Proceedings of the
47th IEEE Conference on Decision and Control
Cancun, Mexico, Dec. 9-11, 2008

Controllability properties of discrete-spectrum Schrödinger equations

Thomas Chambrion, Paolo Mason, Mario Sigalotti, and Ugo Boscain

Abstract— **We state an approximate controllability result for the bilinear Schrödinger equation in the case in which the uncontrolled Hamiltonian has discrete non-resonant spectrum. This result applies both to bounded or unbounded domains and to the case in which the control potential is bounded or unbounded. In addition we get some controllability properties for the density matrix. Finally we show, by means of specific examples, how these results can be applied.**

I. Introduction

In this paper we study the controllability of the bilinear Schrödinger equation. Its importance is due to applications to modern technologies such as Nuclear Magnetic Resonance, laser spectroscopy, and quantum information science (see for instance [1], [2], [3], [4]).

Many controllability results are available when the state space is finite dimensional, e.g., for spin systems or for molecular dynamics when one neglects interactions with highly excited levels (see for instance [5], [6]). When the state space is infinite-dimensional the controllability problem appears to be much more intricate.

We consider the controllability problem for the following bilinear system representing the Schrödinger equation driven by one external field

$$i\frac{d\psi}{dt}(t) = (H_0 + u(t)H_1)\psi(t). \tag{1}$$

Here the wave function ψ evolves in an infinite-dimensional Hilbert space, H_0 is a self-adjoint operator called *drift Hamiltonian* (i.e. the Hamiltonian responsible for the evolution when the external field is not active), $u(t)$ is a scalar control function, and H_1 is a self-adjoint operator describing the interrelation between the system and the external field.

The reference case is the one in which the Hilbert space is $L^2(\Omega)$ where Ω is either $\mathbf{R}^d$ or a bounded domain of $\mathbf{R}^d$, and equation (1) reads

$$i\frac{\partial\psi}{\partial t}(t,x) = \left(-\Delta + V(x) + u(t)W(x)\right)\psi(t,x), \tag{2}$$

where Δ is the Laplacian (with Dirichlet boundary condition in the case in which Ω is bounded) and V and W are suitably regular functions defined on Ω. However the setting of the paper covers more general cases (for instance Ω can be a Riemannian manifold and Δ the corresponding Laplace-Beltrami operator).

Besides the fact that one cannot expect exact controllability on the whole Hilbert sphere (see [7], [8]) and some negative result (in particular [9], [10]) only few approximate controllability results are available and concern mainly special situations. It should be mentioned, however, that several results on efficient steering of the Schrödinger equation without any controllability assumptions are available, e.g. [11], [12], [13]. (For optimal control results for finite dimensional quantum systems see, for instance, [14], [15], [16], [17].)

In [18], [19] Beauchard and Coron study the controllability of a quantum particle in a 1D potential well with $W(x) = x$. Their results are highly nontrivial and are based on Coron's return method (see [20]) and Nash–Moser's theorem. In particular, they prove that the system is exactly controllable in the unit sphere of the Sobolev space H^7 (implying in particular approximate controllability in L^2). One of the most interesting corollaries of this result is exact controllability between eigenstates.

A different result is given in [21], where adiabatic methods are used to prove approximate controllability for systems having conical eigenvalue crossings in the space of controls.

Another controllability result has been proved by Mirrahimi in [22] using Strichartz estimates and concerns approximate controllability for a certain class of systems such that $\Omega = \mathbf{R}^d$ and whose drift Hamiltonian has mixed spectrum (discrete and continuous).

The aim of the present paper is to state a general approximate controllability result for a large class of systems for which the drift Hamiltonian H_0 has discrete spectrum satisfying a non-resonance condition, while H_1 couples each pair of distinct eigenstates of H_0. The proof of this controllability result relies on finite-dimensional techniques applied to the Galerkin approximations and it is presented in [23].

A feature of our method is that the infinite-dimensional system inherits, in a suitable sense, controllability results for the group of unitary transformations from those of the Galerkin approximations. This permits to extract controllability properties for the *density matrix*. Let us stress that, as it happens in finite dimension, controllability properties for the density matrix cannot in general be deduced from those of the wave function (see for instance [24]).

The paper is organized as follows. In Section II we present the general functional analysis setting and we state our main result (Theorem 2.4) for the control system (1).We also show how this result applies to the Schrödinger equation (2) when

T. Chambrion is with Institut Élie Cartan, UMR 7502 Nancy-Université/CNRS/INRIA, BP 239, 54506 Vandœuvre-lès-Nancy, France, Thomas.Chambrion@iecn.u-nancy.fr.

P. Mason is with I.A.C-C.N.R., Viale del Policlinico 137, 00161 Rome, Italy, p.mason@iac.cnr.it.

M. Sigalotti is Institut Élie Cartan, UMR 7502 INRIA/Nancy-Université/CNRS, BP 239, 54506 Vandœuvre-lès-Nancy, France, mario.sigalotti@inria.fr.

U. Boscain is with SISSA, via Beirut 2-4, 34014 Trieste, Italy and Le2i, CNRS, Université de Bourgogne, BP 47870, 21078 Dijon Cedex, France, boscain@sissa.it.

978-1-4244-3124-3/08/$25.00 ©2008 IEEE

Ω is both bounded or unbounded. In Section III we give a sketch of the proof of the main result. In Section IV we extend Theorem 2.4 to the controlled evolution of the density matrix (Theorem 4.2). Finally in Section V we show how Theorem 2.4 and Theorem 4.2 can be applied to specific cases, namely the harmonic oscillator and the 3D potential well, for suitable controlled potentials. In particular, we show how to get controllability results even in cases in which V does not satisfy the required non-resonance hypothesis, using perturbation arguments.

