On the control of quantum oscillators

Pierre Rouchon *

Technical report A/320 Centre Automatique et Systèmes Ecole des Mines de Paris 30 June 2002

We consider, as in [3], a quantum system described by the following Schrödinger equation

$$i\hbar\dot{\psi} = (H_0 + uH_1)\psi$$

where ψ is the complex probability amplitude vector (belongs to an Hilbet space of finite or infinite dimension), H_0 is the free Hamiltonian and H_1 is the Hamiltonian associated to the scalar control u (corresponding to a classical electro-magnetic field). We discuss here the controllability and/or the following motion planning problem: for two pure states, ψ_a and ψ_b of free energy E_b and E_b ($H_0\psi_a = E_a\psi_a$ and $H_0\psi_b = E_b\psi_b$), find an open-loop control $[0,T] \ni t \mapsto$ u(t) steering the state ψ form ψ_a at t = 0 to the state ψ_b at t = T > 0. It seems that according to [10], such motion planning problem is meaning full. In this report, we consider several Hamiltonian H_0 and H_1 :

- The 1D harmonic oscillator where $\psi(q,t)$ is an L^2 complex function of $q \in \mathbb{R}$ the space position, $H_0 = p^2/2 + q^2/2$ and $H_1 = -q$. p corresponds to the operator $i/\hbar \frac{\partial}{\partial q}$ and q to the multiplication by q.
- A 1D particle with $H_0 = p^2/2 + V(q)$ and $H_1 = -q$ in the quasi-classic approximation ($\hbar \approx 0$).
- A two states system $\psi \in \mathbb{C}^2$ where we exploit the fictitious spin description.
- A three state systems where the control u is designed under weak field approximation and averaging argument.

For each system we show how to exploit flatness based ideas to solved explicitly the motion planing problem.

^{*}Ecole des Mines de Paris, Centre Automatique et Systèmes, 60 B
d Saint-Michel, 75272 Paris cedex 06 FRANCE. pierre.rouchon@ensmp.fr.

1 The harmonic oscillator

Consider the 1D wave packet of an harmonic oscillator $\psi(q, t)$ of configuration $q \in \mathbb{R}$. It satisfies

$$i\hbar\dot{\psi} = (H_0 + uH_1)\psi = \left(\frac{1}{2m}p^2 + \frac{m\omega^2}{2}q^2 - u(t)q\right)\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + \frac{m\omega^2}{2}q^2\psi - uq\psi$$

 $(m, \text{ and } \omega \text{ are parameters})$. Roughly speaking, when the Lie algebra spanned by the operator H_0/i and H_1/i (see [8] for a precise formulation in finite dimension) corresponds to the set of all anti-Hermitean operators (excepted iI), the system is controllable.

Up to suitable time, space and control scaling we can suppose that $H_0 = p^2/2 + q^2/2$ and $H_1 = -q$ and [q, p] = i. Since [q, F(p)] = iF'(p) and [F(q), p] = iF'(q) for any function F, we have

$$[H_0, H_1] = \imath p, \quad [H_0, p] = -\imath q, \quad [H_1, p] = -\imath.$$

Thus this Lie algebra is of finite dimension. Such system is far from being controllable.

The controllable part just coincides with the dynamics of the average position $\langle q \rangle = \int_{-\infty}^{+\infty} q |\psi(t,q)|^2 dq$. Its dynamics given by the classical Ehrenfest theorem (see, e.g,[7]) corresponds then to the classical oscillator

$$\dot{\langle q \rangle} = \langle p \rangle, \quad \dot{\langle p \rangle} = - \langle q \rangle + u$$

which is trivially controllable.

The uncontrollable part corresponds in fact to a Schrödinger dynamics without control. Consider the following change of independent variables $(t, x) \mapsto$ $(t, z = q - \langle q \rangle)$. Then the Schrödinger equation reads with $\psi(t, q) = \exp(i \langle p \rangle z) \phi(t, z)$

$$i\dot{\phi} = (P^2/2 + Z^2/2)\phi + (\langle q \rangle^2/2 - \langle p \rangle^2/2 - u \langle q \rangle)\phi$$

where $P = i \frac{\partial}{\partial z}$ and $Z \equiv z$. The following phase change

$$\phi(t,z) = \exp\left(-i \int_0^t (\langle q \rangle^2 / 2 - \langle p \rangle^2 / 2 - u \langle q \rangle)\right) \varphi(t,z)$$

(gauge transformation since ϕ and φ represent the same physical system) yields to

$$\imath \dot{\varphi} = (P^2/2 + Z^2/2)\varphi.$$

This corresponds to the noncontrollable part. This means that the dynamics of $\phi(t,q)$ can be decomposed into two part, a controllable one of dimension 2, an uncontrollable one of infinite dimension.

