

# Controllability of the Schrödinger Equation via Intersection of Eigenvalues

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**Abstract**—We introduce two models of controlled infinite dimensional quantum system whose Hamiltonian operator has a purely discrete spectrum. For any couple of eigenstates we construct a path in the space of controls that approximately steers the system from one eigenstate to the other. To this purpose we use the adiabatic theory for quantum systems, and therefore the strategy requires large times.

**keywords:** Quantum Control, Controllability of PDEs, Adiabatic Theory,  $\delta$ -like Interactions

## I. INTRODUCTION

The issue of designing an efficient transfer of population between different energy levels is crucial in atomic and molecular physics (see e.g. [17]). In the experiments, excitation and ionization are often induced by means of a sequence of laser pulses. From the point of view of mathematics, the description of such processes translates into the problem of controlling the Schrödinger equation.

In recent years, such a problem has attracted increasing attention, in both communities of control theorist (see for instance [16]), and experts in quantum dynamics (see for instance [6]). Many results are available in the case that the Hilbert space of the states of the system has finite dimension (see e.g. [5], [12] and references therein). Despite that, only few controllability properties have been proven for the Schrödinger equation as a PDE (see for instance [16]) and in particular no satisfactory global controllability results are available.

In this paper we introduce two toy models and propose a method to prove approximate controllability of the Schrödinger equation. More specifically, given two arbitrary eigenstates of the uncontrolled system, we construct a path in the space of controls that steers the system from the first to the second; the target is reached only approximately, but the accuracy of the approximation can be arbitrarily improved slowing the process down and correspondingly raising its duration. Our main technical tool is the adiabatic theorem ([4], [10], [14], [19]), which requires slowly varying controls and gives explicit estimates of the error. It is worth pointing out that in order to apply our method we need a Hamiltonian with purely point spectrum that degenerates for some values of the controls. This seems to be in contradiction with the claimed use of the the adiabatic theory, which requires that during the whole time evolution the eigenvalues remain separated by a non vanishing gap (“gap condition”). The main idea is that such a difficulty can be overcome by a

decoupling between the levels other than the adiabatic one. We stress that our strategy can be applied in many situations in which classical control theory would be too difficult or cumbersome. Besides, it provides explicit expressions of controls (motion planning), and most of all is very robust, in the sense that similar controls produce similar population transfers (see for instance [8], [20]).

Let us describe our two models. The former is the simplest generalization to infinite dimension of three-level models that describe STIRAP processes (see for instance [8], [20]). As in that cases, it is given in the representation of the eigenfunction of the uncontrolled Hamiltonian, namely as an infinite dimensional matrix. The full Hamiltonian reads  $H(u, v) = H_0 + uB_1 + vB_2$ , where the drift (or “free”) Hamiltonian  $H_0$  has discrete spectrum and shows no degeneracies. The couplings  $B_1$  and  $B_2$  couple levels  $E_i$  and  $E_{i+1}$  for  $i$  even and odd, respectively. For every value of the real controls  $u$  and  $v$  the spectrum of  $H(u, v)$  remains discrete, but degeneracies can occur at isolated points in the space of the controls. This phenomenon holds generically for Hamiltonians depending on two parameters, and one refers to it as to the “conical crossing” of eigenvalues (see e.g. [9]). Assume that at time zero  $u = v = 0$  and the system lies in the ground state of the drift  $H_0$ . The adiabatic theorem asserts that, employing slow varying controls  $u(\varepsilon t)$  and  $v(\varepsilon t)$  such that for any  $t$   $H(u(\varepsilon t), v(\varepsilon t))$  has no degeneracies, then at time  $t$  the system lies close to the ground state of  $H(u(\varepsilon t), v(\varepsilon t))$ . As widely known, the situation becomes more complicated when the system is driven near eigenvalue intersections. Nevertheless, we exhibit paths in the control space that pass exactly through an eigenvalue intersection and force the system to perform a transition from the old to a new level. As we explain later, to this task we need to move controls along a surface, so we must have at our disposal at least two controls.

The second model consists of the Schrödinger picture of a quantum particle in a one-dimensional infinite potential well with some additional controlled external fields. Here, the main obstacle to be overcome is that in a one dimensional quantum system the presence of degeneracies in the discrete spectrum is a highly nonstandard feature. In particular the non degeneracy of the ground state holds in any dimension for systems subject to a locally integrable potential ([13]). Therefore our strategy consists in producing degeneracies by means of potentials with non integrable singularities. To this

purpose we use point interaction potentials (Dirac's  $\delta$  and  $\delta'$ ) with a possibly infinite strength.

We consider a particle confined to the interval  $(-\pi/2, \pi/2)$ , whose Hamiltonian reads

$$H(u, v, w) := -\partial_x^2 + u\delta(x - \pi/2) + v\delta'(x - \pi/2) + w\theta(x - \pi/2) \quad (1)$$

where  $\theta$  denotes the Heaviside function, and take  $H(0, 0, 0) = -\partial_x^2$  as the drift Hamiltonian. In contrast with the previous model, here we exploit an intersection obtained letting the control  $u$  and  $v$  diverge. We highlight that, though not proven in the present paper, our schema can be generalized for any symmetric (coercive) potential replacing the infinite well. It is worth mentioning that, unlike the first toy model, in this case it seems extremely difficult to prove that it is possible to steer the system from two eigenstates using classical control theory.

### A. Definitions of Controllability

Let us introduce the notions of controllability that we need in the following.

