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BILINEAR CONTROL OF DISCRETE SPECTRUM SCHRÖDINGER OPERATORS

K. AMMARI AND Z. AMMARI

ABSTRACT. The bilinear control problem of the Schrödinger equation $i\frac{\partial}{\partial t}\psi(t) = (A + u(t)B)\psi(t)$, where $u(t)$ is the control function, is investigated through topological irreducibility of the set $\mathfrak{M} = \{e^{-it(A+uB)}, u \in \mathbb{R}, t > 0\}$ of bounded operators. Under an appropriate assumption on B , this allows to prove the approximate controllability of such systems when the uncontrolled Hamiltonian A has a simple discrete spectrum.

1. INTRODUCTION

Since the early days of quantum mechanics, chemists and physicists have been interested in controlling molecular systems at the atomic scale. From a theoretical standpoint, this is a control problem for infinite dimensional quantum systems.

This area of study has recently experienced a growing development with various applications on a wide variety of physical and chemical systems (see [5],[6]). Most of these applications are described by linear differential equations in which the control inputs appear as linear coefficients, and are then part of bilinear control theory. In this context, various mathematical results are known (see for instance [1],[4],[10],[9],[2],[8],[7] and references therein).

The purpose of this paper is to study the approximate controllability of the bilinear control system given formally by the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(t) = (A + u(t)B)\psi(t), \quad (1.1)$$

where $u(t)$ is the control function, A is the uncontrolled Hamiltonian and B is a given external field. The operator A is assumed to have a simple pure point spectrum and no continuous spectrum (i.e., each eigenvalue is of multiplicity one and A has a complete set of eigenvectors). We were inspired by the recent work [3], where the same problem has been studied using techniques of finite dimension. Here, we present a different approach which relies on the analysis of invariant subspaces of the following set of bounded operators

$$\mathfrak{M} = \{e^{-it(A+uB)}, u \in U, t > 0\},$$

where U is a given subset of \mathbb{R} . This method provides strong results and gives, in the case of bounded operators, a necessary and sufficient condition for approximate controllability of (1.1) (see Proposition 5.1).

The paper is organized as follows. In Section 2 we give some useful definitions. The approximate controllability is studied in Section 3. Section 4 contains the main

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result on the bilinear control of discrete spectrum schrödinger operators. The last section is devoted to some application examples.

2. SCHRÖDINGER CONTROL SYSTEM

Consider for a non-empty subset U of \mathbb{R} a family of self-adjoint operators

$$(H(u), u \in U)$$

acting on a Hilbert space \mathcal{H} such that all the domains $D(H(u)), u \in U$, contain a common subspace D dense in \mathcal{H} . For any piecewise-constant function $u(t) = \sum_{j=0}^{n-1} 1_{[t_j, t_{j+1})}(t)u_j$, the abstract Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(t) = H(u(t))\psi(t), \quad (2.1)$$

admits a unique weak solution in $C^0([0, t_n], \mathcal{H})$ for any initial condition $\psi(0) \in \mathcal{H}$, in the sense that $i\partial_t \langle \psi(t), \phi \rangle = \langle \psi(t), H(u(t))\phi \rangle$ for any $\phi \in D$ and almost everywhere for $t \in [0, t_n]$. This solution is explicitly given by

$$\psi(t) = \begin{cases} e^{-itH(u_0)}\psi(0) & 0 \leq t < t_1 \\ e^{-i(t-t_1)H(u_1)}e^{-it_1H(u_0)}\psi(0) & t_1 \leq t < t_2 \\ \vdots & \vdots \\ e^{-i(t-t_{n-1})H(u_{n-1})} \dots e^{-it_1H(u_0)}\psi(0) & t_{n-1} \leq t < t_n. \end{cases}$$

This justifies the following definition, introduced in [3], for approximate controllability of a Schrödinger system $(H(u), u \in U)$. The principal is that for any initial and target states we can find a sequence of controls $u_1, \dots, u_k \in U$ such that starting from the initial state and evolving the system during a period of times $t_1, \dots, t_k > 0$ with the dynamics of $H(u_1), \dots, H(u_k)$, we end up as close as we want to the target state. Due to the unitarity of the evolution of (2.1) the initial and target states have, a fortiori, the same norm. So that, the controllability question reduces to the Hilbert sphere $\mathcal{S} = \{\psi \in \mathcal{H} : \|\psi\| = 1\}$.