The above computations are classical (see, e.g.,[2]). Less classical is the interpretation in terms of decompositions into controllable and uncontrollable parts. It is the infinite dimensional analogue of decomposition for the nonlinear

system of finite dimension $\dot{\xi} = f(\xi, u)$ via a nonlinear change of coordinates $\xi \mapsto \chi$ (see, e.g., [6]) where

$$\chi = (\chi_1, \chi_2), \quad \dot{\chi}_1 = g_1(\chi_1), \quad \dot{\chi}_2 = g_2(\chi_1, \chi_2, u).$$

The uncontrollable part corresponds then to the autonomous dynamics on χ_1 . The following question becomes then natural. Take the controlled Schrödinger equation (infinite dimension case)

$$i\dot{\psi} = (H_0 + \sum_{1}^{n} u_i H_i)\psi$$

and assume that the Lie algebra spanned by the anti-Hermitean operators H_0/i and H_1/i is of finite dimension. Does there exists a decomposition into a finite dimensional controllable part and an infinite dimensional uncontrollable part.

2 The classical limit

Let us begin with an analogy: assume that the classical dynamics of a particle corresponds to the rigid dynamics of a mechanical system. In robotics, a standard approximation to include the small amplitude by high frequency flexible dynamics consists in adding some flexible modes and in controlling them by perturbation methods once the control of the rigid part is solved. Can we do the same thing for a quantum particle in the classical limit $\hbar \approx 0$.

We will consider in a first step a 1D wave packet $\psi(q,t)$ with Hamiltonian $H = p^2/2 + V(q) - uq$ where $p = \frac{\hbar}{i} \frac{\partial}{\partial q}$ and the mass *m* is set to one. The motion of ψ satisfies

$$i\hbar\psi = H\psi$$

Since \hbar is close to zero, the support of ψ is concentrated around the average position $\langle q \rangle$ whose motion is given by Erhenfest equation:

$$\langle q \rangle = \langle p \rangle, \quad \langle p \rangle = - \langle V'(q) \rangle + u$$

where $\langle \rangle$ corresponds to the average operator. Following [7, Chap VI], we perform the following Taylor development

$$V'(q) = V'(\langle q \rangle) + (q - \langle q \rangle)V''(\langle q \rangle) + (q - \langle q \rangle)^2 V'''(\langle q \rangle) + \dots$$

that is valid when the potential V is smooth and admits small variations on the support of ψ . Since the support of the wave packet ψ is essentially around $\langle q \rangle$ we have

$$\langle V' \rangle \approx V'(\langle q \rangle) + \frac{\chi}{2} V'''(\langle q \rangle)$$

where $\chi = \langle (q - \langle q \rangle)^2 \rangle$ is the square of the standard deviation of q. For small \hbar , an approximation of the mean motion of the wave-packet is thus

$$\dot{\langle q \rangle} = \langle p \rangle, \quad \dot{\langle p \rangle} = -V'(\langle q \rangle) - -\frac{\chi}{2}V'''(\langle q \rangle) + u.$$

Now we have to compute an approximation of the χ dynamics. Classical computations using Heisenberg relation $[q, p] = i\hbar$ and the general formula that gives the time derivation of $\langle A \rangle$ for any observable A,

$$\imath\hbar\frac{d\left\langle A\right\rangle }{dt}=\left\langle \left[A,H\right]\right\rangle +\imath\hbar\left\langle \frac{\partial A}{\partial t}\right\rangle$$

yields to the following approximated dynamics for χ ,

$$\begin{split} \chi &= \eta \\ \dot{\eta} &= 2(\varpi - \chi V''(\langle q \rangle)) \\ \dot{\varpi} &= -\eta V''(\langle q \rangle) \end{split}$$

where $\varpi = \left\langle (p - \langle p \rangle)^2 \right\rangle$ and

$$\eta = \langle (p - \langle p \rangle)(q - \langle q \rangle) + (q - \langle q \rangle)(p - \langle p \rangle) \rangle$$