**Definition 1.1:** Consider a quantum mechanical system whose evolution is described by a self adjoint Hamiltonian depending on  $m$  real parameters in the form  $H(u_1, \dots, u_m) = H_0 + u_1 B_1 + \dots + u_m B_m$ . Assume that for every value of the parameters  $u_1, \dots, u_m$  the spectrum of  $H(u_1, \dots, u_m)$  is discrete. Assume moreover that the drift Hamiltonian  $H_0 = H(0, \dots, 0)$  has a discrete, non degenerate spectrum  $E_0 < E_1 < E_2 < \dots$ , being  $\Phi_0, \Phi_1, \Phi_2, \dots$  the corresponding eigenvectors. We say that such a system is:

- finite-time state to state controllable (f-SSC for short) in the class  $\mathcal{K}$  if for every  $j, l \in \mathbb{N}$  there exist open loop controls  $u_1(\cdot), \dots, u_m(\cdot) \in \mathcal{K}$  steering the system from  $\Phi_j$  to  $\Phi_l$  in finite time  $T(j, l)$ .
- approximately state to state controllable (a-SSC for short) in the class  $\mathcal{K}$ , if for every  $j, l \in \mathbb{N}$  and  $\varepsilon > 0$  there exists a time  $T(j, l, \varepsilon)$  and open loop controls  $u_1(\cdot), \dots, u_m(\cdot) \in \mathcal{K}$ , steering the system from  $\Phi_j$  to a state  $\Phi_{app}$  arbitrarily close to the space spanned by  $\Phi_l$ . Namely, there exists  $\varphi \in [0, 2\pi[$  such that

$$\|e^{-i\varphi} \Phi_{app} - \Phi_l\|_{L^2} \leq \varepsilon. \quad (2)$$

### B. The Adiabatic Theorem

Roughly speaking, the adiabatic theorem states that the eigenvectors are approximately preserved by time evolution provided that the time-dependence of the Hamiltonian is suitably slow. More precisely, let  $H(\varepsilon t)$  be a slowly time-dependent Hamiltonian with purely discrete spectrum,  $\lambda_j(\varepsilon t)$  its  $j^{\text{th}}$  eigenvalue and  $P_j(\varepsilon t)$  the orthogonal projection on the space  $\mathcal{H}_j(\varepsilon t)$  of the eigenvectors associated to  $\lambda_j(\varepsilon t)$ . Clearly, the time evolution  $U_\varepsilon(t, s)$  generated by  $H(\varepsilon t)$  preserves  $\mathcal{H}_j(\varepsilon t)$  if and only if it fulfils the following intertwining property (see [19] and references therein)

$$P_j(\varepsilon t)U_\varepsilon(t, s) = U_\varepsilon(t, s)P_j(\varepsilon s). \quad (3)$$

Since  $\frac{d}{dt}(U_\varepsilon(s, t)P_j(\varepsilon t)U_\varepsilon(t, s)) = \varepsilon U_\varepsilon(s, t)\dot{P}_j(\varepsilon t)U_\varepsilon(t, s)$ , where the dot denotes the derivative w.r.t.  $t$ , then relation (3) is satisfied at the zero.th order in  $\varepsilon$  only. In fact, (3) is exactly satisfied by the evolution  $U_a^\varepsilon(t, s)$  generated by the so-called ‘‘adiabatic Hamiltonian’’ associated to the  $j^{\text{th}}$  level, that reads

$$H_a(\varepsilon t) := H(\varepsilon t) - 2i\varepsilon P_j(\varepsilon t)\dot{P}_j(\varepsilon t) + i\varepsilon \dot{P}_j(\varepsilon t) \quad (4)$$

The adiabatic theorem estimates the difference between the time evolutions  $U_\varepsilon$  and  $U_a^\varepsilon$ .

**Theorem 1.2:** Consider a family  $H(t)$  of self adjoint operators on a Hilbert space  $\mathcal{H}$ , with  $t$  in the possibly unbounded interval  $(t_1, t_2)$ . Suppose that:

- 1) all  $H(t)$ 's have a common dense domain  $\mathcal{D}$ .
- 2)  $H(\cdot) \in \mathcal{C}_b^2((t_1, t_2), \mathcal{L}(\mathcal{D}, \mathcal{H}))$ , where  $\mathcal{L}(\mathcal{D}, \mathcal{H})$  denotes the space of bounded linear operators from  $\mathcal{D}$  to  $\mathcal{H}$  provided that  $\mathcal{D}$  is endowed with the norm of the graph of  $H(t_1)$ :

$$\|T\|_{\mathcal{L}(\mathcal{D}, \mathcal{H})} := \sup_{v \in \mathcal{D} \setminus \{0\}} \frac{\|Tv\|_{\mathcal{H}}}{\|v\|_{\mathcal{H}} + \|H(t_1)v\|_{\mathcal{H}}}$$

- 3) for every  $t$ , the spectrum  $\sigma(H(t))$  of  $H(t)$  is discrete and non degenerate, i.e.  $\sigma(H(t)) = \{\lambda_j(t), j = 0, \dots, n, \dots, \lambda_i(t) < \lambda_k(t) \text{ if } i < k\}$ .
- 4) Fixed  $j \in \mathbb{N}$ , the following gap condition is satisfied:
$$g := \inf_{t \in (t_1, t_2)} \min(\lambda_{j+1}(t) - \lambda_j(t), \lambda_j(t) - \lambda_{j-1}(t)) > 0$$

Let  $U_\varepsilon$  and  $U_a^\varepsilon$  be the two-parameter propagators generated by  $H(\varepsilon t)$  and  $H_a(\varepsilon t)$  defined in (4) respectively. Then, for any  $t$  and  $t_0$  in  $(t_1, t_2)$ ,

$$\|U_\varepsilon(t, t_0) - U_a^\varepsilon(t, t_0)\| < C\varepsilon(1 + \varepsilon|t - t_0|) \quad (5)$$

where the constant  $C$  depends on  $g$  and possibly diverges as  $g$  vanishes.

