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Approximate controllability via adiabatic techniques for the three input controlled Schrödinger equation

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Abstract— **We present a constructive method to control the bilinear Schrödinger equation by means of three controlled external fields. The method is based on adiabatic techniques and works if the spectrum of the Hamiltonian admits eigenvalue intersections, with respect to variations of the controls, and if the latter are conical. We provide sharp estimates of the relation between the error and the controllability time, namely by following adiabatically special curves in the space of controls.**

I. Introduction

Interesting issues in quantum control concern the controllability of the bilinear Schrödinger equation

$$i\frac{d\psi}{dt} = \left(H_0 + \sum_{k=1}^{m} u_k(t)H_k\right)\psi(t), \tag{1}$$

where ψ belongs to the Hilbert sphere $\mathbf{S}$ of a (finite or infinite dimensional) complex separable Hilbert space $\mathcal{H}$ and $H_0, \dots, H_m$ are self-adjoint operators on $\mathcal{H}$. The controls $u_1, \dots, u_m$ are scalar-valued and represent the action of external fields. H_0 describes the "internal" dynamics of the system, while $H_1, \dots, H_m$ the interrelation between the system and the controls.

The controllability problem aims at establishing whether, for every pair of states ψ_0 and ψ_1, there exist controls $u_k(\cdot)$ and a time T such that the solution of (1) with initial condition $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$.

While the case where $\mathcal{H}$ is a finite dimensional Hilbert space has been widely understood [9], in the infinite dimensional case the answer is far from being given. In particular, negative results have been proven when $\mathcal{H}$ is infinite-dimensional (see [2], [18]). Hence one has to look for weaker controllability properties as, for instance, approximate controllability (see for instance [6], [8], [13], [14]), or controllability between subfamilies of states (in particular the eigenstates of H_0, which are the most relevant physical states) and other regular states (see [3], [4]).

In most of the results in the literature only the single-input case is considered. In this exposition we study the case $m = 3$ that exhibit conical intersection between the eigenvalues of the Hamiltonian, and we look both for controllability results and explicit expressions of the external fields realizing the transition. The idea is to use slowly varying controls, taking advantage of the adiabatic theorem, and climb the energy levels through the conical intersections.

Adiabatic methods are well-known tools in quantum mechanics. Typical results in adiabatic theory state that slow (i.e. adiabatic) changes in the environment produce small changes in the population density associated with isolated portions of the spectrum (see for instance [17]).

The applications of adiabatic methods in quantum control, as a tool for obtaining controllability results, have already been exploited in previous papers (see for instance [1], [12], [7]). Roughly speaking, the basic idea is the following: assume that there are two eigenvalues of the controlled Hamiltonian that are (locally) well separated from the rest of the spectrum and that cross conically at some value $\bar{\mathbf{u}}$ of the control; then we can produce an (approximate) controlled population transfer between the two levels by slowly tuning the control function along a smooth path passing through $\bar{\mathbf{u}}$.

Direct application of the adiabatic theorem leads to a precision of the order of the square root of the control speed. In this presentation (see also [7]), we propose some special paths in space of control that remarkably improve the precision of the transfer, that is the error is of the order of the control speed. From a practical point of view, this means that to obtain the same precision we reduce the duration of the process, whose extent constitute one of the main disadvantages of the implementation of the adiabatic techniques.

We remark moreover that this result allows us to control the population inside some portion of the discrete spectrum, if well separated from the rest, even in the presence of continuos spectrum.

II. Main results

The dynamics of the quantum system are described by the time-dependent Schrödinger equation

$$i\frac{d\psi}{dt} = H(\mathbf{u}(t))\psi(t). \tag{2}$$

where $\mathbf{u} = (u_1, u_2, u_3) \in \mathbb{R}^3$ and $H(\mathbf{u}) = H_0 + u_1H_1 + u_2H_2 + u_3H_3$, where H_i are self-adjoint possibly unbounded linear operators on the Hilbert space $\mathcal{H}$, for every $i = 0, \dots, 3$. The operators H_1, H_2, H_3 are Kato-small with respect to H_0, that is for $i = 1, 2, 3$ $\mathcal{D}(H_0) \subset \mathcal{D}(H_i)$ and for every $\alpha > 0$ there exists $\beta > 0$ such that $\|H_i\psi\| \leq \alpha\|H_0\psi\| + \beta\|\psi\|$ for every $\psi \in \mathcal{D}(H_0)$.