Definition 2.1. The system $(H(u), u \in U)$ is said *approximately controllable* if for every $\psi_0, \psi_1 \in \mathcal{S}$ and every $\varepsilon > 0$ there exist $k \in \mathbb{N}$, $t_1, \dots, t_k > 0$ and $u_1, \dots, u_k \in U$ such that

$$\left\| \psi_2 - e^{-it_k H(u_k)} \dots e^{-it_1 H(u_1)} \psi_1 \right\| < \varepsilon.$$

We denote by $\mathcal{B}(\mathcal{H})$ the algebra of all bounded operators on \mathcal{H} containing in particular the identity operator $\mathbb{1}$. It is worth to recall the following definitions.

- **Invariant subspace:** A subspace $E \subset \mathcal{H}$ is said invariant for $A \in \mathcal{B}(\mathcal{H})$ if E is closed and $AE \subset E$ (i.e., $\forall \psi \in E, A\psi \in E$). Similarly, E is said invariant for a set of bounded operators \mathfrak{M} if E is invariant for each $A \in \mathfrak{M}$. In which case, we also say E is \mathfrak{M} -invariant.
- **Commutant:** The commutant for a set of bounded operators \mathfrak{M} is the subalgebra of $\mathcal{B}(\mathcal{H})$ defined by

$$\mathfrak{M}' = \{T \in \mathcal{B}(\mathcal{H}) : TA = AT, \forall A \in \mathfrak{M}\}.$$

- **Topological irreducibility:** A set of bounded operators \mathfrak{M} is said topologically irreducible if the only invariant subspaces for \mathfrak{M} are \mathcal{H} and $\{0\}$ (i.e., \mathfrak{M} have no proper invariant subspace).

- Reducing subspace: A subspace E is said reducing for $A \in \mathcal{B}(\mathcal{H})$ if E and E^\perp are invariant subspaces of A .

3. APPROXIMATE CONTROLLABILITY

In all the following we set

$$\begin{aligned}\mathfrak{M} &:= \{e^{-itH(u)}, u \in U, t > 0\}, & \mathfrak{M}^* &:= \{e^{itH(u)}, u \in U, t > 0\}, \\ \mathfrak{R} &:= \{\prod_{k=1}^n e^{-it_k H(u_k)}, \forall n \in \mathbb{N}; u_1, \dots, u_n \in U; t_1, \dots, t_n > 0\}.\end{aligned}$$

We first state a necessary condition for the approximate controllability.

Proposition 3.1. *If $(H(u), u \in U)$ is approximately controllable then the commutant \mathfrak{M}' consists of multiples of the identity operator (i.e. $\mathfrak{M}' = \mathbb{C}\mathbb{1}$).*

Proof. Let ψ, ϕ be two analytic vectors of $H(u)$ and $T \in \mathfrak{M}'$ (see [12, Section X.6] for a definition of analytic vectors). The functions

$$f(t) = \langle \psi, T e^{-itH(u)} \phi \rangle \quad \text{and} \quad g(t) = \langle \psi, e^{-itH(u)} T \phi \rangle, \quad t > 0,$$

admit analytic extension to a strip $\Sigma_\theta := \{z \in \mathbb{C} : |\text{Im}(z)| < \theta\}$. Since T satisfies

$$\langle \psi, T e^{-itH(u)} \phi \rangle = \langle \psi, e^{-itH(u)} T \phi \rangle, \quad t > 0,$$

we get

$$\tilde{f}(z) = \langle \psi, T e^{-izH(u)} \phi \rangle = \langle \psi, e^{-izH(u)} T \phi \rangle = \tilde{g}(z)$$

for any $z \in \Sigma_\theta$, where \tilde{f} and \tilde{g} are respectively the analytic extensions to Σ_θ of f and g . In particular, we have

$$\langle \psi, T e^{itH(u)} \phi \rangle = \langle \psi, e^{itH(u)} T \phi \rangle, \quad \forall t > 0.$$