Notice that if at time  $t_0$  the system lies in an eigenstate of  $H(\varepsilon t_0)$  associated to the eigenvalue  $\lambda_j(t_0)$ , then estimate (5) gives

$$\|\psi_\varepsilon(t) - \psi_a^\varepsilon(t)\| < C\varepsilon(1 + \varepsilon|t - t_0|) \quad (6)$$

where  $\psi_\varepsilon(t)$  represents the actual state of the system and  $\psi_a^\varepsilon(t)$  is eigenvector of  $H(\varepsilon t)$  relative to the eigenvalue  $\lambda_j(\varepsilon t)$ . Furthermore, if the  $j^{\text{th}}$  level of  $H(t)$  is non degenerate at any time  $t$ , and  $\Phi_j(t)$  is the associated eigenvector, then  $H_a(\varepsilon t)\Phi_j(\varepsilon t) = \lambda_j(\varepsilon t)\Phi_j(\varepsilon t) - i\varepsilon \dot{P}_j(\varepsilon t)\Phi_j(\varepsilon t)$  and

$$U_a^\varepsilon(t, t_0)\Phi_j(\varepsilon t_0) = \exp\left(-i \int_0^t ds \lambda_j(\varepsilon s)\right) \Phi_j(\varepsilon t). \quad (7)$$

The paper is organized as follows. In Section II we present the first toy model. After studying the spectrum of the Hamiltonian, we introduce the concept of climbing path and prove that the adiabatic theorem can be applied to climbing paths even if the gap condition is not satisfied (see Theorem 2.5). As a corollary we get that the system is a-SSC (see Corollary 2.6). In Section III, we present the second model. In this case, using locally non integrable controlled potentials, we prove that the system is a-SSC (see Theorem 3.2).

## II. AN INFINITE DIMENSIONAL TOY MODEL

### The model and the spectrum of the Hamiltonian.

Let us consider an infinite dimensional quantum system endowed with a purely discrete spectrum and suppose that its energy levels are non degenerate. Let  $E_j$  be the energy of the  $j$ .th level with  $E_j < E_k$  for  $j < k$  and let  $E_0$  be the energy of the ground state. In the basis of the eigenstates of the energy, the Hamiltonian is represented by an infinite diagonal matrix, whose  $j^{\text{th}}$  element equals  $E_j$ . In the following we refer to this Hamiltonian as to the drift or free Hamiltonian. We have at our disposal two real controls  $u$  and  $v$  that couple energy levels by pairs in such a way that the infinite matrix representing the controlled Hamiltonian reads

$$H(u, v) = \begin{pmatrix} E_0 & \alpha_0 u & 0 & 0 & 0 & \cdots \\ \alpha_0 u & E_1 & \beta_0 v & 0 & 0 & \cdots \\ 0 & \beta_0 v & E_2 & \alpha_1 u & 0 & \cdots \\ 0 & 0 & \alpha_1 u & E_3 & \beta_1 v & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (8)$$

Here the coefficients  $\alpha_j$ 's and  $\beta_j$ 's (that we assume to be greater than zero) implement the fact that different pairs of levels react in different manners to the presence of the external fields. The matrix (8) defines a linear operator  $\hat{H}(u, v)$  acting on the Hilbert space  $\ell^2$  of all complex sequences  $\{x_j\}$  such that  $\sum_{j=0}^{\infty} |x_j|^2 < \infty$ . Moreover, for technical reasons we assume that the sequence of the  $E_j$ 's diverges, and the quantities  $\alpha_j/|E_{2j}|^\mu$  and  $\beta_j/|E_{2j}|^\mu$  vanish as  $j$  goes to infinity for some  $0 < \mu < 1$ . These hypotheses yield some remarkable consequences in terms of spectral properties of  $\hat{H}(u, v)$ , namely:

**Proposition 2.1:** *Under the hypotheses previously stated on the coefficients  $E_j, \alpha_j, \beta_j$ , the operator  $H(u, v)$  defined in (8) and acting on  $\ell^2$ , satisfies the following:*

- (i)  $\hat{H}(u, v)$  is self-adjoint.
- (ii) The spectrum of  $\hat{H}(u, v)$  is purely discrete.
- (iii) If both  $u$  and  $v$  are different from zero, then all eigenvalues are non degenerate.
- (iv) The spectrum of  $\hat{H}(u, v)$  is equal to the spectrum of  $\hat{H}(|u|, |v|)$ .

Owing to (i), (ii) and (iii) and using perturbation theory [11], one can prove that there exists a unique countable set of continuous functions  $\lambda_j : \mathbb{R}^2 \rightarrow \mathbb{R}$  such that

- A.  $\lambda_j(u, v)$  is an eigenvalue of  $\hat{H}(u, v)$ .
- B.  $\lambda_j(u, v) \leq \lambda_{j+1}(u, v)$  for any  $j \in \mathbb{N}$ ,  $u, v \in \mathbb{R}$  and  $\lambda_j(u, v) < \lambda_{j+1}(u, v)$  for any  $j \in \mathbb{N}$ ,  $u, v > 0$ .