Thus the quantum analogue of a rigid dynamics perturbed by the first flexible mode reads now .

$$\begin{aligned} \langle q \rangle &= \langle p \rangle \\ \langle \dot{p} \rangle &= -V'(\langle q \rangle) - \frac{\chi}{2} V'''(\langle q \rangle) + u \\ \dot{\chi} &= \eta \\ \dot{\eta} &= 2(\varpi - \chi V''(\langle q \rangle)) \\ \dot{\varpi} &= -\eta V''(\langle q \rangle) \end{aligned}$$
(1)

It seems that such an approximated model has never been used for control design. First of all, the quantity $I = \chi \varpi - \eta^2/4$ is an invariant: $\dot{I} = 0$. It is strongly related to the Heisenberg principle. Assume $I > \hbar^2$. Since $\chi \varpi = I + \eta^2/4$, we have $\Delta q \cdot \Delta p = \sqrt{\chi \varpi} \ge \hbar$. The above model is valid for χ , ϖ and η small such that $I \ge \hbar^2$.

Notice also that, for any I > 0, the restriction of the dynamics on the manifold $\chi \varpi - \eta^2/4 = I$ is flat with χ as flat output [5]. This results from the following computations. Assume that instead of knowing the control $t \mapsto u(t)$ (direct problem), we know $t \mapsto \chi(t)$ (inverse problem). Then $\eta = \dot{\chi}$ and $\varpi = (I + \eta^2/4)/\chi$. Since $V''(\langle q \rangle) = (\varpi - \dot{\eta}/2)/\chi$, $\langle q \rangle$ is an implicit function of $(\chi, \dot{\chi}, \ddot{\chi})$. It is then easy to seen that $\langle p \rangle$ and u are implicit functions of $(\chi, \dot{\chi}, \ddot{\chi}, \chi^{(3)})$, and $(\chi, \dot{\chi}, \ddot{\chi}, \chi^{(3)}, \chi^{(4)})$, respectively. The inverse problem admits no dynamics and thus χ is the flat output.

Let us now sketch a possible use of the flat output χ to design an open-loop steering control from a local minimum of V to another one. It is easy to see that, in regions where V''(q) > 0, the dynamics of (χ, η, ϖ) is stable (neutrally) and that in regions where V''(q) < 0 it is unstable (hyperbolically). If the goal is to steer from a stable steady-state to another one we have to cross such unstable region where the support of wave packet tends to grow exponentially in time. More precisely, assume that we start with the steady-state

$$(\langle q \rangle, \langle p \rangle, \chi, \eta, \varpi) = (q_1, 0, \chi_1, 0, V''(q_1)\chi_1)$$

and finish with another stable steady-state

$$(\langle q \rangle, \langle p \rangle, \chi, \eta, \varpi) = (q_2, 0, \chi_2, 0, V''(q_2)\chi_2)$$

with $q_1 \neq q_2$, $V'(q_1) = V'(q_2) = 0$, $V''(q_1) > 0$, $V''(q_2) > 0$ and $V''(q_1)(\chi_1)^2 = V''(q_2)(\chi_2)^2$. Then exists a region between q_1 and q_2 where V'' < 0. This unstable zone where the potential V is concave avoids a quasi-static (adiabatic) strategy. Bounds on the control u avoids also an impulse strategy where a large u on a short time can steer $\langle q \rangle$ from q_1 to q_2 in a time much smaller than $\sqrt{1/|V''(q)|}$. Using flatness based method it is possible to design a steering control u(t) that is not too large with a steering time of the same order of the natural time-constant $\sqrt{1/|V''(q)|}$. However, such design method has to pass through singularities corresponding to potential inflexion V'''(q) = 0.