Since the set of analytic vectors of a self-adjoint operator is dense in \mathcal{H} , we see that $T e^{itH(u)} = e^{itH(u)} T$ for any $t > 0$ and $u \in U$. Therefore, by taking the adjoint we obtain that $T^* \in \mathfrak{M}'$. Hence, there exists a self-adjoint operator $C \in \mathfrak{M}'$, for instance $C = T + T^*$. Moreover, by functional calculus any spectral projection $1_\Delta(C)$ belongs to \mathfrak{M}' . If C is not a multiple of the identity then there exists an orthogonal projection $1_\Delta(C) \neq \mathbb{1}$ and hence we will have

$$\prod_{k=1}^n e^{-it_k H(u_k)} 1_\Delta(C) = 1_\Delta(C) \prod_{k=1}^n e^{-it_k H(u_k)}, \quad \forall n \in \mathbb{N}.$$

This contradicts the approximate controllability of the system $(H(u), u \in U)$. ■

We also have the following sufficient condition for the approximate controllability.

Proposition 3.2. *If \mathfrak{M} is topologically irreducible then $(H(u), u \in U)$ is approximately controllable.*

Proof. If the statement of the proposition is false then there exists $\psi \in \mathcal{S}$ such that $\mathfrak{R}\psi^\perp := \{T\psi, T \in \mathfrak{R}\}^\perp \neq \{0\}$. This closed subspace is \mathfrak{M}^* -invariant since for any $\phi \in \mathfrak{R}\psi^\perp$

$$\langle e^{itH(u)} \phi, \prod_{k=1}^n e^{-it_k H(u_k)} \psi \rangle = 0.$$

So that $\mathfrak{M}(\mathfrak{R}\psi^\perp) \subset \mathfrak{R}\psi^\perp$. Hence \mathfrak{M}^* is not topologically irreducible and consequently \mathfrak{M} neither since a subspace E is \mathfrak{M}^* -invariant iff E^\perp is \mathfrak{M} -invariant. ■

In the following particular situation we provide a necessary and sufficient condition for the approximate controllability.

Proposition 3.3. *Assume that for each $u \in U$ the spectrum of $H(u)$ does not separate the plane (i.e., $\sigma(H(u)) \neq \mathbb{R}$, $\forall u \in U$). Then $\mathfrak{M} = \mathbb{C}\mathbb{1}$ iff \mathfrak{M} is topologically irreducible.*

Proof. Suppose that \mathfrak{M} is not topologically irreducible, then there exists a proper \mathfrak{M} -invariant subspace E . Let P denote the orthogonal projection on E and let $R_\mu(H(u))$ be the resolvent $(\mu\mathbb{1} - H(u))^{-1}$, $\text{Im}(\mu) \neq 0$. The following relation holds:

$$e^{-itH(u)}P = Pe^{-itH(u)}P, \quad \forall t > 0, \forall u \in U. \quad (3.1)$$

Actually, under the assumption of non-separating spectrum $e^{-itH(u)}P = Pe^{-itH(u)}$ holds true for any $u \in U$ and $t > 0$. For any $\psi, \phi \in \mathcal{H}$, the two functions

$$f(\mu) = \langle \psi, R_\mu(H(u))P\phi \rangle \quad \text{and} \quad g(\mu) = \langle \psi, PR_\mu(H(u))P\phi \rangle$$

are analytic on the resolvent set $\varrho(H(u))$ which is a connected open subset of \mathbb{C} . Using the resolvent formula

$$\text{Im}(\mu) > 0, \quad R_\mu(H(u)) = -i \int_0^{+\infty} e^{it\mu} e^{-itH(u)} dt,$$

and the relation (3.1), we easily see that $f(\mu) = g(\mu)$, for $\text{Im}(\mu) > 0$ and hence $f = g$. Repeating the same argument yields

$$\langle \psi, \prod_{k=1}^n R_{\mu_k}(H(u))P\phi \rangle = \langle \psi, P \prod_{k=1}^n R_{\mu_k}(H(u))P\phi \rangle$$

