CONTROL OF A QUANTUM PARTICLE IN A MOVING POTENTIAL WELL

Pierre Rouchon *

* *Ecole des Mines de Paris, Centre Automatique et Systèmes, 60 Bd Saint-Michel, 75272 Paris cedex 06 FRANCE. (pierre.rouchon@ensmp.fr)*

Abstract: The control is the potential well absolute position. For two kinds of potential shape (periodic and box), we propose approximated solutions to the stead-state motion planing problem: steering in finite time the particle from an initial well position to a final well position, the initial and final particle energies being identical. This problem is a quantum analogue of the water tank problem, where a tank filled with liquid is moved from one position where the surface is horizontal to another position where the surface is also horizontal.

Keywords: Quantum system, controllability, motion planning, operational calculus, Gevrey functions.

1. INTRODUCTION

We consider the control of a quantum particle represented by a probability complex amplitude $\mathbb{R} \ni q \mapsto \psi(q,t)$ solution of

$$\imath \frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial q^2} + (V(q) + \ddot{v}q)\psi \qquad (1)$$

This 1-D Schrödinger equation describes the non relativistic motion of a single charged particle (mass $m = 1$, $\hbar = 1$) with a potential V in a non Galilean frame z of absolute position v, corresponding to the position of the well. Changes of independent variables $(t,q) \mapsto (t,z)$ and dependent variable $\psi \mapsto \phi$, transform (1) into (2) where the control appears as a shift on the space variable. These classical transformations are as follows (see, e.g., (Butkovskiy and Samoilenko, 1984)). The transformations $q = z - v$ and

$$\psi(t, z-v) = \exp\left(\imath\left(-z\dot{v} - v\dot{v} + \frac{1}{2}\int_0^t \dot{v}^2\right)\right)\phi(t,z)$$

yield

$$\imath \frac{\partial \phi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \phi}{\partial z^2} + V(z-v)\phi \qquad (2)$$

corresponding to the Schrödinger equation in a Galilean frame q.

Controllability depends strongly on the shape of the potential V. We will discuss here some preliminary results with the following potential shape.

- The periodic potential, $V(q) = V(q+a)$, where impulsive controls achieve iso-energy translations with amplitudes multiple of the period a.
- The box potential (see figure 1), $V(q) = 0$ for $q \in [-1/2, 1/2]$ and $V(q) = +\infty$ for q outside $[-1/2, 1/2]$. This problem admits strong similarity with the water tank problem: around any state of definite energy, the linear tangent approximate system is not controllable but it is "steady-state" controllable in the sense of (Petit and Rouchon, 2002). We guess that, as for the water-tank system (Coron, 2002), the nonlinear dynamics is locally controllable around any state of definite energy.

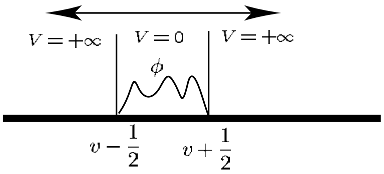

Fig. 1. Quantum particle in a moving box

2. PERIODIC POTENTIAL

Take (1) with a periodic potential (period $a > 0$):

$$V(q+a) = V(q), \forall q.$$

The goal is to solve approximatively the transition between two bounded states of the same energy ψ_1 and ψ_2 such that

$$\psi_2(q) = \psi_1(q - ka)$$

where $k \in \mathbb{Z}$.

Take the form (2) with v as control. Take any C^2 function $[0,1] \ni \alpha \mapsto y(\alpha) \in \mathbb{R}$ such that

$$y(0) = \dot{y}(0) = \ddot{y}(0) = \dot{y}(1) = \ddot{y}(1), \quad y(1) = ka$$

Then, for $\varepsilon > 0$ small enough the control

$$[0,T] \ni t \mapsto v(t) = \begin{cases} 0 & \text{for } t < 0 \\ y(t/\varepsilon) & \text{for } t \in [0,\varepsilon] \\ a & \text{for } t > \varepsilon. \end{cases}$$

steers, approximatively, from ψ_1 to ψ_2. This is obvious with (2): $v(t)$ is close to a step between 0 and ka; since $V(z - ka) = V(z)$, the influence of such variation of v on ϕ solution of (2) remains small ($O(\varepsilon)$). Thus ϕ remains closed to $\psi_1(z)$ during the impulse. Thus, up to a phase shift the real state $\psi(\varepsilon, q)$ corresponds to $\phi(\varepsilon, z) = \psi_1(z) = \psi_1(q - ka) = \psi_2(q)$.