Such quasi-classic approximations can be easily extended to any quantum system with configuration variables q_i , impulsion variable p_i , free Hamiltonian $H_0(p,q)$ and controlled Hamiltonian $H_i(q)$ associated to the scalar control u_i . This is not the case of the WKB method [7] that becomes quite nasty when the number of q_i exceeds 1. We just gives here the approximated model for a single particle, with n degree of freedom $(q_1, ..., q_n)$ and with the following Hamiltonian

$$H_0 = \sum_{i=1}^n p_i^2 / 2 + V(q), \quad H_i(q) = q_i$$

The approximated dynamics reads for i = 1, ..., n:

$$\begin{split} & \langle \dot{q}_i \rangle = \langle p_i \rangle \\ & \langle \dot{p}_i \rangle = -V_{,i}(\langle q \rangle) - \chi^{jk} V_{,ijk}(\langle q \rangle) + u_i \end{split}$$

where we have used Einstein summation convention,

$$\chi^{jk} = \langle (q_j - \langle q_j \rangle)(q_k - \langle q_k \rangle) \rangle,$$

 $V_{,i}$ stands for $\frac{\partial V}{\partial q_i}$ and $V_{,ijk}$ stand for $\frac{\partial^3 V}{\partial q_i \partial q_j \partial q_k}$. The dynamics of the χ^{jk} are then

$$\begin{split} \chi^{jk} &= \eta^{jk} \\ \eta^{jk} &= 2\varpi^{jk} - \chi^{jl} V_{,kl}(\langle q \rangle) - \chi^{kl} V_{,jl}(\langle q \rangle) \\ \varpi^{jk} &= -\frac{1}{2} \left(\eta^{jl} V_{,kl}(\langle q \rangle) + \eta^{kl} V_{,jl}(\langle q \rangle) \right) \end{split}$$

where

$$\eta^{jk} = \langle (q_j - \langle q_j \rangle) (p_k - \langle p_k \rangle) + (p_j - \langle p_j \rangle) (q_k - \langle q_k \rangle) \rangle$$

$$\varpi^{j,k} = \langle (p_j - \langle p_j \rangle) (p_k - \langle p_k \rangle) \rangle.$$

3 Two states systems

Consider now a two states system. Its wave function ψ belongs to $\mathbb{C}^2.$ The Schrödinger equation

$$\imath\hbar\psi = (H_0 + uH_1)\psi$$

involves now the 2×2 Hermitean matrices H_0 and H_1 :

$$H_0 = \begin{pmatrix} -E/2 & 0\\ 0 & E/2 \end{pmatrix}, \quad H_1 = \begin{pmatrix} h_1 & b\\ b^* & h_2 \end{pmatrix}$$

with $E, h_1, h_2 \in \mathbb{R}$ and $b \in \mathbb{C}^*$. With $\psi = (a_1, a_2) \in \mathbb{C}^2$, the density matrix is defined by

$$\rho = \left|\phi\right\rangle\left\langle\phi\right| = \begin{pmatrix} |a_1|^2 & a_1^*a_2\\ a_1a_2^* & |a_2|^2 \end{pmatrix}$$

In terms of Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

it reads

$$\rho = 1 + \lambda \sigma_x + \mu \sigma_y + \nu \sigma_z$$

with $\vec{S} = (\lambda, \mu, \nu) \in \mathbb{S}^2$. This corresponds to a classical change of coordinates (spin coordinates, see [4]) where the meaningless absolute phase is removed: : $\phi = (a_1, a_2) \in \mathbb{C}^2/\{0\}$ and $\tilde{\phi}(\tilde{a}_1, \tilde{a}_2) \in \mathbb{C}^2/\{0\}$ are the probabilities amplitudes of the same physical state if and only if exists $\theta \in \mathbb{S}^1$ such that $a = \exp(i\theta)\tilde{a}$. Notice that $\vec{S} \in \mathbb{S}^2$ comes from $|a_1|^2 + |a_2|^2 = 1$. In the spin coordinates the dynamics reads

$$\dot{\vec{S}} = \vec{S} \wedge (\omega_0 \vec{B}_0 + \frac{u}{\hbar} \vec{B}_1)$$

where $\omega_0 = E/\hbar$ and

$$\vec{B}_0 = \begin{pmatrix} 0\\0\\1 \end{pmatrix}, \quad \vec{B}_1 = \begin{pmatrix} -2\Re(b)\\2\Im(b)\\h_1 - h_2 \end{pmatrix}$$