We are interested in controlling (2) inside some portion of the discrete spectrum of $H(\mathbf{u})$. Since we use adiabatic techniques, such portion of spectrum must be well separated

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from its complement in the spectrum of the Hamiltonian, and this property must hold uniformly for $\mathbf{u}$ belonging to some domain in $\mathbb{R}^3$. All these properties are formalized by the following notion.

Definition 2.1: Let ω be a domain in $\mathbb{R}^3$. A map Σ that associates with each $\mathbf{u} \in \omega$ a subset $\Sigma(\mathbf{u})$ of the discrete spectrum of $H(\mathbf{u})$ is said to define a *separated discrete spectrum* on ω if there exist two continuous functions $f_1, f_2 : \omega \to \mathbb{R}$ such that

- $f_1(\mathbf{u}) < f_2(\mathbf{u})$ and $\Sigma(\mathbf{u}) \subset [f_1(\mathbf{u}), f_2(\mathbf{u})] \qquad \forall \mathbf{u} \in \omega$.
- there exists $\Gamma > 0$ such that

$$\inf_{\mathbf{u}\in\omega} \inf_{\lambda \in \mathrm{Spec}(H(\mathbf{u}))\setminus\Sigma(\mathbf{u})} \mathrm{dist}(\lambda, [f_1(\mathbf{u}), f_2(\mathbf{u})])) > \Gamma.$$

Notation From now on we label the eigenvalues belonging to $\Sigma(\mathbf{u})$ in such a way that $\Sigma(\mathbf{u}) = \{\lambda_0(\mathbf{u}), \dots, \lambda_k(\mathbf{u})\}$, where $\lambda_0(\mathbf{u}) \le \cdots \le \lambda_k(\mathbf{u})$ are counted according to their multiplicity (note that the separation of Σ from the rest of the spectrum guarantees that k is constant). Moreover we denote by $\phi_0(\mathbf{u}), \dots, \phi_k(\mathbf{u})$ an orthonormal family of eigenstates corresponding to $\lambda_0(\mathbf{u}), \dots, \lambda_k(\mathbf{u})$. Notice that in this notation λ_0 does not need to be the ground state of the system.

Our techniques rely on the existence of conical intersections between the eigenvalues, which constitute a well-known notion in molecular physics (see for instance [5], [11], [17]). In this paper we will adopt the following definition, consistent with the one already given in [7] for the two-input case.

Definition 2.2: We say that $\bar{\mathbf{u}} \in \mathbb{R}^3$ is a *conical intersection* between the eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ has multiplicity two and there exists a constant $c > 0$ such that for any unit vector $\mathbf{v} \in \mathbb{R}^3$ and $t > 0$ small enough we have that

$$\lambda_{j+1}(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_j(\bar{\mathbf{u}} + t\mathbf{v}) > ct\,. \tag{3}$$

It is worth noticing that conical intersections are not pathological phenomena. On the contrary, in physically interesting cases they often happen to be generic.

In this framework, we will be concerned with the following notion of controllability.

Definition 2.3: Let Σ be a separated discrete spectrum on ω. We say that (2) is approximately *spread-controllable* on Σ if for every $\mathbf{u}^0, \mathbf{u}^1 \in \omega$ such that $\Sigma(\mathbf{u}^0)$ and $\Sigma(\mathbf{u}^1)$ are non-degenerate, for every $\bar{\phi} \in \{\phi_0(\mathbf{u}^0), \dots, \phi_k(\mathbf{u}^0)\}$, $p \in [0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2 = 1$, and every $\varepsilon > 0$ there exist $T > 0$, $\vartheta_0, \dots, \vartheta_k \in \mathbb{R}$ and a piecewise $\mathcal{C}^1$ control $\mathbf{u}(\cdot) : [0,T] \to \mathbb{R}^m$ such that

$$\|\psi(T) - \sum_{j=0}^{k} p_j e^{i\vartheta_j} \phi_j(\mathbf{u}^1)\| \le \varepsilon, \tag{4}$$

where $\psi(\cdot)$ is the solution of (2) with $\psi(0) = \bar{\phi}$.