II. Mathematical framework and statement of the main result

Hereafter $\mathbf{N}$ denotes the set of strictly positive integers. Definition 2.1 below provides the abstract mathematical framework that will be used to formulate the controllability results later applied to the Schrödinger equation (2).

Definition 2.1: Let $\mathscr{H}$ be a complex Hilbert space and U be a subset of $\mathbf{R}$. Let A, B be two, possibly unbounded, operators on $\mathscr{H}$ with values in $\mathscr{H}$ and denote by $D(A)$ and $D(B)$ their domains. The control system (A, B, U) is the formal controlled equation

$$\frac{d\psi}{dt}(t) = A\psi(t) + u(t)B\psi(t), \qquad u(t) \in U. \tag{3}$$

We say that (A, B, U) is a skew-adjoint discrete-spectrum control system if the following conditions are satisfied: (H1) A and B are skew-adjoint, (H2) there exists an orthonormal basis $(\phi_n)_{n\in\mathbf{N}}$ of $\mathscr{H}$ made of eigenvectors of A, (H3) $\phi_n \in D(B)$ for every $n \in \mathbf{N}$.

In order to give a meaning to the evolution equation (3), at least when u is constant, we should ensure that the sum $A + uB$ is well defined. The standard notion of sum of operators seen as quadratic forms (see [25]) is not always applicable under the sole hypotheses (H1), (H2), (H3). An adapted definition of $A + uB$ can nevertheless be given as follows: hypothesis (H3) guarantees that the sum $A + uB$ is well defined on $V = \mathrm{span}\{\phi_n \mid n \in \mathbf{N}\}$. Any skew-Hermitian operator $C : V \to \mathscr{H}$ admits a unique skew-adjoint extension $\mathcal{E}(C)$. We identify $A + uB$ with $\mathcal{E}(A|_V + uB|_V)$.

Let us notice that when $A + uB$ is well defined as sum of quadratic forms and is skew-adjoint then the two definitions of sum coincide. This happens in particular for the Schrödinger equation (2) in most physically significant situations.

A crucial consequence of what precedes is that for every $u \in U$ the skew-adjoint operator $A+uB$ generates a group of unitary transformations $e^{t(A+uB)} : \mathscr{H} \to \mathscr{H}$. In particular, the unit sphere $\mathcal{S}$ of $\mathscr{H}$ satisfies $e^{t(A+uB)}(\mathcal{S}) = \mathcal{S}$ for every $u \in U$ and every $t \geq 0$.

Due to the dependence of the domain $D(A + uB)$ on u, the solutions of (3) cannot in general be defined in classical (strong, mild or weak) sense. Let us mention that, in some relevant cases in which the spectrum of A has a nontrivial continuous component the solution can be defined as in [26], [27] by means of Strichartz estimates.

We will say that the *solution of (3)* with initial condition $\psi_0 \in \mathscr{H}$ and corresponding to the piecewise constant control $u : [0, T] \to U$ is the curve $t \mapsto \psi(t)$ defined by

$$\psi(t) = e^{(t-\sum_{l=1}^{j-1} t_l)(A+u_jB)} \circ \cdots \circ e^{t_2(A+u_2B)} \circ e^{t_1(A+u_1B)}(\psi_0), \tag{4}$$

where $\sum_{l=1}^{j-1} t_l \leq t < \sum_{l=1}^{j} t_l$ and $u(\tau) = u_j$ if $\sum_{l=1}^{j-1} t_l \leq \tau < \sum_{l=1}^{j} t_l$. Notice that such a $\psi(\cdot)$ satisfies, for every $n \in \mathbf{N}$ and almost every $t \in [0, T]$, the differential equation

$$\frac{d}{dt}\langle \psi(t), \phi_n\rangle = -\langle \psi(t), (A + u(t)B)\phi_n\rangle. \tag{5}$$

Remark 2.2: The notion of solution introduced above makes sense in very degenerate situations and can be enhanced when B is bounded. Indeed, well-known results assert that in this case if $u \in L^1([0, T], U)$ then there exists a unique weak (and mild) solution $\psi \in \mathcal{C}([0, T], \mathscr{H})$ which coincides with the curve (4) when u is piecewise constant. Moreover, if $\psi_0 \in D(A)$ and $u \in \mathcal{C}^1([0, T], U)$ then ψ is differentiable and it is a strong solution of (3). (See [7] and references therein.)

Definition 2.3: Let (A, B, U) be a skew-adjoint discrete-spectrum control system. We say that (A, B, U) is approximately controllable if for every $\psi_0, \psi_1 \in \mathcal{S}$ and every $\varepsilon > 0$ there exist $k \in \mathbf{N}$, $t_1, \ldots, t_k > 0$ and $u_1, \ldots, u_k \in U$ such that

$$\|\psi_1 - e^{t_k(A+u_kB)} \circ \cdots \circ e^{t_1(A+u_1B)}(\psi_0)\| < \varepsilon.$$

Let, for every $n \in \mathbf{N}$, $i\lambda_n$ denote the eigenvalue of A corresponding to ϕ_n ($\lambda_n \in \mathbf{R}$). Our general result is the following.

Theorem 2.4: Let $\delta > 0$ and $(A, B, (0, \delta))$ be a skew-adjoint discrete-spectrum control system. If the elements of the sequence $(\lambda_{n+1} - \lambda_n)_{n\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent and if $\langle B\phi_n, \phi_{n+1}\rangle \neq 0$ for every $n \in \mathbf{N}$, then $(A, B, (0, \delta))$ is approximately controllable.

Recall that the elements of the sequence $(\lambda_{n+1} - \lambda_n)_{n\in\mathbf{N}}$ are said to be $\mathbf{Q}$-linearly independent if for every $N \in \mathbf{N}$ and $(q_1, \ldots, q_N) \in \mathbf{Q}^N \setminus \{0\}$ one has $\sum_{n=1}^{N} q_n(\lambda_{n+1} - \lambda_n) \neq 0$.