This simple impulsive control overcomes the following difficulty: such transitions necessarily requires to reach energies in the continuous part of the spectrum. Moreover straightforward extensions to $2D$ or $3D$ periodic potentials can be done.

3. THE MOVING BOX

As illustrated on figure 1 take (2), with $V(z) = 0$ for $z \in [-\frac{1}{2}, \frac{1}{2}]$ and $V(z) = +\infty$ for z outside $[-\frac{1}{2}, \frac{1}{2}]$. The dynamics reads:

$$\imath \frac{\partial \phi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \phi}{\partial z^2}, \quad z \in [v - \frac{1}{2}, v + \frac{1}{2}],$$
$$\phi(v - \frac{1}{2}, t) = \phi(v + \frac{1}{2}, t) = 0$$

where v is the position of the box and z is an absolute position (Galilean frame). Otherwise stated (see (1))

$$\imath \frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial q^2} + \ddot{v} q \psi, \quad q \in [-\frac{1}{2}, \frac{1}{2}],$$
$$\psi(-\frac{1}{2}, t) = \psi(\frac{1}{2}, t) = 0$$

where $q = z - v$ is the relative position with respect to the box. ψ and ϕ are related via

$$\psi(t, z - v) = \exp\left(\imath\left(-z\dot{v} - \nu\dot{v} + \frac{1}{2}\int_0^t \dot{v}^2\right)\right)\phi(t,z).$$

3.1 Modal decomposition

For $v = 0$, the system admits a non-degenerate discrete spectrum (see, e.g.,(Messiah, 1962)):

$$\begin{aligned} \omega_{2n} &= 2n^2\pi^2 \\ \psi_{2n}(q) &= 2\sin(2n\pi q) \end{aligned} \quad (3)$$

$$\begin{aligned} \omega_{2n+1} &= 2\left(n + \frac{1}{2}\right)^2 \pi^2 \\ \psi_{2n+1}(q) &= 2\cos\left((2n+1)\pi q\right) \end{aligned} \quad (4)$$

Set $\psi(t,q) = \sum_{n \geq 1} a_n(t)\psi_n(q)$ in $\imath\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial q^2} + \ddot{v} q \psi$, to obtain, for each integer $n \geq 1$,

$$\imath \frac{d}{dt} a_{2n} = -\omega_{2n} a_{2n} + \ddot{v}\left(\sum_{k \geq 0} a_{2k+1} \int_{-\frac{1}{2}}^{\frac{1}{2}} q\psi_{2n}(q)\psi_{2k+1}(q)\, dq\right)$$
$$\imath \frac{d}{dt} a_{2n+1} = -\omega_{2n+1} a_{2n+1} + \ddot{v}\left(\sum_{k \geq 1} a_{2k} \int_{-\frac{1}{2}}^{\frac{1}{2}} q\psi_{2n+1}(q)\psi_{2k}(q)\, dq\right).$$

For any integers $\alpha \geq 1$ and $\beta \geq 0$:

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} q\psi_{2\alpha}(q)\psi_{2\beta+1}(q)\, dq = (-1)^{\alpha+\beta}\left(\frac{1}{\left[\left(\alpha + \beta + \frac{1}{2}\right)\pi\right]^2} + \frac{1}{\left[\left(\alpha - \beta - \frac{1}{2}\right)\pi\right]^2}\right)$$

Notice that odd (resp. even) modes are connected via the control v to even (resp. odd) modes (selection rules).

3.2 Tangent linearization

Denote by $\bar{\psi}$ any state of definite energy $\bar{\omega}$ in (3) or (4). Set

$$\psi(t,q) = \exp(-\imath\bar{\omega}t)(\bar{\psi}(q) + \Psi(q,t))$$

in (2). Then Ψ satisfies

$$\imath\frac{\partial \Psi}{\partial t} + \bar{\omega}\Psi = -\frac{1}{2}\frac{\partial^2 \Psi}{\partial q^2} + \ddot{v} q(\bar{\psi} + \Psi)$$
$$0 = \Psi(-\frac{1}{2}, t) = \Psi(\frac{1}{2}, t).$$

The tangent linear system is obtained, assuming Ψ and $\ddot{v}$ small and neglecting the second order term $\ddot{v} q \Psi$:

$$\begin{aligned} \imath\frac{\partial \Psi}{\partial t} + \bar{\omega}\Psi &= -\frac{1}{2}\frac{\partial^2 \Psi}{\partial q^2} + \ddot{v} q \bar{\psi} \\ \Psi(-\frac{1}{2}, t) &= \Psi(\frac{1}{2}, t) = 0 \end{aligned} \quad (5)$$