for any $\mu_k \in \mathbb{C} \setminus \mathbb{R}$. By Stone-Weierstrass theorem polynomials in $(x \pm i)^{-1}$ are dense in the space of continuous functions vanishing at infinity $C_\infty(\mathbb{R})$. Therefore, for any $v \in C_\infty(\mathbb{R})$, we have

$$\langle \psi, v(H(u))P\phi \rangle = \langle \psi, Pv(H(u))P\phi \rangle.$$

Thus, for any $\varepsilon > 0$, $e^{-\varepsilon H(u)^2} e^{itH(u)}P = Pe^{-\varepsilon H(u)^2} e^{itH(u)}P$, with $t \in \mathbb{R}$. Since the strong limit $s - \lim_{\varepsilon \rightarrow 0} e^{-\varepsilon H(u)^2} = \mathbb{1}$ holds, we conclude that

$$e^{itH(u)}P = Pe^{itH(u)}P, \quad \forall t \in \mathbb{R}.$$

This means that E is a proper reducing subspace for each $A \in \mathfrak{M}$ and hence P is a non-trivial projection belonging to \mathfrak{M}' . This contradicts $\mathfrak{M}' = \mathbb{C}\mathbb{1}$. \blacksquare

Remark 3.4. We notice that if either \mathcal{H} is finite dimension or $H(u), u \in U$, are bounded operators then the assumption of non separating spectrum is satisfied.

Remark 3.5. We recall that an operator $A \in \mathcal{B}(\mathcal{H})$ is said completely normal if it is normal and every invariant subspace is reducing. Therefore, if $e^{-itH(u)}$ are completely normal operators for any $u \in U$ and $t > 0$ the conclusion of Proposition 3.3 holds true.

4. BILINEAR CONTROL SYSTEM

In this section we consider a specific Schrödinger system, often called bilinear control system. Let A, B be two self-adjoint operators on \mathcal{H} . We assume for $u \in U$:

- (H1) There exists a self-adjoint extension $H(u)$ of $A + uB$ defined on $D(A) \cap D(B)$.
- (H2) A has simple eigenvalues with an orthonormal basis $(\phi_n)_{n \in \mathbb{N}}$ of eigenvectors.
- (H3) $\phi_n \in D(B)$ for every $n \in \mathbb{N}$.

We assign to this bilinear control system (A, B, U) a graph $G = (\mathbb{N}, \Gamma)$, where Γ is a subset of unordered pairs in $\mathbb{N} \times \mathbb{N}$, given by

$$\Gamma := \{\{i, j\} \in \mathbb{N}^2 : \langle \phi_i, B\phi_j \rangle \neq 0\}.$$

We say that G is connected if for every pair $\{i, j\} \in \mathbb{N}^2$, the graph G contains a path connecting i and j , i.e.,

$$\forall \{i, j\} \in \mathbb{N}^2, \exists \{i_0, i_1\}, \dots, \{i_{k-1}, i_k\} \in \Gamma : i_0 = i \text{ and } i_k = j.$$

Theorem 4.1. *Let (A, B, U) be a bilinear control system satisfying (H1)-(H3) such that $0 \in U$ and $U \neq \{0\}$. Then $(H(u), u \in U)$ is approximately controllable if the graph*

$$G = (\mathbb{N}, \Gamma) \text{ is connected.} \quad (4.1)$$

Proof. Let E be a \mathfrak{M} -invariant subspace and P the orthogonal projection on E . It follows that

$$e^{-itH(u)}P = Pe^{-itH(u)}P, \quad \forall u \in U, \forall t > 0.$$

In particular, if $u = 0$ we get the relation $e^{-itA}P = Pe^{-itA}P$, $t > 0$. By the spectral theorem

$$e^{-it\lambda_n} \|P\phi_n\|^2 = \langle \phi_n, e^{-itA}P\phi_n \rangle = \langle P\phi_n, e^{-itA}P\phi_n \rangle = \int_{\mathbb{R}} e^{-itx} d\mu_{P\phi_n} = \hat{\mu}_{P\phi_n}(t),$$