Under suitable assumptions on the domain Ω and on the potentials V, W it turns out that the Schrödinger equation (2) falls into the previous abstract setting (see for instance [28, Theorem 1.2.2] and [29, Theorems XIII.69 and XIII.70]).

In particular we have the following result.

Corollary 2.5: Let Ω be an open subset of $\mathbf{R}^d$, V, W be two real-valued functions defined on Ω, and U be a subset of $\mathbf{R}$. Assume either that (i) Ω is bounded, V, W belong to $L^\infty(\Omega, \mathbf{R})$ or that (ii) $\Omega = \mathbf{R}^d$, V, W belong to $L^1_{\mathrm{loc}}(\mathbf{R}^d, \mathbf{R})$, the growth of W at infinity is at most exponential and, for every $u \in U$, $\lim_{\|x\|\to+\infty}(V(x) + uW(x)) = +\infty$ and $\inf_{x\in\mathbf{R}^d}(V(x) + uW(x)) > -\infty$. Denote by $(\lambda_k)_{k\in\mathbf{N}}$ the sequence of eigenvalues of $-\Delta + V$ and by $(\phi_k)_{k\in\mathbf{N}}$ an orthonormal basis of $L^2(\Omega, \mathbf{C})$ of corresponding real-valued eigenfunctions. Assume, in addition to (i) or (ii), that U contains the interval $(0, \delta)$ for some $\delta > 0$, that the elements of $(\lambda_{k+1} - \lambda_k)_{k\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent, and that $\int_\Omega W(x)\phi_k\phi_{k+1}\, dx \neq 0$ for every $k \in \mathbf{N}$. Then the controlled Schrödinger equation (2) associated with Ω, V, W and U is approximately controllable.

III. Scheme of the proof

In this section we briefly outline the main steps leading to the proof of Theorem 2.4 (details can be found in [23]).

First step. First remark that, if $u \neq 0$, $e^{t(A+uB)} = e^{tu((1/u)A+B)}$. Theorem 2.4 is therefore equivalent to the following property: if the terms $(\lambda_{n+1} - \lambda_n)_{n\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent and if $\langle B\phi_n, \phi_{n+1}\rangle \neq 0$ for every $n \in \mathbf{N}$, then for every $\delta, \varepsilon > 0$ and every $\psi_0, \psi_1 \in \mathcal{S}$ there exist $k \in \mathbf{N}$, $t_1, \ldots, t_k > 0$ and $u_1, \ldots, u_k > \delta$ such that

$$\|\psi_1 - e^{t_k(u_k A+B)} \circ \cdots \circ e^{t_1(u_1 A+B)}(\psi_0)\| < \varepsilon. \quad (6)$$

In other words, the system for which the roles of A and B as drift and controlled field are inverted, namely,

$$\frac{d\psi}{dt}(t) = u(t)A\psi(t) + B\psi(t), \qquad u(t) \in U, \quad (7)$$

is approximately controllable provided that the control set U contains a half-line. The notion of solution of (7) corresponding to a piecewise constant control function is defined as in (4).

Second step. Let, for every $j,k \in \mathbf{N}$, $b_{jk} = \langle B\phi_j, \phi_k\rangle$ and $a_{jk} = \langle A\phi_j, \phi_k\rangle = i\lambda_j\delta_{jk}$. Define, for every $n \in \mathbf{N}$, the two complex-valued $n\times n$ matrices $A^{(n)} = (a_{jk})_{1\le j,k\le n}$ and $B^{(n)} = (b_{jk})_{1\le j,k\le n}$. These two matrices give rise to the Galerkin approximations of (7). To these finite-dimensional systems we can apply the following controllability result.

Proposition 3.1: Let $\mathfrak{A} = (\alpha_{jk})_{j,k=1}^n$, $\mathfrak{B} = (\beta_{jk})_{j,k=1}^n$ be two skew-symmetric $n \times n$ matrices and assume that $\mathfrak{A}$ is diagonal and $\mathfrak{B}$ is connected (i.e. for every pair of indices $j,k \in \{1,\ldots,n\}$ there exists a finite sequence $r_1,\ldots,r_l \in \{1,\ldots,n\}$ such that $\beta_{jr_1}\beta_{r_1r_2}\cdots\beta_{r_{l-1}r_l}\beta_{r_lk} \neq 0$). Assume moreover that $|\alpha_{jj} - \alpha_{kk}| \neq |\alpha_{ll} - \alpha_{mm}|$ if $\{j,k\} \neq \{l,m\}$. Then the control system $(\overline{\Sigma}) : \dot{x} = u\mathfrak{A}x + \mathfrak{B}x$ is controllable in $\mathcal{S}_n$ with piecewise constant controls with values in $\overline{U} \subset \mathbf{R}$, provided that $\overline{U}$ contains at least two points.

Third step. Given $u : [0,T] \to \mathbf{R}$ let us represent the matrix $M(t) = e^{-v(t)A^{(N)}}B^{(N)}e^{v(t)A^{(N)}}$, where $v(t) = \int_0^t u(\tau)d\tau$, in block form as follows

$$M(t) = \begin{pmatrix} M^{(n,n)}(t) & M^{(n,N-n)}(t) \\ M^{(N-n,n)}(t) & M^{(N-n,N-n)}(t) \end{pmatrix}, \quad (8)$$

where the superscripts indicate the dimensions of each block.