We prove here below via operational computations that (5) is not controllable but steady-state controllable. We give explicit formulae for the control $[0,T] \ni t \mapsto \ddot{v}(t)$, steering in finite time from $\Psi = 0$, $v = \dot{v} = 0$ at $t = 0$ to $\Psi = 0$, $v = a$, $\dot{v} = 0$ at $t = T$ for any $T > 0$. Computations are similar to those we have proposed for heat or Euler-Bernouilli dynamics where ultra-distributions and Gevrey functions of order ≤ 1 appear (Laroche *et al.*, 2000; Fliess *et al.*, 1996; Rouchon, 2001).

Set $s = d/dt$. Standard computations show that the general solution of

$$(\imath s + \bar{\omega})\Psi = -\frac{1}{2}\Psi'' + s^2 v q \bar{\psi}$$

is

$$\Psi = A(s,q)a(s) + B(s,q)b(s) + C(s,q)v(s)$$

where

$$A(s,q) = \cos\left(q\sqrt{2\imath s + 2\bar{\omega}}\right)$$
$$B(s,q) = \frac{\sin\left(q\sqrt{2\imath s + 2\bar{\omega}}\right)}{\sqrt{2\imath s + 2\bar{\omega}}}$$
$$C(s,q) = (-\imath s q \bar{\psi}(q) + \bar{\psi}'(q)).$$

3.3 Case $q \mapsto \bar{\phi}(q)$ even.

The boundary conditions imply

$$A(s,1/2)a(s) = 0, \quad B(s,1/2)b(s) = -\psi'(1/2)v(s).$$

The element $a(s)$ is a torsion element (Mounier, 1998), thus the system is not controllable. Nevertheless, for steady-state controllability, we have $a \equiv 0$ (as for the water tank (Petit and Rouchon, 2002)) and we have the following parameterization[1]:

$$b(s) = -\bar{\psi}'(1/2)\frac{\sin\left(\frac{1}{2}\sqrt{-2\imath s + 2\bar{\omega}}\right)}{\sqrt{-2\imath s + 2\bar{\omega}}}\, y(s) \qquad (6)$$
$$v(s) = \frac{\sin\left(\frac{1}{2}\sqrt{2\imath s + 2\bar{\omega}}\right)}{\sqrt{2\imath s + 2\bar{\omega}}}\,\frac{\sin\left(\frac{1}{2}\sqrt{-2\imath s + 2\bar{\omega}}\right)}{\sqrt{-2\imath s + 2\bar{\omega}}} y(s)$$
$$\Psi(s,q) = B(s,q)b(s) + C(s,q)v(s)$$

The entire functions of s appearing in this formulae are of order less than $1/2$, i.e., their module for s large is bounded by $\exp(M\sqrt{|s|})$ for some $M > 0$, independent of $s \in \mathbb{C}$ and $q \in [-1,1]$. The above formulae (6) admit then a clear interpretation in the time domain, as for the heat equation with the Holmgren series solution (Valiron, 1950), when y is a C^∞ time function of Gevrey order less than 1: i.e. $\exists M > 0$ and $\exists \sigma \in [0,1]$ such that, $\forall t$, $\forall n$, $|y^{(n)}(t)| \leq M^n \Gamma(1 + (\sigma+1)n)$ where Γ is the Gamma function[2]. This results from the following fact: to an entire function of s, $F(s)$, of order $\leq 1/2$ is associated a series $\sum_{n\geq 0} a_n s^n$ with coefficient a_n satisfying $|a_n| \leq K^n/\Gamma(1+2n)$ for all n, with some constant $K > 0$ independent of n. To $F(s)y(s)$ corresponds in the time domain, the series,

$$\sum_{n\geq 0} a_n y^{(n)}(t)$$

that is absolutely convergent when y is a Gevrey function of order $\sigma < 1$. Take $T > 0$ and $D \in \mathbb{R}$. Steering (5) from $\Psi = 0$, $v = 0$ at time $t = 0$, to $\Psi = 0$, $v = D$ at $t = T$ is possible with the following Gevrey function of order σ:

$$[0,T] \ni t \mapsto y(t) = \begin{cases} 0 & \text{for } t \leq 0 \\ \bar{D}\dfrac{\exp\left(-\left(\frac{T}{t}\right)^{\frac{1}{\sigma}}\right)}{\exp\left(-\left(\frac{T}{t}\right)^{\frac{1}{\sigma}}\right) + \exp\left(-\left(\frac{T}{T-t}\right)^{\frac{1}{\sigma}}\right)} & \text{for } 0 < t < T \\ \bar{D} & \text{for } t \geq T \end{cases}$$

with $\bar{D} = \frac{2\bar{\omega}D}{\sin^2(\sqrt{\bar{\omega}/2})}$. The fact that this function is of Gevrey order σ results from its exponential decay of order σ around 0 and 1 (see, e.g., (Ramis, 1993; Ramis, 1978)).