Set $\tau = \omega_0 t$, $' = d/d\tau$ and $v = \frac{\|\vec{B}_1\|}{\omega_0 \hbar} u$ the new control. The dynamics becomes

$$\vec{S}' = \vec{S} \wedge (\vec{B}_0 + v\vec{J})$$

where \vec{J} is the unitary vector $\frac{1}{\|\vec{B}_1\|}\vec{B}_1$. Denote by $\alpha \in]0, \pi[$ the angle between \vec{B}_0 and \vec{J} and consider the ortho-normal frame $(\vec{I}, \vec{J}, \vec{K})$ with $\vec{K} = \vec{B}_0 \wedge \vec{J} / \sin \alpha$ and $\vec{I} = \vec{J} \wedge \vec{K}$. Set $\vec{S} = x\vec{I} + y\vec{J} + z\vec{K}$ $((x, y, z) \in \mathbb{R}^3$ with $x^2 + y^2 + z^2 = 1)$. Then the dynamics reads

$$x' = -z(\cos \alpha + u), \quad y' = z \sin \alpha, \quad z' = x(\cos \alpha + u) - y \sin \alpha,$$

since $\vec{B}_0 = \sin \alpha \vec{I} + \cos \alpha \vec{J}$. Notice that $x^2 + y^2 + z^2$ is invariant. The restriction of the dynamics on \mathbb{S}^2 is flat with y as flat output:

$$z = y' / \sin \alpha$$
, $x = \pm \sqrt{1 - y^2 - (y')^2 / \sin^2 \alpha}$.

Let us now find a **smooth** control $[0,T] \ni t \mapsto u(t), u(0) = 0$ and u(T) = 0, steering from -E/2 to +E/2. When u = 0, the state of energy -E/2 corresponds, in the spin-coordinates, to $(x, y, z) = (-\sin \alpha, -\cos \alpha, 0)$ and the state of energy +E/2 to $(x, y, z) = (\sin \alpha, \cos \alpha, 0)$.

Assume to simplify that $\alpha = \pi/2$ (a similar construction exists for over values of α). Set $p(\tau) = (1 - \tau)\tau^2(2 - \tau)^2$. Simple computations show that the function $f(\tau) = 1 - p^2(\tau) - (p')^2(\tau)$ is non negative on [0, 2], reaches 0 only for $\tau = 1$ with f''(1) > 0. Thus the function $g : \mathbb{R} \to \mathbb{R}$ defined by

$$g(\tau) = \begin{cases} -1 & \text{if } \tau < 0\\ -\sqrt{f(\tau)} & \text{if } \tau \in [0,1]\\ \sqrt{f(\tau)} & \text{if } \tau \in [1,2]\\ 1 & \text{if } \tau > 2. \end{cases}$$

is C^2 . The control

$$w(\tau) = -g'(\tau)/p'(\tau)$$

is well defined even for τ around 1. It steers the system from (-1, 0, 0) at $\tau = 0$ to (1, 0, 0) at $\tau = 2$. The steering trajectory is

$$x(\tau) = g(\tau), \quad y(\tau) = p(\tau), \quad z(\tau) = p'(\tau).$$

The interest of the above computations relies on the fact that the control u is smooth. This is not the case for standard steering control of $\pm 1/2$ spin systems [1]: u is then piecewise constant and discontinuous; the steering trajectory is a collection of Lamor precessions over finite time interval.

4 Three states system

Consider now a three states system with three energy levels $E_1 < E_2 < E_3$ corresponding to the physical case illustrated on figure 1. It corresponds to the reduced model of a 1D particule in the potential V(q) admitting two minima with bounded state ψ_1 and ψ_2 of low energy E_1 and E_2 separated by a potential barrier and a third bounded state ψ_3 of energy E_3 passing over the barrier. The supports of the ψ_i , i = 1, 2, 3 are roughly sketched by the dashed horizontal lines. The three states model is a finite dimensional approximation of $i\hbar\dot{\psi} =$ $(p^2/2m + V(q) - uq)\psi$ then entries (1, 2) and (2, 1) in H_1 are negligible. We have the following dynamics

$$\begin{split} \imath\hbar\dot{\alpha}_{1} &= (E_{1} + u\langle q\rangle_{1})\alpha_{1} + u\langle q\rangle_{13}\,\alpha_{3}\\ \imath\hbar\dot{\alpha}_{2} &= (E_{2} + u\langle q\rangle_{2})\alpha_{2} + u\langle q\rangle_{23}\,\alpha_{3}\\ \imath\hbar\dot{\alpha}_{3} &= (E_{3} + u\langle q\rangle_{3})\alpha_{3} + u\langle q\rangle_{31}^{*}\,\alpha_{1} + u\langle q\rangle_{32}^{*}\,\alpha_{2} \end{split}$$