Claim 3.2: There exists a sequence of piecewise constant control functions $u_k : [0,T] \to (\delta,\infty)$ such that the sequence of matrix-valued curves

$$t \mapsto M_k(t) = e^{-v_k(t)A^{(N)}}B^{(N)}e^{v_k(t)A^{(N)}},$$

where $v_k(t) = \int_0^t u_k(\tau)d\tau$, converges uniformly w.r.t. t to

$$t \mapsto \bar{M}(t) = \begin{pmatrix} M^{(n,n)}(t) & 0_{n\times(N-n)} \\ 0_{(N-n)\times n} & M^{(N-n,N-n)}(t) \end{pmatrix}$$

in the integral sense $\int_0^t M_k(\tau)d\tau \overset{k\to\infty}{\to} \int_0^t \bar{M}(\tau)d\tau$.

Fourth step. Let us fix two states $\psi_0, \psi_1 \in \mathscr{H}$. Our aim is to approximately steer the system between ψ_0 and ψ_1. Let $\varepsilon > 0$. Let Π_n be the projection on the space generated by the first n eigenvectors of A. Then, if we take n large enough and we apply Proposition 3.1 and Claim 3.2 with a suitable N it is possible to prove the following.

Claim 3.3: For k large enough,

$$\|\Pi_n(e^{-v_k(T)A}\psi^k(T)) - \Pi_n(e^{-v(T)A}\psi_1)\| < \varepsilon \quad (9)$$

where $u(\cdot)$ is a control connecting $\Pi_n(\psi_0)$ to $\Pi_n(\psi_1)$ in the Galerkin approximation, $v(t) = \int_0^t u(\tau)d\tau$, $v_k(t) = \int_0^t u_k(\tau)d\tau$ and $\psi^k(\cdot)$ is the trajectory associated to $u_k(\cdot)$ starting from ψ_0.

Fifth step. The last step of the proof consists in showing that it is possible to get rid of the differences of phase in an arbitrary short time so that

$$\|\Pi_n(\psi^k(T)) - \Pi_n(\psi_1)\| < \varepsilon.$$

Finally the proof of Theorem 2.4 can be completed showing that the "queues" $\|\psi_1 - \Pi_n(\psi_1)\|$ and $\|\psi^k(T) - \Pi_n(\psi^k(T))\|$ can be made arbitrary small by choosing a suitably large n and a suitably small ε.

IV. Controllability for density matrices

A. Physical motivations

A *density matrix* (sometimes called density operator) is a non-negative, self-adjoint operator of trace class [29, Vol. I] on a Hilbert space. The trace of a density matrix is normalized to one. As a consequence of the definition a density matrix is a compact operator (hence with discrete spectrum) and can always be written as a weighted sum of projectors,

$$\rho = \sum_{j=1}^{\infty} P_j\varphi_j\varphi_j^*, \quad (10)$$

where $P_j \in [0,1]$, $\sum_j P_j = 1$, and $\varphi_j\varphi_j^*$ is the *orthogonal projector* on the space spanned by φ_j with $\varphi_j^*(\cdot) = \langle\varphi_j, \cdot\rangle$. Here $\{\varphi_j\}_{j\in\mathbf{N}}$ is a set of normalized vectors not necessarily orthogonal.

The density matrix is used to describe the evolution of systems whose initial wave function is not known precisely, but only with a certain probability, or when one is dealing with an ensemble of identical systems that cannot be prepared precisely in the same state. More precisely (10) describes a system whose state is known to be φ_j with probability P_j, $j \in \mathbf{N}$.

The time evolution of the density matrix is determined by the evolutions of the states φ_j, namely

$$\rho(t) = \mathbf{U}(t)\rho(0)\mathbf{U}^*(t) \quad (11)$$

where $\mathbf{U}(t)$ is the operator of temporal evolution (the resolvent) and $\mathbf{U}^*(t)$ its adjoint. Notice that the spectrum of $\rho(t)$ is constant along the motion.

B. Statement of the result

Fix $\delta > 0$ and let $(A, B, (0,\delta))$ be a skew-adjoint discrete-spectrum control system on a Hilbert space $\mathscr{H}$, $(\varphi_j)_{j\in\mathbf{N}}$ an orthonormal basis of $\mathscr{H}$ (not necessarily of eigenvectors of

A), $\{P_j\}_{j\in N}$ a sequence of non-negative numbers such that $\sum_{j=1}^{\infty} P_j = 1$, and denote by ρ the density matrix

$$\rho = \sum_{j=1}^{\infty} P_j \varphi_j {\varphi_j}^*.$$

Definition 4.1: Two density matrices ρ_0 and ρ_1 are said to be *unitarily equivalent* if there exists a unitary transformation $\mathbf{U}$ of $\mathscr{H}$ such that $\rho_1 = \mathbf{U}\rho_0\mathbf{U}^*$.

Obviously the controllability question for the evolution of the density matrix makes sense only for pairs (ρ_0, ρ_1) of initial and final density matrices that are unitarily equivalent. Notice that this is a quite strong assumption, since it implies that the eigenvalues of ρ_0 and ρ_1 are the same. Controllability results in the case of density matrices that are not unitarily equivalent have been obtained in the case of open systems (i.e. systems evolving under a suitable nonunitary evolution) in the finite-dimensional case. See for instance [30].

For density matrices the following generalization of Theorem 2.4, proved in [23], holds.

Theorem 4.2: Let ρ_0 and ρ_1 be two unitarily equivalent density matrices. Then, under the hypotheses of Theorem 2.4, for every $\varepsilon > 0$ there exists a piecewise constant control steering the density matrix from ρ_0 ε-approximately to ρ_1 i.e. there exist $k \in \mathbf{N}$, $t_1, \ldots, t_k > 0$ and $u_1, \ldots, u_k \in (0, \delta)$ such that setting $\mathbf{V} = e^{t_k(A+u_kB)} \circ \cdots \circ e^{t_1(A+u_1B)}$, one has $\|\rho_1 - \mathbf{V}\rho_0\mathbf{V}^*\| < \varepsilon$, where $\|\cdot\|$ denotes the operator norm on $\mathscr{H}$.