3.4 Case $q \mapsto \bar{\phi}(q)$ odd.

The boundary conditions imply

$$B(s,1/2)b(s) = 0, \quad A(s,1/2)a(s) = -\psi'(1/2)v(s).$$

b is a torsion element and thus the system is not controllable. Nevertheless, as for the even case, we have the following parameterization:

$$a(s) = -\bar{\psi}'(1/2)\cos\left(\frac{1}{2}\sqrt{-2\imath s + 2\bar{\omega}}\right) y(s) \qquad (7)$$
$$v(s) = \cos\left(\frac{1}{2}\sqrt{2\imath s + 2\bar{\omega}}\right)\cos\left(\frac{1}{2}\sqrt{-2\imath s + 2\bar{\omega}}\right) y(s)$$
$$\Psi(s,q) = A(s,q)a(s) + C(s,q)v(s).$$

As for the even case, with

$$[0,T] \ni t \mapsto y(t) = \begin{cases} 0 & \text{for } t \leq 0 \\ \bar{D}\dfrac{\exp\left(-\left(\frac{T}{t}\right)^{\frac{1}{\sigma}}\right)}{\exp\left(-\left(\frac{T}{t}\right)^{\frac{1}{\sigma}}\right) + \exp\left(-\left(\frac{T}{T-t}\right)^{\frac{1}{\sigma}}\right)} & \text{for } 0 < t < T \\ \bar{D} & \text{for } t \geq T \end{cases}$$

where $\bar{D} = \frac{D}{\cos^2(\sqrt{\bar{\omega}/2})}$, we can steer (5) from $\Psi = 0$, $v = 0$ at time $t = 0$, to $\Psi = 0$, $v = D$ at $t = T$.

3.5 Practical computations

The above method for computing the steering control requires to develop in series of s and to calculate high order time derivatives of y. All these calculations can be bypassed with Cauchy

[1] Remember that v is associated to a real quantity and the operator $\frac{\sin\left(\frac{1}{2}\sqrt{2\imath s+2\bar{\omega}}\right)}{\sqrt{2\imath s+2\bar{\omega}}}\frac{\sin\left(\frac{1}{2}\sqrt{-2\imath s+2\bar{\omega}}\right)}{\sqrt{-2\imath s+2\bar{\omega}}}$ is a real operator.

[2] Analytic functions are Gevrey functions of order $\sigma = 0$.

formula. Take a bounded measurable function $t \mapsto Y(t)$ corresponding to the position set-point for v. From this function, we deduce a complex entire function $\zeta \mapsto y(\zeta)$ via convolution with a Gaussian kernel with standard deviation ε

$$y(\zeta) = \frac{1}{\varepsilon\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left(-\frac{(\zeta - t)^2}{2\varepsilon^2}\right) Y(t)\ dt$$

Consider, e.g, the relation giving the control v in the even case: $v(s) = F(s)y(s)$ where

$$F(s) = \frac{\sin\left(\frac{1}{2}\sqrt{2\imath s + 2\bar{\omega}}\right)}{\sqrt{2\imath s + 2\bar{\omega}}} \frac{\sin\left(\frac{1}{2}\sqrt{-2\imath s + 2\bar{\omega}}\right)}{\sqrt{-2\imath s + 2\bar{\omega}}}$$

is an entire function of order less than 1 (order 1/2 in fact but 1 is enough here). Thus $F(s) = \sum_{n\geq 0} a_n s^n$ where $|a_n| \leq K^n/\Gamma(1+n)$ with $K > 0$ independent of n. In the time domain $F(s)y(s)$ corresponds to $\sum_{n\geq 0} a_n y^{(n)}(t)$. But

$$y^{(n)}(t) = \frac{\Gamma(n+1)}{2\imath\pi} \oint_\gamma \frac{y(t+\xi)}{\xi^{n+1}}\ d\xi$$

where γ is a closed path around zero. Thus $\sum_{n\geq 0} a_n y^{(n)}(t)$ becomes