Conical intersections may be characterized by the non-degeneracy of the following matrix, which we call *conicity matrix*.

Definition 2.4: We define the *conicity matrix* associated with $(\psi_j, \psi_{j+1}) \in \mathcal{D}(H_0) \times \mathcal{D}(H_0)$ as

$$\mathcal{M}(\psi_j, \psi_{j+1}) = \begin{pmatrix} \langle\psi_j, H_1\psi_{j+1}\rangle & \langle\psi_j, H_1\psi_{j+1}\rangle^* & \langle\psi_{j+1}, H_1\psi_{j+1}\rangle - \langle\psi_j, H_1\psi_j\rangle \\ \langle\psi_j, H_2\psi_{j+1}\rangle & \langle\psi_j, H_2\psi_{j+1}\rangle^* & \langle\psi_{j+1}, H_2\psi_{j+1}\rangle - \langle\psi_j, H_2\psi_j\rangle \\ \langle\psi_j, H_3\psi_{j+1}\rangle & \langle\psi_j, H_3\psi_{j+1}\rangle^* & \langle\psi_{j+1}, H_3\psi_{j+1}\rangle - \langle\psi_j, H_3\psi_j\rangle \end{pmatrix}.$$

Proposition 2.5: Assume that $\{\lambda_j, \lambda_{j+1}\}$ is a separated discrete spectrum with $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$. Let $\{\psi_j, \psi_{j+1}\}$ be an orthonormal basis of the eigenspace associated with the double eigenvalue. Then $\bar{\mathbf{u}}$ is a conical intersection if and only if $\mathcal{M}(\psi_j, \psi_{j+1})$ is nonsingular.

Let us focus on the band constituted by the two eigenvalues $\{\lambda_j, \lambda_{j+1}\}$, assumed to be well separated from the rest of the spectrum and conically intersecting in 0. We are interested in the dynamics inside the two-dimensional space generated by the eigenvalues corresponding to λ_j, and λ_{j+1}.

Under some regularity assumptions, we can construct a $\mathcal{C}^1$ representation of these dynamics into $\mathbb{C}^2$. These dynamics are described by a Hamiltonian function on $\mathbb{C}$ called *effective Hamiltonian*. Explicit estimates show that the off-diagonal terms of this Hamiltonian are responsible of the reduced precision of adiabatic approximation in the presence of eigenvalues intersection (that is, the term of the order of the square root of the control speed).

Let us now introduce the following vectors

$$\boldsymbol{m}(\psi_j, \psi_{j+1}) = (\langle\psi_j, H_1\psi_{j+1}\rangle, \langle\psi_j, H_2\psi_{j+1}\rangle, \langle\psi_j, H_3\psi_{j+1}\rangle)^T, \tag{5}$$

and

$$\begin{aligned} X(\psi_j, \psi_{j+1}) &= \frac{\boldsymbol{m}(\psi_j, \psi_{j+1}) \times \boldsymbol{m}^*(\psi_j, \psi_{j+1})}{2i} \qquad (6) \\ &= (\mathfrak{Im}(m_2 m_3^*), \mathfrak{Im}(m_3 m_1^*), \mathfrak{Im}(m_1 m_2^*))^T\,, \end{aligned}$$

Theorem 2.6: Let $\bar{\mathbf{u}}$ be a conical intersection between λ_j and λ_{j+1}. There is a neighbourhood of $\bar{\mathbf{u}}$ such that the vector field

$$\mathcal{X}_P(\mathbf{u}) = X(\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u})) \tag{7}$$

satisfies the following properties:

1) all integral curves of $\mathcal{X}_P$ starting from a point of $U \setminus \bar{\mathbf{u}}$ reach $\bar{\mathbf{u}}$ in finite time; moreover, they are smooth up to the singularity included;
2) along these integral curves, the reduced Hamiltonian is diagonal.

We remark that property 2) implies that the adiabatic evolution along the integral curves of $\mathcal{X}_P$ conserves the populations, and moreover the precision of adiabatic approximation is of the order of the control speed.