Remark 4.3: As Corollary 2.5 is a particularization of Theorem 2.4 to the controlled Schrödinger equation, the hypotheses of Corollary 2.5 imply ε-approximate controllability of the corresponding density matrix.

V. Examples

A. Perturbation of the spectrum

The scope of Section V is to show how the general controllability results obtained in the previous sections can be applied in specific cases. In particular, we want to show how the conditions on the spectrum of the Schrödinger operator appearing in the hypotheses of Corollary 2.5 can be checked in practice.

Throughout this section we assume that one of the hypotheses (i) or (ii) of Corollary 2.5 holds true. Thus, (A, B, U) is a well-defined controlled Schrödinger equation, where $A = -i(-\Delta + V)$ and $B = -iW$.

The study of the examples below is based on the simple idea that, even if the hypotheses of Corollary 2.5 are not satisfied by the operators A and B, one can anyway ensure that they hold true for $A_\mu = -i(-\Delta + V + \mu W)$ and $B_\mu = -iW$ for some μ in the interior of U. This is enough to conclude that the system $\dot{\psi} = A\psi + uB\psi$, $u \in U$, is approximately controllable, since the replacement of (A, B) by (A_μ, B_μ) corresponds to a reparameterization of U that sends u into a new control $u - \mu \in U - \mu$ and V into $V + \mu W$. Although the spectrum of A_μ is not in general explicitly computable, we can nevertheless deduce some crucial properties about it by applying standard perturbation arguments. Theorem 5.1 recalls, in a simplified version suitable for our purposes, some classical perturbation results describing the dependence on μ of the spectrum of $-\Delta + V + \mu W$. (See [31, Chapter VII, Remark 4.22], [32, §II.10, Theorem 1] and also [33].)

Theorem 5.1: Let U be an open interval containing zero. Assume either that (i) Ω is bounded, V, W belong to $L^\infty(\Omega)$ or that (ii) $\Omega = \mathbf{R}^d$, V belongs to $L^1_{\mathrm{loc}}(\mathbf{R}^d)$, W belongs to $L^\infty(\mathbf{R}^d)$, $\lim_{\|x\|\to+\infty} V(x) = +\infty$ and $\inf_{x\in\mathbf{R}^d} V(x) > -\infty$. In both cases (i) and (ii) assume that each eigenvalue of the Schrödinger operator $-\Delta + V$ is simple. Denote by $(\lambda_k)_{k\in\mathbf{N}}$ the sequence of eigenvalues of $-\Delta + V$ and by $(\phi_k)_{k\in\mathbf{N}}$ the corresponding eigenfunctions. Then, for any k in $\mathbf{N}$, there exist two analytic curves $\Lambda_k : U \to \mathbf{C}$ and $\Phi_k : U \to L^2(\Omega)$ such that:

- $\Lambda_k(0) = \lambda_k$ and $\Phi_k(0) = \phi_k$;
- for any μ in U, $(\Lambda_k(\mu))_{k\in\mathbf{N}}$ is the family of eigenvalues of $\Delta - V + \mu W$ counted according to their multiplicities and $(\Phi_k(\mu))_{k\in\mathbf{N}}$ is an orthonormal basis of corresponding eigenfunctions;
- $\Lambda'_k(0) = \int_\Omega W(x)|\phi_k(x)|^2 dx$.

We check below that if the derivatives $\Lambda'_k(0)$ are $\mathbf{Q}$-linearly independent then for almost every $\mu \in U$ the eigenvalues of $-\Delta + V + \mu W$ are $\mathbf{Q}$-linearly independent. This fact is used in the following to apply Corollary 2.5 to situations in which the uncontrolled Schrödinger operator has a resonant spectrum.

Setting $b_{jk} = \langle B\phi_j, \phi_k\rangle$ for any pair of integers $j, k \in \mathbf{N}$, one has

$$b_{jk} = \int_\Omega W(x)\phi_j(x)\phi_k(x)dx. \tag{12}$$

In particular, $\Lambda'_k(0) = \int_\Omega W(x)|\phi_k(x)|^2 dx$ is equal to b_{kk}.

From the analitic dependence of the eigenvalues with respect to μ it is possible to show the following result.

Proposition 5.2: Let U be an open interval containing zero and assume that Ω, V and W satisfy one of the hypotheses (i) or (ii) of Theorem 5.1 and that the eigenvalues of $-\Delta + V$ are simple. If the elements of the sequence $(b_{kk})_{k\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent, then for almost every μ in U the elements of $(\Lambda_k(\mu))_{k\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent.

The other crucial hypothesis of Corollary 2.5 is that $b_{j,j+1} \neq 0$ for every $j \in \mathbf{N}$. Still by an analyticity argument one checks that either such hypothesis is always false or it is true for almost every $\mu \in U$.

Corollary 5.3: Let U be an open interval containing zero and assume that Ω, V and W satisfy one of the hypotheses (i) or (ii) of Theorem 5.1 and that the eigenvalues of $-\Delta + V$ are simple. Assume moreover that the elements of the sequence $(b_{kk})_{k\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent and that $b_{j,j+1} \neq 0$ for every $j \in \mathbf{N}$. Then the controlled Schrödinger equation associated with Ω, V, W and $\tilde{U}$ is approximately controllable for every $\tilde{U} \subset U$ with nonempty interior.