Figure 1: A three states system: steering from E_1 to E_2 without reaching E_3 via active tunnelling control.

where

$$\langle q \rangle_i = \int |\psi_i|^2 q \, dq, \quad \langle q \rangle_{ij} = \int \psi_i^* \psi_j q \, dq$$

and $\psi = \alpha_1 \psi_1 + \alpha_2 \psi_2 + \alpha_3 \psi_3$ with $a_i \in \mathbb{C}$. Change the phase as follows

$$\alpha_i = \exp\left(-iE_3t - \int_0^t u(s) \langle q \rangle_3 / \hbar \, ds\right) \, a_i, \quad i = 1, 2, 3$$

Then

$$\dot{a}_1 = (\omega_{13} + ue_1)a_1 + ub_1a_3 \dot{a}_2 = (\omega_{23} + ue_2)a_2 + ub_2a_3 \dot{a}_3 = ub_1^*a_1 + ub_2^*a_2$$

$$(2)$$

where $\omega_{13} = (E_1 - E_3)/\hbar$ and $\omega_{23} = (E_2 - E_3)/\hbar$ are the Bohr frequencies, $e_i = (\langle q \rangle_i - \langle q \rangle_3)/\hbar$, $b_1 = \langle q \rangle_{13}/\hbar$ and $b_2 = \langle q \rangle_{23}/\hbar$.

Finding explicit open-loop control $[0,T] \ni t \mapsto u(t)$ steering from the pure state of energy E_1 , a = (1,0,0), to the pure state E_2 , a = (0,1,0) without passing via the intermediate state E_3 is not so obvious. We propose here an open-loop design mixing standard perturbation techniques (see, e.g., [7]) and flatness based steering methods.

Assume that the control u is small, $|ub_i|, |ue_j| \ll \omega_{13}, \omega_{23}$ and varies slowly (time constant much smaller than $T_{23} = 2\pi/\omega_{23}$ and $T_{13} = 2\pi/\omega_{13}$ the Bohr periods). Set $b_1 = r_1 \exp(i\theta_1), b_2 = r_2 \exp(i\theta_2)$ with r_i and θ_i real. Set

$$u = \frac{2v_1(t)}{r_1}\cos(\omega_{13}t) + \frac{2v_2(t)}{r_2}\cos(\omega_{23}t)$$

with v_1 and v_2 small amplitude. Then classical averaging techniques show that the solutions of (2) are close to the solution of the average system

$$\dot{x}_1 = v_1 x_3
\dot{x}_2 = v_2 x_3
\dot{x}_3 = -v_1 x_1 - v_2 x_2$$
(3)

where

$$a_1 = \exp(i(\theta_1 - \omega_{13}t))x_1, \quad a_2 = \exp(i(\theta_2 - \omega_{23}t))x_2, \quad a_3 = ix_3$$

Notice that when one of the v_i is constant and the other one is zero we recover the classical Rabi oscillations [7]. They can be used to steer, in a first step, the state from energy E_1 to energy E_3 with v_1 constant $\neq 0$ and $v_2 = 0$ and then, in a second step, to steer the system from E_3 to E_2 with $v_1 = 0$ and v_2 constant $\neq 0$. We will see that we can mix these two steps to steer directly the system from E_1 to E_2 without reaching the energy E_3 .