A peculiarity of conical intersections is that, when approaching the singularity from different directions, the eigenstates corresponding to the intersecting eigenvalues have different limits. This property is crucial for control purposes, since corners (i.e., $\mathcal{C}^1$ singularities) at the intersection induce a distribution of the population between the concerned levels, as explained in the following proposition.

Proposition 2.7: Let $\mathbf{v}_0, \mathbf{v} \in \mathbb{R}^3$ be two unit vectors, and call ϕ_j^0, ϕ_{j+1}^0 the limits as $t \to 0^+$ of the eigenstates

$\phi_j(r_0(t)), \phi_{j+1}(r_0(t))$ along a straight line $r_0(t) = \mathbf{u} + t\mathbf{v}_0$, and $\phi_j^{\mathbf{v}}, \phi_{j+1}^{\mathbf{v}}$ the limit basis along the straight line $r_{\mathbf{v}}(t) = \mathbf{u} + t\mathbf{v}$.

Then, up to phases, the following relation holds:

$$\begin{pmatrix} \phi_j^{\mathbf{v}} \\ \phi_{j+1}^{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} \cos\Xi & e^{-i\beta}\sin\Xi \\ -e^{i\beta}\sin\Xi & \cos\Xi \end{pmatrix} \begin{pmatrix} \phi_j^0 \\ \phi_{j+1}^0 \end{pmatrix}, \quad (8)$$

where the parameters $\Xi = \Xi(\mathbf{v})$ and $\beta = \beta(\mathbf{v})$ satisfy the following equations:

$$\tan 2\Xi(\mathbf{v}) = (-1)^{\xi} \frac{2|\langle \phi_j^0, H_{\mathbf{v}}\phi_{j+1}^0 \rangle|}{\langle \phi_j^0, H_{\mathbf{v}}\phi_j^0 \rangle - \langle \phi_{j+1}^0, H_{\mathbf{v}}\phi_{j+1}^0 \rangle} \quad (9)$$

$$\beta(\mathbf{v}) \overset{(\mathrm{mod}\, 2\pi)}{=} \arg\langle \phi_j^0, H_{\mathbf{v}}\phi_{j+1}^0 \rangle + \xi\pi, \quad (10)$$

where $H_{\mathbf{v}} = \sum_{i=1}^m H_i v_i$ and $\xi = 0, 1$.

Remark 2.8: Up to phases, the limits of the eigenstates $\phi_j(\gamma(t)), \phi_{j+1}(\gamma(t))$ along any $\mathcal{C}^1$ curve passing through the conical intersection at $t = 0$ depend only on the unit vector $\frac{\dot\gamma(0)}{\|\dot\gamma(0)\|}$.

Controlling the incoming and the outgoing directions $\mathbf{v}_0$ and $\mathbf{v}$, we can take advantage of the above result to induce the desired distribution of probability between the two levels. It is worth noticing that it is always possible to choose integral paths of non-mixing field through the conical intersection in order to achieve the previous goal, thanks to the following proposition.

Proposition 2.9: For every unit vector $\mathbf{v}$ in $\mathbb{R}^3$ there exists an integral curve $\gamma : [-\eta, 0] \to \omega$ of $\mathcal{X}_P$ with $\gamma(0) = 0$, $\eta > 0$, such that

$$\lim_{t\to 0^-} \frac{\dot\gamma(t)}{\|\dot\gamma(t)\|} = \mathbf{v}.$$

The strategy to induce a prescribed probability distribution between two levels is described by the following proposition.