B. 1D harmonic oscillator

In this section we study the Schrödinger equation describing the evolution of the controlled one-dimensional harmonic oscillator,

$$i\frac{\partial\psi}{\partial t}(t,x) = -\frac{\partial^2\psi}{\partial x^2}(t,x) + \left(x^2 - u(t)W(x)\right)\psi(t,x), \quad (13)$$

where ψ is the wave function depending on the time t and on a space variable $x \in \mathbf{R} = \Omega$. Recall that $u(\cdot)$ is a piecewise-continuous function with values in a subset U of $\mathbf{R}$. Notice that the potential corresponding to the uncontrolled Schrödinger operator is $V(x) = x^2$. The control system (13) has been studied, among others, by Mirrahimi and Rouchon who proved its non-controllability in the case where W is the identity function (see [9]).

From classical results we know that the spectrum of $-\Delta + V$ is discrete. Its explicit expression is

$$\{\lambda_k = 2k+1 \mid k \geq 0\},$$

and therefore $\lambda_{k+1} - \lambda_k$ are $\mathbf{Q}$-linearly dependent. Each λ_k is a simple eigenvalue whose corresponding eigenfunction is

$$\phi_k(x) = \sigma_k e^{-\frac{x^2}{2}} H_k(x) \quad (14)$$

where $\sigma_l = 1/\sqrt{l!2^l\sqrt{\pi}}$ and $H_k(x) = (-1)^k e^{x^2}\frac{d^k}{dx^k}e^{-x^2}$ is the k^{th} Hermite polynomial.

In order to apply Corollary 5.3 we would like first of all to ensure that the elements

$$b_{kk} = (-1)^k\sigma_k^2 \int_{\mathbf{R}} W(x)H_k(x)\frac{d^k}{dx^k}e^{-x^2}dx, \qquad k \geq 0, \quad (15)$$

are $\mathbf{Q}$-linearly independent. Notice that for $W(x) = x$ (i.e., the non-controllable case pointed out by Mirrahimi and Rouchon), since each function ϕ_k^2 is even, $b_{kk} = \int W\phi_k^2 = 0$.

The existence of controlled potentials W for which the elements of $(b_{kk})_{k\in\mathbf{N}}$ are $\mathbf{Q}$-linearly independent can be easily inferred from the linear independence of the functions ϕ_k^2. The proposition below provides some explicit W with such a property (and such that the corresponding Schrödinger equation is controllable). The potentials W will be chosen in $L^\infty(\mathbf{R})$ and it turns out that the corresponding solutions in the sense (4) coincide with mild or strong solutions, depending on the regularity of the initial condition.

Proposition 5.4: (1) If W is even, then system (13) is not approximately controllable. (2) If W has the form $W : x \mapsto e^{ax^2+bx+c}$, with $a, b, c \in \mathbf{R}$ such that $a < 0$ and the two numbers $\sqrt{1-a}$ and b are algebraically independent, then system (13) is approximately controllable, provided that U has nonempty interior.

Proof: Since each function ϕ_k has the same parity as the integer k, then $\phi_k\phi_j$ has the same parity as the integer $j+k$. If W is even, then (12) shows that for every (j,k) such that $j+k$ is odd, $b_{jk} = 0$. It turns out that the spaces spanned by the sets $\{\phi_k \mid k \text{ even}\}$ and $\{\phi_k \mid k \text{ odd}\}$ are invariant by the dynamics of system (13). In particular, there is no way to steer system (13) from ϕ_1 to a point ε-close to ϕ_2 if ε is smaller than $\sqrt{2}$. This proves (1).

In order to prove (2) one needs to apply Corollary 5.3 (with U playing the role of $\tilde{U}$ and $\mathbf{R}$ the role of U) with W having the special form $W : x \mapsto e^{ax^2+bx+c}$.

After rather standard computations (see [23] for the details) it is possible to prove, if $j+k$ is even, that

$$b_{jk} = \sigma_j\sigma_k\sqrt{\pi}e^{c-\frac{b^2}{4a-4}}S_{j,k}(b)$$

where $S_{j,k}$ is a nonzero polynomial with coefficients in $\mathbf{Q}(\sqrt{1-a})$ of degree exactly $j+k$.

Since b is transcendental over $\mathbf{Q}(\sqrt{1-a})$ then $b_{jk} \neq 0$ as soon as j and k have the same parity. Moreover, the elements of the sequence $(\Lambda_k'(0))_{k\geq 0} = (b_{kk})_{k\geq 0}$ are $\mathbf{Q}$-linearly independent.

To conclude the proof let us check that each matrix $(b_{jk})_{j,k=0}^n$ is connected. Fix $j,k \in \{0,\ldots,n\}$. We should prove the existence of a sequence $r_1,\ldots,r_l \in \{0,\ldots,n\}$ such that $b_{jr_1}b_{r_1r_2}\cdots b_{r_{l-1}r_l}b_{r_lk} \neq 0$. If j and k have the same parity then we are done since $b_{jk} \neq 0$. Otherwise, a simple computation shows that

$$b_{01} = \frac{be^{c-\frac{b^2}{4a-4}}}{\sqrt{2}(1-a)^{\frac{3}{2}}} \neq 0$$

and we can conclude by taking $\{r_1, r_2\} = \{0,1\}$. ■

C. 3D potential well

Consider the Schrödinger equation

$$i\frac{\partial\psi}{\partial t}(t,x) = -\Delta\psi(t,x) + u(t)W(x)\psi(t,x), \quad (16)$$

where ψ depends on the time t and on the space variable $x = (x_1,x_2,x_3) \in \Omega = (0,l_1)\times(0,l_2)\times(0,l_3)$ and satisfies the Dirichlet boundary condition $\psi|_{\partial\Omega} = 0$. Notice that the potential corresponding to the uncontrolled Schrödinger operator is $V(x) = 0$. For every W measurable bounded, solutions in the sense (4) coincide with mild or strong solutions, depending on the regularity of the initial condition.