Up to phase shifts that are not important from physical reasons, we have to find v_1 and v_2 steering the state x from (1,0,0) to (0,1,0). Thus we can suppose that the components of x remain real during the motion (notice that umust be real thus, v_1 and v_2 are also real). Conservation of probability means that $I = x_1^2 + x_2^2 + x_3^2$ is invariant and equal to 1 and we have (with the positive branch $x_3 = \sqrt{1 - x_1^2 - x_2^2}$):

$$\dot{x}_1 = v_1 \sqrt{1 - x_1^2 - x_2^2}, \quad \dot{x}_2 = v_2 \sqrt{1 - x_1^2 - x_2^2}$$

with x_1 and x_2 as flat output. Take any increasing smooth bijection $s \mapsto \sigma(s)$ from [0, 1] to [0, 1] with

$$\sigma(0) = 0, \quad \sigma(1) = 1, \quad \frac{d^i \sigma}{ds^i}(0) = \frac{d^i \sigma}{ds^i}(1) = 0, \quad i = 1, 2, 3.$$

Set $x_1 = 1 - \sigma(t/T)$ and $x_2 = \sigma(t/T)$. Then the control

$$v_1(t) = \frac{-\sigma'(t/T)}{T\sqrt{2\sigma(t/T)(1-\sigma(t/T))}}$$
$$v_2(t) = \frac{\sigma'(t/T)}{T\sqrt{2\sigma(t/T)(1-\sigma(t/T))}}$$

is well defined for $t \in [0, T]$, is smooth and satisfies $v_i(0) = v_i(T) = 0$, i = 1, 2. Moreover it steers the average state x from (1, 0, 0) at t = 0 to (0, 1, 0) at t = T. Notice that when $T \gg T_{13}, T_{23}$, we automatically satisfy the averaging assumptions.

The simulations here are based on model (2) with σ a polynomial of degree 7. We have considered three different cases:

- the standard case of figure 2: the b_i and e_i are closed to one; the ratio of the Bohr frequency is irrational.
- the resonant case of figure 3: the ratio of the Bohr frequency is rational $\omega_{23} = 2\omega_{13}$.
- the ill conditioned case of figure 4: the system is close to a non controllable one; $\omega_{23} \approx \omega_{13}$. This case requires larger transition times T.

Such control designs can be extended to quantum oscillators with more than 3 states. It seems that this design method produces steering trajectories similar to [9].



Figure 2: Active tunneling from E_1 to E_2 without reaching $E_3 > E_1, E_2$; the standard case.



Figure 3: Active tunneling from E_1 to E_2 without reaching $E_3 > E_1, E_2$; the resonant case $E_3 - E_2 = 2(E_3 - E_1)$.



Figure 4: Active tunneling from E_1 to E_2 without reaching $E_3 > E_1, E_2$; the ill conditioned case $E_3 - E_2 \approx (E_3 - E_1)$.

References

- A. Abragam. Principles of Nuclear Magnetism. Oxford University Press, 1961.
- [2] A.G. Butkovskiy and Y.I. Samoilenko. Control of Quantum-Mechnical Processes and Systems, volume 56 of Mathematics and its Applications (Soviet Series. Kluver Academic Publishers, Dortrecht/Boston/London, 1984. English edition 1990.
- [3] E. Cancès, C. Lebris, and M. Pilot. Contrôle optimal bilinéaire sur une équation de Schrödinger. Comptes Rendus de l'Académie des Sciences, Paris, Sèrie 1, 330:567–571, 2000.
- [4] C. Cohen-Tannoudji, B. Diu, and F. Lalo. Mècanique Quantique, volume I& II. Hermann, Paris, 1977.
- [5] M. Fliess, J. Lévine, Ph. Martin, and P. Rouchon. A Lie-Bäcklund approach to equivalence and flatness of nonlinear systems. *IEEE AC*, 44:922–937, 1999.
- [6] A. Isidori. Nonlinear Control Systems. Springer, New York, 2nd edition, 1989.
- [7] A. Messiah. Quantum Mechanics, volume I&II. North Holland Publ. Co., Amsterdam, 1962.
- [8] V. Ramakrishna, M. Salapaka, M. Dahleh, and H. Rabitz. Controllability of molecular systems. *Phys. Rev. A*, 51(2), 1995.
- [9] G. Turinici. Controlabilité exacte de la population des états propres dans les systèmes quantiques bilinéaires. C. R. Acad. Sci. Paris, Sèrie 1, 330:327– 332, 2000.
- [10] G. Turinici. Controllable quantities for bilinear quantum systems. In Proceedings of the 39th IEEE Conference on Decision and Control, pages 1364– 1369, 2000.