weaker assumption, namely $\mu'(0) \pm \mu'(1) \neq 0$, but only in *large* time T.

Moreover, under appropriate assumptions on μ, references [15, 10] propose explicit motions that are impossible in small time T, with small controls in L^2. Thus, a positive minimal time is required for local exact controllability, even if information propagates at infinite speed. This minimal time is due to nonlinearities; its characterization is an open problem.

Actually, assumption $\mu'(0) \pm \mu'(1) \neq 0$ is not necessary for local exact controllability in large time. For instance, the quantum box, i.e.

$$\begin{cases} i\partial_t \psi(t,x) = -\partial_x^2 \psi(t,x) - u(t) x \psi(t,x), \quad x \in (0,1), \\ \psi(t,0) = \psi(t,1) = 0, \end{cases} \tag{3.3}$$

is treated in [4]. Of course, these results are proved with additional technics: power series expansions and Coron's return method [16].

There is no contradiction between the negative result of Section 2 and the positive result of Theorem 1. Indeed, the wave function cannot be steered between any 2 points ψ_0, ψ_f of $H^2 \cap H^1_0$, but it can be steered between any 2 points ψ_0, ψ_f of $H^3_{(0)}$, which is smaller than $H^2 \cap H^1_0$. In particular, $H^3_{(0)}((0,1),\mathbb{C})$ has an empty interior in $H^2_{(0)}((0,1),\mathbb{C})$. Thus there is no incompatibility between the reachable set to have empty interior in $H^2 \cap H^1_0$ and the reachable set to coincide with $H^3_{(0)}$.

3.2 Open problems in multi-D or with continuous spectrum

The linearization principle used to prove Theorem 1 does not work in multi-D: the trigonometric moment problem, associated to the controllability of the linearized system, cannot be solved. Indeed, its frequencies, which are the eigenvalues of the Dirichlet-Laplacian operator, do not satisfy a required gap condition [32].

The study of a toy model [5] suggests that if local controllability holds in 2D (with a priori bounded L^2-controls) then a positive minimal time is required, whatever μ is. The appropriate functional frame for such a result is an open problem.

In 3D or in presence of continuous spectrum, we conjecture that local exact controllability does not hold (with a priori bounded L^2-controls) because the gap condition in the spectrum of the Dirichlet-Laplacian operator is violated (see [6] for a toy model from nuclear magnetic resonance and ensemble controllability as originally stated in [23]). Thus, exact controllability should be investigated with controls that are not a priori bounded in L^2; this requires new technics. We refer to [28] for precise negative results.

Finally, we emphasize that exact controllability in multi-D but in *infinite* time has been proved in [28, 29], with technics similar to one used in the proof of Theorem 1.

4 Approximate controllability

Different approaches have been developed to prove approximate controllability.

4.1 Lyapunov technics

Due to measurement effect and back-action, closed loop controls in the Schrödinger frame are not appropriate. However, closed loop controls may be computed via numerical simulations and then applied to real quantum systems in open loop, without measurement. Then, the strategy consists in designing damping feedback laws, thanks to a controlled Lyapunov functions, which encodes the distance to the target. In finite dimension, the convergence proof relies on LaSalle invariance principle. In infinite dimension, this principle works when the trajectories of the closed loop system are compact (in the appropriate space), which is often difficult to prove. Thus two adaptations have been proposed: approximate convergence [9, 25] and weak convergence [11] to the target.

4.2 Variational methods and global exact controllability

The global approximate controllability of (1.1), in any Sobolev space, is proved in [27], under generic assumtions on (V,μ), with Lyapunov technics and variational arguments.

Theorem 2 *Let $V,\mu \in C^\infty(\overline{\Omega},\mathbb{R})$ and $(\lambda_j)_{j\in\mathbb{N}^*}$, $(\varphi_j)_{j\in\mathbb{N}^*}$ be the eigenvalues and normalized eigenvectors of $(-\Delta+V)$. Assume $\langle \mu\varphi_j,\varphi_1\rangle \neq 0$, for all $j \geqslant 2$ and $\lambda_1-\lambda_j \neq \lambda_p-\lambda_q$ for all $j,p,q\in\mathbb{N}^*$ such that $\{1,j\}\neq\{p,q\}$, $j\neq 1$. Then, for every $s>0$, the system (1.1) is globally approximately controllable in $H^s_{(V)} := D[(-\Delta+V)^{s/2}]$, the domain of $(-\Delta+V)^{s/2}$: for every $\epsilon,\delta>0$ and $\psi_0\in\mathcal{S}\cap H^s_{(V)}$, there exists a time $T>0$ and a control $u\in C_0^\infty((0,T),\mathbb{R})$ such that the solution of (1.1) with initial condition $\psi(0)=\psi_0$ satisfies $\|\psi(T)-\varphi_1\|_{H^{s-\delta}_{(V)}}<\epsilon$.*

This theorem is of particular importance. Indeed, in 1D and for appropriate choices of (V,μ), *global* exact controllability of (1.1) in H^{3+} can be proved by combining

- global appoximate controllability in H^3 given by Theorem 2,
- local exact controllability in H^3 given by Theorem 1,
- time reversibility of the Schrödinger equation (i.e. if $(\psi(t,x),u(t))$ is a trajectory then so is $(\psi^*(T-t,x),u(T-t))$ where ψ^* is the complex conjugate of ψ).