Proposition 2.10: Let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j, λ_{j+1}. Let $\gamma : [0,1] \to \omega$ be a curve such that for some $\tau_0 \in (0,1)$ $\gamma(\tau_0) = \bar{\mathbf{u}}$, $\gamma|_{[0,\tau_0]}$ and $\gamma|_{[\tau_0,1]}$ are integral curves of non-mixing field, and

$$\lim_{\tau\to\tau_0^-} \dot\gamma(\tau) = \mathbf{v}_0 \qquad \lim_{\tau\to\tau_0^+} \dot\gamma(\tau) = \mathbf{v} \quad (11)$$

for some unit vectors $\mathbf{v}_0, \mathbf{v}$. Let ϕ_j^0, ϕ_{j+1}^0 be limits as $\tau \to \tau_0^-$ of the eigenstates $\phi_j(\gamma(\tau)), \phi_{j+1}(\gamma(\tau))$, respectively. Then there exists $C > 0$ such that, for any $\varepsilon > 0$,

$$\|\psi(1/\varepsilon) - p_1 e^{i\vartheta_j}\phi_j(\gamma(1)) - p_2 e^{i\vartheta_{j+1}}\phi_{j+1}(\gamma(1))\| \le C\varepsilon \quad (12)$$

where $\vartheta_j,\ \vartheta_{j+1} \in \mathbb{R}$, $\psi(\cdot)$ is the solution of equation (2) with $\psi(0) = \phi_j(\gamma(0))$ corresponding to the control $\mathbf{u} : [0, 1/\varepsilon] \to \omega$ defined by $\mathbf{u}(t) = \gamma(\varepsilon t)$,

$$p_1 = |\cos(\Xi(\mathbf{v}))|,\ p_2 = |\sin(\Xi(\mathbf{v}))|,$$

and $\Xi(\cdot)$ is defined according to Proposition 2.7.

Assume that we are given the desired probability distribution (p_1, p_2). To induce the transition from an eigenstate to a distributed state, we construct the control path $\mathbf{u}(\cdot)$ as follows. We define $\eta \in [0, \pi/2]$ such that $(p_1, p_2) = (\cos\eta, \sin\eta)$, and we consider a closed path $\gamma(\cdot)$ such that

- the path passes through the conical intersection $\bar{\mathbf{u}}$
- it is tangent to $\mathcal{X}_P$ in a punctured neighbourhood of $\bar{\mathbf{u}}$
- we choose $\mathbf{v}_0$ and $\mathbf{v}$ in (11) in such a way that they satisfy

$$\Xi(\mathbf{v}) = \eta.$$

Then we slow down the path $\gamma(\cdot)$ until the required precision is attained.

By applying the previous method iteratively it is not difficult to get the following controllability result.

Theorem 2.11: Consider $H(\mathbf{u}) = H_0 + u_1H_1 + u_2H_2 + u_3H_3$, where H_i are self-adjoint operators on a separable Hilbert space $\mathcal{H}$, $i = 0, \dots, 3$, where H_1, H_2, H_3 are Kato-small with respect to H_0. Let $\Sigma : \mathbf{u} \mapsto \{\lambda_0(\mathbf{u}), \dots, \lambda_k(\mathbf{u})\}$ define a separated discrete spectrum on $\omega \subset \mathbb{R}^3$ and assume that there exist conical intersections $\mathbf{u}_j \in \omega,\ j = 0, \dots, k-1$, between the eigenvalues λ_j, λ_{j+1}, with $\lambda_l(\mathbf{u}_j)$ simple if $l \neq j, j+1$. Then, for every $\mathbf{u}^0$ and $\mathbf{u}^1$ such that $\Sigma(\mathbf{u}^0)$ and $\Sigma(\mathbf{u}^1)$ are non-degenerate, for every $\bar\phi \in \{\phi_0(\mathbf{u}^0), \dots, \phi_k(\mathbf{u}^0)\}$, and $p \in [0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2 = 1$, there exist $C > 0$ and a continuous control $\gamma(\cdot) : [0,1] \to \mathbb{R}^m$ with $\gamma(0) = \mathbf{u}^0$ and $\gamma(1) = \mathbf{u}^1$, such that for every $\varepsilon > 0$

$$\|\psi(1/\varepsilon) - \sum_{j=0}^k p_j e^{i\vartheta_j}\phi_j(\mathbf{u}^1)\| \le C\varepsilon, \quad (13)$$

where $\psi(\cdot)$ is the solution of (2) with $\psi(0) = \bar\phi$, $\mathbf{u}(t) = \gamma(\varepsilon t)$, and $\vartheta_0, \dots, \vartheta_k \in \mathbb{R}$ are some phases depending on ε and γ. In particular, (2) is approximately spread controllable on Σ.

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