The spectrum of the Schrödinger operator is

$$\left\{\lambda_{k_1,k_2,k_3} = \pi^2\left(\frac{k_1^2}{l_1^2} + \frac{k_2^2}{l_2^2} + \frac{k_3^2}{l_3^2}\right) \mid k_1,k_2,k_3 \geq 1\right\}.$$

For the sake of simplicity, assume that $(l_1l_2)^2$, $(l_1l_3)^2$, and $(l_2l_3)^2$ are $\mathbf{Q}$-linearly independent, so that all the eigenvalues are simple and the perturbation result appearing in Theorem 5.1 can be applied. (The case of multiple eigenvalues can be treated similarly, applying a refined perturbation argument as the one used in [33].)

The normalized eigenfunction corresponding to λ_{k_1,k_2,k_3} is given, up to sign, by

$$\phi_{k_1,k_2,k_3}(x_1,x_2,x_3) = \\ = \frac{2^{\frac{3}{2}}}{\sqrt{l_1l_2l_3}}\sin\left(\frac{k_1x_1\pi}{l_1}\right)\sin\left(\frac{k_2x_2\pi}{l_2}\right)\sin\left(\frac{k_3x_3\pi}{l_3}\right). \quad (17)$$

Proposition 5.5: Let $(l_1l_2)^2$, $(l_1l_3)^2$, and $(l_2l_3)^2$ be $\mathbf{Q}$-linearly independent and define $W(x) = e^{\alpha\cdot x}$ with $\alpha = (\alpha_1,\alpha_2,\alpha_3) \in \mathbf{R}^3$. Assume that $\alpha_1,\alpha_2,\alpha_3$ are nonzero and that $(\pi/\alpha_1l_1)^2$, $(\pi/\alpha_2l_2)^2$, $(\pi/\alpha_3l_3)^2$ are algebraically independent. Then the control system (16) is approximately controllable.

In order to prove Proposition 5.5 we will need the following technical result (whose proof can be found in [23]).

Lemma 5.6: Let β be a real number transcendental over a field $\mathbf{F}$ with $\mathbf{Q} \subset \mathbf{F} \subset \mathbf{R}$. Then the elements of the family $\left(\frac{1}{1+q\beta}\right)_{q\in\mathbf{Q}}$ are $\mathbf{F}$-linearly independent.

Proof of Proposition 5.5. Theorem 5.1 and Fubini's theorem imply that the eigenvalues $\Lambda_{k_1,k_2,k_3}(\mu)$ of $-\Delta + \mu W$ on Ω for the Dirichlet boundary value problem satisfy

$$\Lambda'_{k_1,k_2,k_3}(0) = \\ = Ck_1^2k_2^2k_3^2 \frac{1}{\left(\frac{4\pi^2}{\alpha_1^2 l_1^2}k_1^2+1\right)\left(\frac{4\pi^2}{\alpha_2^2 l_2^2}k_2^2+1\right)\left(\frac{4\pi^2}{\alpha_3^2 l_3^2}k_3^2+1\right)}, \tag{18}$$

where

$$C = \frac{64(e^{\alpha_1 l_1}-1)(e^{\alpha_2 l_2}-1)(e^{\alpha_3 l_3}-1)\pi^6}{(\alpha_1 l_1 \alpha_2 l_2 \alpha_3 l_3)^3}.$$

Let $\beta_j = 4\pi^2/(\alpha_j^2 l_j^2)$, $j = 1,2,3$. The $\mathbf{Q}$-linear independence of the elements of $(\Lambda'_{k_1,k_2,k_3}(0))_{k_1,k_2,k_3\in\mathbf{N}}$ is obtained from the expression above thanks to three nested applications of Lemma 5.6 with $\mathbf{F} = \mathbf{Q}(\beta_1,\beta_2)$ and $\beta = \beta_3$, $\mathbf{F} = \mathbf{Q}(\beta_1)$ and $\beta = \beta_2$, and $\mathbf{F} = \mathbf{Q}$ and $\beta = \beta_1$. In order to complete the proof, let us check that every matrix $B^{(n)}$ is connected. (The conclusion then follows from Corollary 5.3.) A straightforward computation shows that for every triples of positive integers (k_1,k_2,k_3) and (h_1,h_2,h_3) the integral

$$\int_\Omega e^{\alpha\cdot x}\phi_{k_1,k_2,k_3}(x)\phi_{h_1,h_2,h_3}(x)dx$$

is different from zero, i.e., every element of $B^{(n)}$ is nonzero. $\square$

References

[1] P. Hübler, J. Bargon, and S. J. Glaser, "Nuclear magnetic resonance quantum computing exploiting the pure spin state of para hydrogen," *J. Chem. Phys.*, vol. 113, no. 6, pp. 2056–2059, 2000.

[2] A. Peirce, M. Dahleh, and H. Rabitz, "Optimal control of quantum mechanical systems: Existence, numerical approximations, and applications," *Phys. Rev. A*, vol. 37, pp. 4950–4964, 1988.

[3] H. Rabitz, H. de Vivie-Riedle, R. Motzkus, and K. Kompa, "Wither the future of controlling quantum phenomena?" *SCIENCE*, vol. 288, pp. 824–828, 2000.

[4] M. Shapiro and P. Brumer, *Principles of the Quantum Control of Molecular Processes*. Principles of the Quantum Control of Molecular Processes, pp. 250. Wiley-VCH, Feb. 2003.

[5] C. Altafini, "Controllability of quantum mechanical systems by root space decomposition of $su(N)$," *J. Math. Phys.*, vol. 43, no. 5, pp. 2051–2062, 2002.

[6] D. D'Alessandro, *Introduction to quantum control and dynamics.* Applied Mathematics and Nonlinear Science Series. Boca Raton, FL: Chapman, Hall/CRC., 2008.