Let us expose this strategy on the quantum box (3.3). First, one can check the assumptions of Theorem 2 with $V(x)=\gamma x$ and $\mu(x)=(1-\gamma)x$ when $\gamma>0$ is small enough. This means that, in (3.3), we consider controls $u(t)$ of the form $\gamma+\tilde{u}(t)$. Thus an initial condition $\psi_0\in H^{3+}_{(0)}$ can be steered arbitrarily close to the first eigenvector $\varphi_{1,\gamma}$ of $(-\partial_x^2+\gamma x)$, in H^3-norm.

Moreover, by a variant of Theorem 1, the local exact controllability of (3.3) holds in $H^3_{(0)}$ around $\varphi_{1,\gamma}$. Therefore the initial condition $\psi_0 \in H^{3+}_{(0)}$ can be steered exactly to $\varphi_{1,\gamma}$ in finite time. By the time-reversibility of the Schrödinger equation, we can also steer exactly the solution from $\varphi_{1,\gamma}$ to any target $\psi_f \in H^{3+}$. Therefore, the solution can be steered exactly from any initial condition $\psi_0 \in H^{3+}_{(0)}$ to any target $\psi_f \in H^{3+}_{(0)}$ in finite time.

4.3 Geometric technics applied to Galerkin approximations

In [12, 14, 13] the authors study the control of Schrödinger PDEs, in the abstract form (1.2) and under technical assumptions on the (unbounded) operators H_0 and H_1 that ensure the existence of solutions with piecewise constant controls u:

1. H_0 is skew-adjoint on its domain $D(H_0)$.
2. There exists a Hilbert basis $(\phi_k)_{k\in\mathbb{N}}$ of $\mathcal{H}$ made of eigenvectors of H_0: $H_0\phi_k = i\lambda_k\phi_k$ and $\phi_k \in D(H_1)$, $\forall k \in \mathbb{N}$.
3. $H_0 + uH_1$ is essentially skew-adjoint (not necessarily with domain $D(H_0)$) for every $u \in [0, \delta]$ for some $\delta > 0$.
4. $\langle H_1\phi_j, \phi_k\rangle = 0$ for every $j, k \in \mathbb{N}$ such that $\lambda_j = \lambda_k$ and $j \neq k$.

Theorem 3 *Assume that, for every $j, k \in \mathbb{N}$, there exists a finite number of integers $p_1, ..., p_r \in \mathbb{N}$ such that*

$$p_1 = j, \quad p_r = k, \quad \langle H_1\phi_{p_l}, \phi_{p_{l+1}}\rangle \neq 0, \forall l = 1, ..., r-1$$

$$|\lambda_L - \lambda_M| \neq |\lambda_{p_l} - \lambda_{p_{l+1}}|, \forall 1 \leqslant l \leqslant r-1, L, M \in \mathbb{N} \text{ with } \{L, M\} \neq \{p_l, p_{l+1}\}.$$

Then for every $\epsilon > 0$ and ψ_0, ψ_f in the unit sphere of $\mathcal{H}$, there exists a piecewise constant function $u : [0, T_\epsilon] \to [0, \delta]$ such that the solution of (1.2) with initial condition $\psi(0) = \psi_0$ satisfies $\|\psi(T_\epsilon) - \psi_f\|_{\mathcal{H}} < \epsilon$.

We refer to [12, 14, 13] for proof and additional results such as estimates on the L^1-norm of the control. Note that H_0 is not necessarily of the form $(-\Delta + V)$, H_1 can be unbounded, δ may be arbitrary small and the two assumptions are generic with respect to (H_0, H_1). The connectivity and transition frequency conditions in Theorem 3 mean physically that each pair of H_0 eigen-states is connected via a finite number of first order (one-photon) transitions and that the transition frequencies between pairs of eigen-states are all different.

Note that, contrary to Theorem 2, Theorem 3 cannot be combined with Theorem 1 to prove global exact controllability. Indeed, functional spaces are different: $\mathcal{H} = L^2(\Omega)$ in Theorem 3, whereas H^3-regularity is required for Theorem 1.

This kind of results applies to several relevant examples such as the control of a particule in a quantum box by an electric field (3.3) and the control of the planar rotation of a linear molecule by means of two electric fields

$$i\partial_t \psi(t,\theta) = \Big(-\partial_\theta^2 + u_1(t)\cos(\theta) + u_2(t)\sin(\theta)\Big)\psi(t,\theta), \quad \theta \in \mathbb{T}$$

where $\mathbb{T}$ is the 1D-torus. However, several other systems of physical interest are not covered by these results such as trapped ions modeled by two coupled quantum harmonic oscillators. In [19], specific methods have been used to prove their approximate controllability.

5 Concluding remarks

The variety of methods developed by different authors to characterize controllability of Schrödinger PDEs with bilinear control is the sign of a rich structure and subtle nature of control issues. New methods will probably be necessary to answer the remaining open problems in the field.

This survey is far from being complete. In particular, we do not consider numerical methods to derive the steering control such as those used in NMR [30] to achieve robustness versus parameter uncertainties or such as monotone algorithms [3, 24] for optimal control [18]. We do not consider also open quantum systems where the state is then the density operator ρ, a non-negative Hermitian operator with unit trace on $\mathcal{H}$. The Schrödinger equation is then replaced by the Lindbald equation

$$\frac{d}{dt}\rho = -\imath[H_0 + uH_1, \rho] + \sum_\nu L_\nu \rho L_\nu^\dagger - \tfrac{1}{2}\big(L_\nu^\dagger L_\nu \rho + \rho L_\nu^\dagger L_\nu\big)$$

with operator L_ν related to the decoherence channel ν. Even in the case of finite dimensional Hilbert space $\mathcal{H}$, controllability of such system is not yet well understood and characterized [1, 22].

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