$$\sum_{n\geq 0} a_n \frac{\Gamma(n+1)}{2\imath\pi} \oint_\gamma \frac{y(t+\xi)}{\xi^{n+1}}\ d\xi =$$

$$\frac{1}{2\imath\pi} \oint_\gamma \left(\sum_{n\geq 0} a_n \frac{\Gamma(n+1)}{\xi^{n+1}}\right) y(t+\xi)\ d\xi$$

where [3]

$$\sum_{n\geq 0} a_n \frac{\Gamma(n+1)}{\xi^{n+1}} = \int_{D_\delta} F(s)\exp(-s\xi)ds = B_1(F)(\xi).$$

is the Borel transform (see, e.g., (Boas, 1954)) of the F that is defined for $\xi \in \mathbb{C}$ large enough, $|\xi| > K$. In the time domain $F(s)y(s)$ corresponds to

$$\frac{1}{2\imath\pi} \oint_\gamma B_1(F)(\xi) y(t+\xi)\ d\xi$$

where γ is a closed path around zero. Since $y(\zeta) = \frac{1}{\varepsilon\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp(-(\zeta - t)^2/2\varepsilon^2) Y(t)\ dt$ we have the following filter to deduce the control from the reference signal $Y(t)$:

$$v(t) = \int_{-\infty}^{+\infty} \left[\oint_\gamma \frac{B_1(F)(\xi)}{\imath\varepsilon(2\pi)^{\frac{3}{2}}} \exp\left(-\frac{(\xi-\tau)^2}{2\varepsilon^2}\right) d\xi\right] Y(t-\tau) d\tau$$

The kernel

$$f(\tau) = \frac{1}{\imath\varepsilon(2\pi)^{\frac{3}{2}}} \oint_\gamma B_1(F)(\xi)\exp(-(\xi-\tau)^2/2\varepsilon^2)\ d\xi$$

can be computed numerically once for all. One can check that $f(\tau)$ is real and vanishes rapidly for $|\tau| \gg \varepsilon$. In fact F is here of order 1/2, thus $B_1(F)$ is defined on $\mathbb{C}/\{0\}$ and admits an essential singularity in 0 and Thus, the contour γ is any contour around 0. Such computations provide a simple numerical method to generate trajectories and to solve approximatively the steady-states motion planning problem for (5). These formulas are used in a Matlab animation that can be obtained upon request from the author.

[3] D_δ is the half line starting from 0 in the complex plane with direction δ chosen to ensure the convergence of the integral.

REFERENCES

Boas, R.P. (1954). *Entire functions.* Academic Press, New York.

Butkovskiy, A.G. and Y.I. Samoilenko (1984). *Control of Quantum-Mechnical Processes and Systems.* Vol. 56 of *Mathematics and its Applications (Soviet Series.* Kluver Academic Publishers. Dortrecht/Boston/London. English edition 1990.

Coron, J.M. (2002). Local controllability of a 1-d tank containing a fluid modeled by the shallow water equations. *ESAIM: COCV* **8**, 513–554.

Fliess, M., H. Mounier, P. Rouchon and J. Rudolph (1996). Systèmes linéaires sur les opérateurs de Mikusiński et commande d'une poutre flexible. In: *ESAIM Proc. "Élasticité, viscoélasticité et contrôle optimal", 8ème entretiens du centre Jacques Cartier, Lyon.* pp. 157–168.

Laroche, B., Ph. Martin and P. Rouchon (2000). Motion planing for the heat equation. *Int. Journal of Robust and Nonlinear Control* **10**, 629–643.

Messiah, A. (1962). *Quantum Mechanics.* Vol. I&II. North Holland Publ. Co.. Amsterdam.

Mounier, H. (1998). Algebraic interpretations of the spectral controllability of a linear delay system. *Forum Math.* **10**, 39–58.

Petit, N. and P. Rouchon (2002). Dynamics and solutions to some control problems for water-tank systems. *IEEE AC* **47**(4), 594–609.

Ramis, J.P. (1978). Dévissage Gevrey. *Astérisque* **59-60**, 173–204.

Ramis, J.P. (1993). *Séries Divergentes et Théories Asymptotiques.* Panoramas et synthèses. Société Mathématique de France.

Rouchon, P. (2001). Motion planning, equivalence, infinite dimensional systems. *Int. J. Applied Mathematics and Computer Science* **11**(1), 165–188.

Schirmer, S. G., H. Fu and A. I. Solomon (2001). Complete controllability of quantum systems. *Physical Review A.*

Valiron, G. (1950). *Equations Fonctionnelles.* 2nd ed.. Masson et Cie, Editeurs, Paris.