[7] J. M. Ball, J. E. Marsden, and M. Slemrod, "Controllability for distributed bilinear systems," *SIAM J. Control Optim.*, vol. 20, no. 4, pp. 575–597, 1982.

[8] G. Turinici, "On the controllability of bilinear quantum systems," in *Mathematical models and methods for ab initio Quantum Chemistry*, ser. Lecture Notes in Chemistry, M. Defranceschi and C. Le Bris, Eds., vol. 74. Springer, 2000.

[9] M. Mirrahimi and P. Rouchon, "Controllability of quantum harmonic oscillators," *IEEE Trans. Automat. Control*, vol. 49, no. 5, pp. 745–747, 2004.

[10] P. Rouchon, "Control of a quantum particle in a moving potential well," in *Lagrangian and Hamiltonian methods for nonlinear control 2003*. Laxenburg: IFAC, 2003, pp. 287–290.

[11] L. Baudouin, O. Kavian, and J.-P. Puel, "Regularity for a Schrödinger equation with singular potentials and application to bilinear optimal control," *J. Differential Equations*, vol. 216, no. 1, pp. 188–222, 2005.

[12] A. Borzì and E. Decker, "Analysis of a leap-frog pseudospectral scheme for the Schrödinger equation," *J. Comput. Appl. Math.*, vol. 193, no. 1, pp. 65–88, 2006.

[13] K. Ito and K. Kunisch, "Optimal bilinear control of an abstract Schrödinger equation," *SIAM J. Control Optim.*, vol. 46, no. 1, pp. 274–287 (electronic), 2007.

[14] U. Boscain, T. Chambrion, and G. Charlot, "Nonisotropic 3-level quantum systems: complete solutions for minimum time and minimum energy," *Discrete Contin. Dyn. Syst. Ser. B*, vol. 5, no. 4, pp. 957–990 (electronic), 2005.

[15] U. Boscain and G. Charlot, "Resonance of minimizers for n-level quantum systems with an arbitrary cost," *ESAIM Control Optim. Calc. Var.*, vol. 10, no. 4, pp. 593–614 (electronic), 2004.

[16] U. Boscain and P. Mason, "Time minimal trajectories for a spin $1/2$ particle in a magnetic field," *J. Math. Phys.*, vol. 47, no. 6, pp. 062 101, 29, 2006.

[17] N. Khaneja, S. J. Glaser, and R. Brockett, "Sub-Riemannian geometry and time optimal control of three spin systems: quantum gates and coherence transfer," *Phys. Rev. A (3)*, vol. 65, no. 3, part A, pp. 032 301, 11, 2002.

[18] K. Beauchard, "Local controllability of a 1-D Schrödinger equation," *J. Math. Pures Appl. (9)*, vol. 84, no. 7, pp. 851–956, 2005.

[19] K. Beauchard and J.-M. Coron, "Controllability of a quantum particle in a moving potential well," *J. Funct. Anal.*, vol. 232, no. 2, pp. 328–389, 2006.

[20] J.-M. Coron, *Control and nonlinearity*, ser. Mathematical Surveys and Monographs. Providence, RI: American Mathematical Society, 2007, vol. 136.

[21] R. Adami and U. Boscain, "Controllability of the Schrödinger equation via intersection of eigenvalues," in *Proceedings of the 44th IEEE Conference on Decision and Control, December 12-15*, 2005, pp. 1080–1085.

[22] M. Mirrahimi, "Lyapunov control of a particle in a finite quantum potential well," in *Proceedings of the 45th IEEE Conference on Decision and Control*, December 13-15, 2006.

[23] T. Chambrion, P. Mason, M. Sigalotti, and U. Boscain, "Controllability of the discrete spectrum Schrödinger equation driven by an external field," *to appear in Annales de l'Institut Henri Poincaré*, 2008.

[24] F. Albertini and D. D'Alessandro, "Notions of controllability for bilinear multilevel quantum systems," *IEEE Trans. Automat. Control*, vol. 48, no. 8, pp. 1399–1403, 2003.

[25] E. B. Davies, *Spectral theory and differential operators*, ser. Cambridge Studies in Advanced Mathematics. Cambridge: Cambridge University Press, 1995, vol. 42.

[26] V. Pierfelice, "Strichartz estimates for the Schrödinger and heat equations perturbed with singular and time dependent potentials," *Asymptot. Anal.*, vol. 47, no. 1-2, pp. 1–18, 2006.

[27] I. Rodnianski and W. Schlag, "Time decay for solutions of Schrödinger equations with rough and time-dependent potentials," *Invent. Math.*, vol. 155, no. 3, pp. 451–513, 2004.

[28] A. Henrot, *Extremum problems for eigenvalues of elliptic operators*, ser. Frontiers in Mathematics. Basel: Birkhäuser Verlag, 2006.

[29] M. Reed and B. Simon, *Methods of modern mathematical physics. IV. Analysis of operators*. New York: Academic Press [Harcourt Brace Jovanovich Publishers], 1978.

[30] C. Altafini, "Controllability properties for finite dimensional quantum Markovian master equations," *J. Math. Phys.*, vol. 44, no. 6, pp. 2357–2372, 2003.

[31] T. Kato, *Perturbation theory for linear operators*, ser. Die Grundlehren der mathematischen Wissenschaften, Band 132. Springer-Verlag New York, Inc., New York, 1966.

[32] F. Rellich, *Perturbation theory of eigenvalue problems*, ser. Assisted by J. Berkowitz. With a preface by Jacob T. Schwartz. New York: Gordon and Breach Science Publishers, 1969.

[33] J. H. Albert, "Genericity of simple eigenvalues for elliptic PDE's," *Proc. Amer. Math. Soc.*, vol. 48, pp. 413–418, 1975.