Roughly speaking, the graph of the spectrum of  $\hat{H}(u, v)$  as a multi-valued function of  $u$  and  $v$  can be represented as a countable family of regular surfaces possibly intersecting along the axes  $u = 0$  and  $v = 0$  only. In order to steer the system from two fixed eigenstates using adiabatic theory, it is essential to classify all possible eigenvalues intersections.

### Intersections along the axis $u = 0$ .

The matrix  $H(0, v)$  is block diagonal. The first block is  $1 \times 1$  and consists of the element  $E_0$ , while the others are  $2 \times 2$

and take the form:

$$\mathbf{B}_j := \begin{pmatrix} E_{2j+1} & \beta_j v \\ \beta_j v & E_{2j+2} \end{pmatrix}, \quad j = 0, 1, 2, \dots \quad (9)$$

The eigenvalues of  $\mathbf{B}_j$  are given by

$$\begin{cases} \Lambda_j^+(v) = E_{2j+2} + \Delta_j \\ \Lambda_j^-(v) = E_{2j+1} - \Delta_j \end{cases} \quad (10)$$

where the quantity  $\Delta_j := \frac{\sqrt{\omega_j^2 + 4\beta_j^2 v^2}}{2} - \omega_j$  with  $\omega_j := E_{2j+2} - E_{2j+1}$  represents the exchange of energy induced by the coupling between the two levels. Notice that turning the presence of the control  $v$  enhances the energy gap between two coupled levels, as shown in Fig.1.

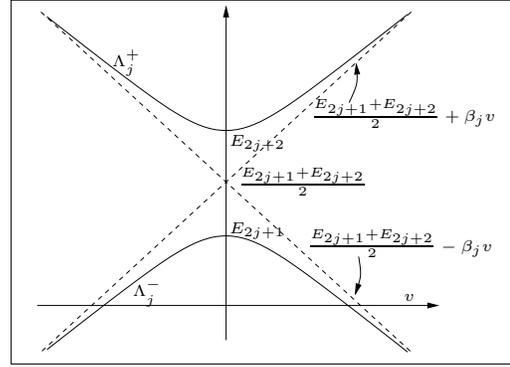


Figure 1

Equalities (10) provide some simple rules in order to classify all crossing of eigenvalues. Set  $\Lambda_{-1}^+ := E_0$  and  $\beta_{-1} := 0$ . Consider a pair of indices  $j$  and  $k$ , with  $j > k$ . Then

- There exists a unique  $v > 0$  such that  $\Lambda_j^+(v) = \Lambda_k^-(v)$ . Conversely, the equation  $\Lambda_j^-(v) = \Lambda_k^+(v)$  has no solutions.
- If  $\beta_j < \beta_k$ , then there exists a unique  $v > 0$  such that  $\Lambda_j^+(v) = \Lambda_k^+(v)$ . Conversely, if  $\beta_j \geq \beta_k$  then the graphs of the functions  $\Lambda_j^+$  and  $\Lambda_k^+$  do not intersect each other.
- If  $\beta_j > \beta_k$ , then there exists a unique  $v > 0$  such that  $\Lambda_j^-(v) = \Lambda_k^-(v)$ . Conversely, if  $\beta_j \leq \beta_k$  then the graphs of the functions  $\Lambda_j^-$  and  $\Lambda_k^-$  do not intersect.

### Intersections along the axis $v = 0$ .

The matrix  $H(u, 0)$  is block diagonal, each block being  $2 \times 2$  and taking the form:

$$\mathbf{A}_j := \begin{pmatrix} E_{2j} & \alpha_j u \\ \alpha_j u & E_{2j+1} \end{pmatrix}, \quad j = 0, 1, 2, \dots$$

The eigenvalues of  $\mathbf{A}_j$  are given by

$$\Gamma_j^-(u) = E_{2j} - D_j, \quad \Gamma_j^+(u) = E_{2j+1} + D_j \quad (11)$$

with  $D_j := \frac{\sqrt{\Omega_j^2 + 4\alpha_j^2 u^2}}{2} - \Omega_j$  and  $\Omega_j := E_{2j+1} - E_{2j}$ . Like in the previous case, a complete classification of the eigenvalue intersections can be done.

**Remark 2.2:** *We want to prevent the reader from identifying functions  $\Lambda_j$ 's and  $\Gamma_j$ 's with the  $\lambda_k$ 's, even for suitable values of  $k$  (for instance,  $\Lambda_j^+(u)$  with  $\lambda_{2j+2}$ ). Such identification is correct if the controls are smaller than the lowest value for which a degeneracy occurs. This is due to*

the fact that the  $\lambda_i$ 's satisfy  $\lambda_i(u, v) \leq \lambda_j(u, v)$ , for  $i < j$  and for every  $(u, v) \in \mathbf{R}^2$ , while the graphs of the functions  $\Lambda_j$ 's (resp. the  $\Gamma_j$ 's) can cross each other.

The results of this Section can be resumed as follows.