where $\mu_{P\phi_n}$ is the spectral measure associated to $P\phi_n$ and $\hat{\mu}_{P\phi_n}$ its Fourier transform. Since $\overline{\hat{\mu}_{P\phi_n}(t)} = \hat{\mu}_{P\phi_n}(-t)$ for any $t > 0$ we easily see that $\hat{\mu}_{P\phi_n}(t) = e^{-it\lambda_n} \|P\phi_n\|^2$ for all $t \in \mathbb{R}$. So that, $\mu_{P\phi_n} = \delta_{\lambda_n} \|P\phi_n\|^2$ and hence by functional calculus we see that $AP\phi_n = \lambda_n P\phi_n$. More precisely, let χ_κ be a bounded sequence of Borel compactly supported functions such that $\chi_\kappa(\lambda_n) = 1$ and $\chi_\kappa(x) \rightarrow 1$ for every $x \in \mathbb{R}$ then by the spectral theorem we get $\lim_{\kappa \rightarrow \infty} \chi_\kappa(A)P\phi_n = P\phi_n$ and

$$\begin{aligned} \|(A - \lambda_n \mathbb{1})\chi_\kappa(A)P\phi_n\|^2 &= \langle P\phi_n, (A - \lambda_n \mathbb{1})^2 \chi_\kappa^2(A)P\phi_n \rangle \\ &= \int_{\mathbb{R}} (x - \lambda_n)^2 \chi_\kappa^2(x) d\mu_{P\phi_n} = 0. \end{aligned}$$

Hence, using the fact that the graph of A is closed and $\lim_{\kappa \rightarrow \infty} (A - \lambda_n)\chi_\kappa(A)P\phi_n = 0$, we see that $P\phi_n \in D(A)$ and $(A - \lambda_n)P\phi_n = 0$. Since the eigenvalues λ_n of A are simple, we conclude that

$$AP\phi_n = c_n \phi_n, \quad \forall n \in \mathbb{N} \text{ and } c_n \in \{0, 1\}.$$

The projection P satisfies the relation $Pe^{-itH(u)}P = e^{-itH(u)}P$, $u \in U$ and $t > 0$ which leads to the following identity

$$c_n c_m \langle \phi_n, e^{-itH(u)}\phi_m \rangle = c_m \langle \phi_n, e^{-itH(u)}\phi_m \rangle, \quad \forall (n, m) \in \mathbb{N}^2. \quad (4.2)$$

By differentiating (4.2), we obtain for all $n, m \in \mathbb{N}$

$$c_n c_m \langle \phi_n, B\phi_m \rangle = c_m \langle \phi_n, B\phi_m \rangle.$$

This implies that if $\langle \phi_n, B\phi_m \rangle \neq 0$ then $c_n = c_m$. It is clear that under the assumption (4.1) that $c_n = 0$ for all $n \in \mathbb{N}$ or $c_n = 1$ for all $n \in \mathbb{N}$. This means that $P = \mathbb{1}$ or $P = 0$ and therefore \mathfrak{M} is topologically irreducible. By Proposition 3.2 we obtain the claimed result. \blacksquare

Remark 4.2. We notice that if $\langle \phi_{n+1}, B\phi_n \rangle \neq 0$ for every $n \in \mathbb{N}$ then (4.1) is satisfied.

We show a non approximate controllability result in the proposition below when the graph G has a finite disconnected component. In Subsection 5.1, we will show that if A and B are bounded then disconnectedness of the graph G implies the non approximate controllability of the system (A, B, U) .

Proposition 4.3. *Let (A, B, U) be a bilinear control system satisfying (H1)-(H3) such that $0 \in U$ and $U \neq \{0\}$. If the graph $G = (\mathbb{N}, \Gamma)$ admits at least one finite connected component then $(H(u), u \in U)$ is not approximately controllable.*

Proof. Suppose that G is a disconnected graph with at least one finite connected component (J, Γ_0) which is a subgraph of G with J a finite subset of \mathbb{N} . Hence, we have

$$\langle \phi_i, B\phi_j \rangle = 0 \quad \forall i \in J^c, \forall j \in J.$$