**Theorem 2.3:** *The set*

$\mathcal{S} := \{(u, v, p) \text{ s.t. } u, v \in \mathbf{R}, p \text{ eigenvalue of } \hat{H}(u, v)\}$  (12) is the union of the graphs of a countable, increasing family of continuous functions  $\lambda_j(u, v)$ , i.e.  $\mathcal{S} = \cup_{j=0}^{\infty} \mathcal{S}_j$  and  $\mathcal{S}_j = \{(u, v, \lambda_j(u, v)) \text{ s.t. } u, v \in \mathbf{R}\}$ . Such graphs intersect one another in a countable set lying in the union of the planes  $u = 0$  and  $v = 0$ . Apart from that points, they are smooth.

Fig. 3 gives an idea of the shape of the three first surfaces belonging to  $\mathcal{S}$ , for some value of the parameters  $E_i$ ,  $\alpha_i$ , and  $\beta_i$ , which could be useful to figure out how to employ the adiabatic theory (see below).

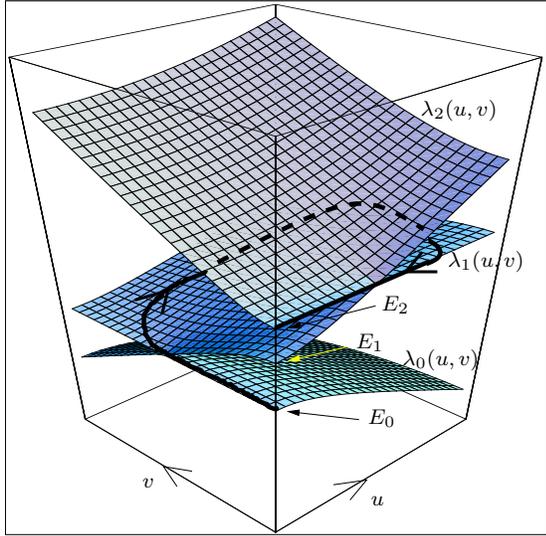


Figure 3

### Controllability via Adiabatic Theory

The Schrödinger equation for the Hamiltonian (8) reads

$$i \frac{d\psi(t)}{dt} = H(u(t), v(t))\psi(t) \quad (13)$$

where  $\psi(t) = (\psi_0(t), \psi_1(t), \dots)$  is a vector in  $\ell^2$ . Before illustrating how to apply the adiabatic theory, let us mention that the controllability of (13) is already known, since if  $u = 0$  or  $v = 0$ , then the variables  $\psi_i$  are coupled by pairs only. Therefore, using standard techniques of control theory on  $SU(2)$ , one can prove f-SSC. In the following we prove a-SSF for (13) by using adiabatic theory. Once chosen a  $C^2$  path  $(u(t), v(t))$  in  $\mathbf{R}^2$ , the operator  $H(u(t), v(t))$  belongs to  $\mathcal{C}_b^2((t_1, t_2), \mathcal{L}(\mathcal{D}, \mathcal{H}))$  and one can apply Theorem 1.2. Since the constant  $C$  supplied by the adiabatic theorem (cfr. formula (5)) diverges as the gap vanishes, then the approximation we get in (2) is as good as the path  $(u(\varepsilon t), v(\varepsilon t))$  stays far from the singularities.

Consider the set  $\mathcal{S}$  defined in (12). A point  $(u, v, p) \in \mathcal{S}$  is called a singularity if  $p = \lambda_i(u, v) = \lambda_j(u, v)$  with  $i \neq j$ . From the analysis preceding theorem (2.3), it follows that the singularities are isolated points and if  $(u, v, p)$  is a singularity then  $uv = 0$ . We denote by  $\mathcal{Z}$  the set of all singularities.

**Definition 2.4:** Consider a map  $\gamma(\cdot) := (u(\cdot), v(\cdot), p(\cdot)) : [0, \tau] \rightarrow \mathcal{S} \subset \mathbf{R}^3$ . We say that this map is a climbing path if:

- it is a  $C^2$  map from  $[0, \tau]$  to  $\mathbf{R}^3$ ;
- $\gamma(0) = (u(0), v(0), p(0)) = (0, 0, E_A)$  and  $\gamma(\tau) = (u(\tau), v(\tau), p(\tau)) = (0, 0, E_B)$  for some  $A, B \in \mathbf{N}$ ;
- it passes through a finite number of singularities. i.e.  $\text{Supp}(\gamma) \cap \mathcal{Z}$  is finite.
- if  $\tau_1, \dots, \tau_n$  are the values of the parameter at which the singularities are met, namely  $\gamma(\tau_i) \in \mathcal{Z}$  for any  $i$ , then there exist intervals  $[a_i, b_i]$  such that  $\tau_i \in ]a_i, b_i[$  and  $u$  or  $v$  constantly vanishes on  $[a_i, b_i]$ .

An example of climbing path is represented in Fig. 3. If a climbing path is slowly gone along, then we can apply the adiabatic theorem and obtain the following result:

**Theorem 2.5:** Consider the family of Hamiltonians  $H(u, v)$  and a climbing path  $\gamma$  on the set  $\mathcal{S}$  defined in (12). Given  $\varepsilon \ll 1$  consider the following parametrization of  $\gamma$ :  $\gamma(\varepsilon t) = (u(\varepsilon t), v(\varepsilon t), p(\varepsilon t))$ , with  $t \in [0, T]$  and  $T := \varepsilon^{-1}\tau$ . Let  $\Phi_j(u, v)$  be the eigenvector corresponding to the eigenvalue  $\lambda_j(u, v)$ . Let  $t_1, \dots, t_n$  be the times at which the singularities are met, namely  $\gamma(\varepsilon t_i) \in \mathcal{Z}$  for any  $i$ . Let  $j_i$  be defined by  $p(\varepsilon t) = \lambda_{j_i}(u(\varepsilon t), v(\varepsilon t))$ ,  $t \in ]t_i, t_{i+1}[$ . Then, for every  $t \in ]t_i, t_{i+1}[$ , we have

$$\left\| \exp \left( i \int_0^{\varepsilon t} ds \lambda_{j_i}(u(s), v(s)) \right) \Phi_{j_i}(u(\varepsilon t), v(\varepsilon t)) - \psi(\varepsilon t) \right\| < C\varepsilon(1 + \varepsilon|t|) \leq C\varepsilon(1 + \tau)$$

where  $\psi(t)$  is the solution of the Schrödinger equation  $i\partial_t \psi(t) = H(u(\varepsilon t), v(\varepsilon t))\psi(t)$  with initial data  $\psi(0) = \Phi_{j_i}(0, 0)$ .

Roughly speaking this theorem states that if the singularities are crossed keeping to zero one of the two controls, then the adiabatic theorem holds true and the system jumps at the singularities from a level to another one. Notice that estimate given in theorem 2.5 holds for  $t = T = \varepsilon^{-1}\tau$  also, with the system passed to the level of energy  $E_B$ . Therefore, we have the following

**Corollary 2.6:** The quantum mechanical system described by the Hamiltonian (8) is a-SSC in the class  $\mathcal{C}_b^2$ .

**Remark 2.7:** We conjecture that the result given by Theorem 2.5, can be generalized to any Hamiltonian having conical intersections. (see for instance [9]).

### III. CONTROLLABILITY VIA SINGULAR POTENTIALS

Consider the evolution problem given on the space  $L^2(0, \pi)$  by

$$\begin{aligned} i\partial_t \psi(x, t) &= H(u(\varepsilon t), v(\varepsilon t), w(\varepsilon t))\psi(x, t), \text{ where} \\ H(u, v, w) &:= -\partial_x^2 + u\delta(x - \pi/2) + v\delta'(x - \pi/2) \\ &\quad + w\theta(x - \pi/2). \end{aligned} \quad (14)$$

Here  $\partial_x^2$  is the second partial derivative w.r.t.  $x$  with Dirichlet boundary conditions (i.e.  $\psi(0, t) = \psi(\pi, t) = 0$ ). The term  $u(\varepsilon t)\delta(x - \pi/2)$  is a Dirac's delta potential whose effect results in the boundary condition

$$\lim_{x \rightarrow \frac{\pi}{2}^+} \partial_x \psi(x, t) - \lim_{x \rightarrow \frac{\pi}{2}^-} \partial_x \psi(x, t) = u(\varepsilon t)\psi(\pi/2, t). \quad (15)$$

Analogously, the term  $v(\varepsilon t)\delta'(x - \pi/2)$  corresponds to the boundary conditions

$$A(t) := \lim_{x \rightarrow \frac{\pi}{2}^-} \partial_x \psi(x, t) = \lim_{x \rightarrow \frac{\pi}{2}^+} \partial_x \psi(x, t) \quad (16)$$

$$\lim_{x \rightarrow \frac{\pi}{2}^+} \psi(x, t) - \lim_{x \rightarrow \frac{\pi}{2}^-} \psi(x, t) = v(\varepsilon t) A(t) \quad (17)$$

Finally, the symbol  $\theta(x - \pi/2)$  denotes the Heaviside function which equals 1 for  $x \geq \pi/2$  and 0 otherwise.

It is well known that the drift Hamiltonian  $H_0 = -\partial_x^2$ , with Dirichlet boundary conditions, is a self-adjoint operator whose spectrum is purely discrete and reads  $E_n = (n + 1)^2$ ,  $n = 0, 1, 2, \dots$ . All levels are non degenerate and the corresponding normalized eigenvectors are  $\phi_n(x) = \sqrt{\frac{2}{\pi}} \sin((n + 1)x)$ . As in the previous model, we control the system switching  $u$  and  $v$  separately on. Therefore we must study the spectra of the operators  $H(u, 0, 0)$  and  $H(0, v, 0)$ .

**The spectra of  $H(u, 0, 0)$  and  $H(0, v, 0)$ .**

The eigenvalues  $F_n(u)$  and the eigenvectors  $\xi_n^u$  satisfy the stationary Schrödinger equation with the boundary condition given by the delta potential, namely

$$\begin{aligned} -\frac{d^2}{dx^2} \xi_n^u(x) &= F_n(u) \xi_n^u(x), \quad x \in (0, \pi/2) \cup (\pi/2, \pi) \\ \xi_n^u(0) &= \xi_n^u(\pi) = 0, \\ \lim_{x \rightarrow \frac{\pi}{2}^+} \frac{d}{dx} \xi_n^u(x) - \lim_{x \rightarrow \frac{\pi}{2}^-} \frac{d}{dx} \xi_n^u(x) &= u \xi_n^u(\pi/2). \end{aligned} \quad (18)$$

Notice that for  $n$  odd one has  $\xi_n^u(\pi/2) = 0$ , thus equations (18) reduce to the equations for the odd levels of the drift Hamiltonian. Therefore, for any  $k \in \mathbf{N}$ ,

$$\begin{aligned} F_{2k+1}(u) &= E_{2k+1} = 4(k + 1)^2, \\ \xi_{2k+1}^u(x) &= \phi_{2k+1}(x) = \sqrt{\frac{2}{\pi}} \sin[2(k + 1)x]. \end{aligned} \quad (19)$$

If  $n$  is even then the condition induced by the delta is effective and reads

$$\{F_{2k}(u), k \in \mathbf{N}\} = \{z^2, \tan(\pi/2 z) = -2zu^{-1}\},$$

$$\begin{aligned} \xi_{2k}^u(x) &= N \left[ \cos(\sqrt{F_{2k}(u)}(x - \pi/2)) \right. \\ &\left. + \frac{u}{2\sqrt{F_{2k}(u)}} \sin(\sqrt{F_{2k}(u)}|x - \pi/2|) \right]. \end{aligned} \quad (20)$$

where  $N$  is a normalization factor. As one can expect, the presence of a  $\delta$  interaction does not affect the subspace of the even functions. Moreover, it appears from identity (20) that such potential produces a discontinuity in the first derivative of  $\xi_{2k}^u$ , embodied in the second term at the r.h.s. Obviously, such term overwhelms the first one as  $u$  grows. We stress that  $H(\infty, 0, 0)$  is still a well defined self-adjoint Hamiltonian. It translates into the condition  $\psi(t, \pi/2) = 0$ , to be satisfied at any time  $t$ . The related eigenvalue problem reads

$$-\frac{d^2}{dx^2} \xi_n^\infty(x) = F_n(\infty) \xi_n^\infty(x), \quad x \in (0, \pi/2) \cup (\pi/2, \pi),$$

$$\xi_n^\infty(0) = \xi_n^\infty(\pi/2) = \xi_n^\infty(\pi) = 0. \quad (21)$$

Notice that the boundary condition (21) splits the problem into two independent parts associated to the intervals  $(0, \pi/2)$  and  $(\pi/2, \pi)$ . The physical picture related to this

condition corresponds to an infinite potential barrier located at the point  $\pi/2$ . In such a way the non degeneracy for the ground state (as far as for the other levels) is broken. In such a case the eigenfunction associate to the  $n^{\text{th}}$  eigenvalue  $F_n(\infty) = 4(n + 1)^2$  reads

$$\xi_n^\infty(\alpha, \beta; x) = [\alpha \chi_{[0, \pi/2]}(x) + \beta \chi_{[\pi/2, \pi]}(x)] \sin(2nx), \quad (22)$$

with  $\alpha^2 + \beta^2 = 4/\pi$ . The eigenvalues  $G_n(v)$  and the eigenvectors  $\eta_n^v$  of  $H(0, v, 0)$  fulfil the system

$$\begin{aligned} -\frac{d^2}{dx^2} \eta_n^v(x) &= G_n(v) \eta_n^v(x), \quad x \in (0, \pi/2) \cup (\pi/2, \pi), \\ \eta_n^v(0) &= \eta_n^v(\pi) = 0, \end{aligned} \quad (23)$$

$$\begin{aligned} \lim_{x \rightarrow \frac{\pi}{2}^+} \frac{d}{dx} \eta_n^v(x) &= \lim_{x \rightarrow \frac{\pi}{2}^-} \frac{d}{dx} \eta_n^v(x) =: A, \\ \lim_{x \rightarrow \frac{\pi}{2}^+} \eta_n^v(x) - \lim_{x \rightarrow \frac{\pi}{2}^-} \eta_n^v(x) &= vA. \end{aligned}$$

Notice that the even levels of the drift Hamiltonian are preserved, i.e.

$$\begin{aligned} G_{2k}(v) &= E_{2k} = (2k + 1)^2, \\ \eta_{2k}^v(x) &= \phi_{2k}(x) = \sqrt{\frac{2}{\pi}} \sin[(2k + 1)x]. \end{aligned} \quad (24)$$

If  $n$  is odd then the condition induced by the delta prime is effective and reads

$$\begin{aligned} \{G_{2k+1}(v), k \in \mathbf{N}\} &= \{z^2, \tan(\pi/2 z) = -zv/2\}, \\ \eta_{2k+1}^v(x) &= N \left[ \sin(\sqrt{G_{2k+1}(v)}(x - \pi/2)) \right. \\ &\left. + \text{sgn}(x - \pi/2) \frac{v\sqrt{G_{2k+1}(u)}}{2} \right. \\ &\left. \cos(\sqrt{G_{2k+1}(v)}|x - \pi/2|) \right]. \end{aligned} \quad (25)$$

where  $N$  is a normalization factor. Notice that the delta prime interaction gives rise to a discontinuity at the point  $x = \pi/2$ . Again, the Hamiltonian  $H(0, \infty, 0)$  is well defined and imposes the condition  $\frac{d}{dx} \psi(t, \pi/2) = 0$ , to be satisfied at any time  $t$ . The related eigenvalue problem reads

$$-\frac{d^2}{dx^2} \eta_n^\infty(x) = G_n(v) \eta_n^\infty(x), \quad x \in (0, \pi/2) \cup (\pi/2, \pi),$$

$$\begin{aligned} \eta_n^\infty(0) &= \eta_n^\infty(\pi) = 0, \\ \frac{d}{dx} \eta_n^\infty(\pi/2) &= 0. \end{aligned} \quad (26)$$

The problem splits in two free (i.e. without potential) problems with mixed boundary conditions: Dirichlet in one boundary point, Neumann in the other. The solution reads  $\eta_n^\infty(\gamma, \sigma; x) = [\gamma \chi_{[0, \pi/2]}(x) + \sigma \chi_{[\pi/2, \pi]}(x)] \sin(2nx)$ , with  $\gamma^2 + \sigma^2 = 4/\pi$ .