Let E be the closed subspace spanned by $(\phi_i)_{i \in J}$. Then, $E \subset D(A) \cap D(B) \subset D(H(u))$. For any $\psi \in E$, we check that $\langle \psi, (A + uB)\phi_j \rangle = 0$ for all $j \in J^c$ and $u \in U$. As a consequence $H(u)\psi$ is orthogonal to any $\phi_j, j \in J^c$ and hence $H(u)\psi \in E$. Since E is finite dimension and $H(u)E \subset E$ then the restriction $H(u) : E \rightarrow E$ is a bounded operator. This, in particular, means that any $\psi \in E$ is an analytic vector for $H(u)$ and the series

$$e^{-itH(u)}\psi = \sum_{k=0}^{\infty} \frac{(-it)^k}{k!} H(u)^k \psi$$

is absolutely convergent in E . So, we conclude that $e^{-itH(u)}E \subset E$ for any $t \in \mathbb{R}$ and any $u \in U$. Hence, E is a reducing subspace for \mathfrak{M} and the orthogonal projection P on E belongs to the commutant \mathfrak{M}' . Thus, we have proved that $\mathfrak{M}' \neq \mathbb{C}\mathbb{1}$ and hence by Proposition 3.1 the system (A, B, U) is not approximately controllable. ■

5. APPLICATION EXAMPLES

5.1. A and B bounded. Let (A, B, U) be a bilinear control system as in Section 4. If A and B are bounded operators then the assumptions (H1) and (H3) are satisfied. Actually, the assumption (4.1) in Theorem 4.1 is a necessary and sufficient condition when A and B are bounded operators.

Proposition 5.1. *Let (A, B, U) be a bilinear control system satisfying (H2) with A and B bounded operators and such that $0 \in U$ and $U \neq \{0\}$. Then $(H(u), u \in U)$ is approximately controllable if and only if the graph $G = (\mathbb{N}, \Gamma)$ is connected.*

Proof. Suppose that the graph G is disconnected and let (J, Γ_0) be one of its connected component. Then $\langle \phi_i, B\phi_j \rangle = 0$ for all $i \in J^c, j \in J$ and the closed subspace E spanned by $(\phi_i)_{i \in J}$ is preserved by $A + uB$ since A and B are bounded. This shows that E is a reducing subspace for \mathfrak{M} and hence $\mathfrak{M}' \neq \mathbb{C}\mathbb{1}$. By Proposition 3.1 we see that (A, B, U) is not approximately controllable. ■

5.2. Harmonic oscillator. We consider a concrete example of a Schrödinger equation describing the evolution of a one-dimensional harmonic oscillator,

$$i \frac{\partial \psi}{\partial t}(t, x) = -\frac{\partial^2 \psi}{\partial x^2}(t, x) + (E(t)x + x^2) \psi(t, x), \quad (5.1)$$

with the strength of the electric field $E(\cdot)$ representing the control function. Here $E(t)$ is a piecewise-continuous function taking values in a subset U of \mathbb{R}_+ . In this

framework, the operator A is the one-dimensional harmonic oscillator

$$A = -\frac{\partial^2}{\partial x^2} + x^2,$$

which is essentially self-adjoint on the Schwartz space $S(\mathbb{R})$ and also on $C_0^\infty(\mathbb{R})$, with explicit discrete spectrum

$$\sigma(A) = \{\lambda_k = 2k + 1 \mid k \in \mathbb{N}\}.$$

Each eigenvalue λ_k is simple with a corresponding eigenfunction

$$\phi_k(x) = \frac{1}{\sqrt{k!2^k\sqrt{\pi}}} H_k(x) e^{-\frac{x^2}{2}}, \quad (5.2)$$

where $H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2}$ is the k^{th} Hermite polynomial. The set $(\phi_k)_{k \in \mathbb{N}}$ spans $L^2(\mathbb{R})$. It is well known that the operator sum $A+ux$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$ and also on $S(\mathbb{R})$ for any $u \in \mathbb{R}$ (see [12, Theorem X.28]). Moreover, we easily check

$$\langle \phi_k, x\phi_{k+1} \rangle = \sqrt{\frac{(k+1)}{2}} \neq 0.$$

Hence, the system (A, x, U) satisfies (H1)-(H3) and consequently it is approximately controllable whenever $0 \in U$ and $U \neq \{0\}$.

Remark 5.2. Several other examples can be found in [3].

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