### Application of the adiabatic theory

Our strategy can be resumed in the following three steps.

#### First step.

At time zero the controls are not active and the system lies in the ground state  $\psi(0) := \phi_0$ . We choose a continuous, increasing, non negative, unbounded function  $u$  and switch a delta interaction with strength  $u(\varepsilon t)$  on. We consider the

splitting of the Hilbert space  $L^2(0, \pi)$  into “even” and “odd” components  $\mathcal{H}_e$  and  $\mathcal{H}_o$  where

$$\begin{aligned}\mathcal{H}_e &= \{\psi \in L^2(0, \pi), \quad \psi(x) = \psi(\pi - x)\} \\ \mathcal{H}_o &= \{\psi \in L^2(0, \pi), \quad \psi(x) = -\psi(\pi - x)\}\end{aligned}$$

and notice that on  $\mathcal{H}_o$  the evolution is free. Moreover, due to invariance of the Dirac’s delta interaction under parity w.r.t.  $x = \pi/2$ ,  $\psi(t)$  belongs at any time to  $\mathcal{H}_e$ , and we can restrict ourselves to consider the time evolution in such space. Here there are no crossings of eigenvalues, so the spectral gap up to a time  $T$  can be computed as  $g(T) := \sup_{0 \leq t \leq T} (F_2(u(\varepsilon t)) - F_0(u(\varepsilon t))) \geq E_2 - F_0(\infty) \geq 5$

**Remark 3.1:** The domain of  $H(u(\varepsilon t), 0, 0)$  involves the boundary conditions (15) and hence is time dependent. It follows that one cannot apply the adiabatic Theorem 1.2 directly since hypothesis 1) is not fulfilled. However one can prove that the conclusions of the adiabatic Theorem 1.2 holds also in our case. To this purpose, one has first to show that the Schrödinger equation  $i\partial_t \psi(x, t) = H(u(\varepsilon t), 0, 0)\psi(x, t)$ , has a strong solution. This can be done using an argument similar to those of [18]. Afterwards a version of the adiabatic theorem adapted to the presence of a  $\delta$ -like potential can be carried out.

Therefore, applying such result to the time evolution of  $\mathcal{H}_e$ , we obtain

$$\begin{aligned}\left\| \exp\left(-i \int_0^{\varepsilon t} ds F_0(u(s))\right) \xi_0^{u(\varepsilon t)} - \psi(t) \right\| \\ < C\varepsilon(1 + \varepsilon|t|)\end{aligned}\quad (27)$$

where  $C$  is a constant not depending on  $T$ .

Formula (27) cannot be naively extended to infinite time, for which  $y = \infty$ , since the adiabatic theorem ceases to hold. Therefore we stop at a conveniently large time  $T_1 = \varepsilon^{-1}\tau_1$ . Notice that the reached energy depends on the product  $\tau_1$  only, therefore it is important to fix such a value as the “target” for this first step. Once fixed it, observe that the more  $\varepsilon$  is small (and consequently  $T_1$  is large), the more the error in replacing the true evolution  $\psi(t)$  with  $\xi_0^{u(\varepsilon t)}$  is small, vanishing in the limit  $\varepsilon \rightarrow 0$ .

*Second step.*

As a second step, we put  $u(t) = \infty$  for  $\varepsilon^{-1}T_1 \leq t \leq T_2$  and approximate the true wave function with the unique even eigenfunction of the ground state of  $H(\infty, 0, 0)$ , which is obtained from definition (22) putting  $\alpha = 1$  and  $\beta = -1$ , namely  $\xi_0^\infty(1, -1, x) = \sqrt{\frac{2}{\pi}}|\sin(2x)|$ . It is easily seen that the error done in replacing the true evolution with  $\xi_0^\infty(1, -1, \cdot)$  can be arbitrarily reduced if we choose a suitably small  $\varepsilon$  and a suitably large  $\varepsilon T_1$ .

*Third step.*

Finally we introduce the Heaviside potential endowed with the control  $w$  as coupling constant. The role of such potential is to turn the wave function, which is still even, to an odd one, turning its component in  $[0, \pi/2]$  upside down. This is easily carried out by letting the control  $u$  fixed at  $\infty$  and setting  $w(t) = 4$ ,  $t \in [T_2, T_2 + \pi/4]$  and turn it off outside such interval. To see that, one has to remember

that the evolution in  $[0, \pi/2]$  is decoupled from the one in  $[\pi/2, \pi]$ , and that in the first half interval such evolution is given by the multiplication by the phase factor  $e^{i4t}$  while in the second it is given by the multiplication by the phase factor  $e^{i8t}$ . In a time interval lasting  $\pi/4$ , in the first half interval a half period is accomplished, while in the second the system performs a complete period. Notice that this step does not increase the error in the estimates. Now, turning all controls off, we have reached the first excited level for the drift Hamiltonian. Following the same strategy, one can jump at any energy level. In particular, to reach an odd level one uses delta interaction, to reach an even one one uses the delta prime. As a consequence we have the following:

**Theorem 3.2:** *Let  $\mathcal{K}$  be the class of piecewise continuous functions from  $\mathbf{R}$  to  $[0, \infty]$ . The quantum mechanical system described by the Hamiltonian (14) is a-SSC in the class  $\mathcal{K}$ .*

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