Control of quantum systems using model-based feedback strategies

Augusto Ferrante
Dipartimento di Elettronica e Informatica
Università di Padova
via Gradenigo 6/A
35131 Padova, Italy.
E-mail:augusto@dei.unipd.it

Michele Pavon
Dipartimento di Matematica Pura e Applicata
Università di Padova
via Belzoni 7
35131 Padova, Italy
and LADSEB-CNR, Italy.
E-mail:michele.pavon@unipd.it

Giorgio Raccanelli
v. L. da Vinci 27
36066 Sandrigo, (VI), Italy
E-mail: giorgioracca@inwind.it

Abstract

New model-based feedback control strategies are presented for the steering problem of a quantum system. Both the infinite and finite dimensional cases are discusses. This approach is illustrated by means of a simple spin system example.

Keywords: Quantum systems, transfer problem, feedback control.

1 Introduction

Miniaturization of electronic circuits and devices, and recent advances in laser technology have brought to the forefront the need and the possibility of controlling systems exhibiting quantum mechanical features. Control of quantum systems is a rapidly growing and evolving field whose applications include quantum computing, control of molecular dynamics, NMR, design of semiconductor nanodevices, control of charged particles in beam accelerators, etc., see [1]-[22] and references therein.

Many important problems involve When the nonlinear problem can be numeri the state (propagator) of the quantum system to a desired target. For instance, the design of external control fields to prepare a quantum system in a selected state is a problem of primary importance in quantum information processing, e.g., for such crucial tasks as initializing a quantum processor's memory in a desired quantum logical state by preparing the underlying physical system in the corresponding physical quantum state according to the selected encoding. Preparation of superposition of states is of great interest in order to exploit its inherent parallelism. An example is the preparation in many-particle qubit systems of entangled states, which offer information manipulation that is not possible with the classical binary bits [23].

The most effective strategies in classical control applications involve *feedback control*. The implementation of classical feedback control for quantum systems, however, poses severe challenges since quantum measurements tend to destroy the state of the system (wave packet reduction) [24, 25]. Nevertheless, the possibility of continuous monitoring and manipulation on the natural time-scale has recently become realistic for some quantum systems [26, 27, 28]. This may be viewed as a first substantial step in the direction of closing the gap between quantum feedback control and classical control theory.

We outline in this paper a different approach to the control of quantum systems. We develop namely model-based feedback control strategies that possess certain desirable properties such as rapid convergence of the state/propagator to the desired target employing low control energy. Once the functional form of these feedback controls has been obtained, plugging them back into the Schrödinger equation, we get a nonlinear initial value problem. When the nonlinear problem can be numerically solved, we can construct explicitly the control functions and then implement them in open-loop on the physical system to achieve the desired transfer (see Figure 1). More information on this approach may be found in our

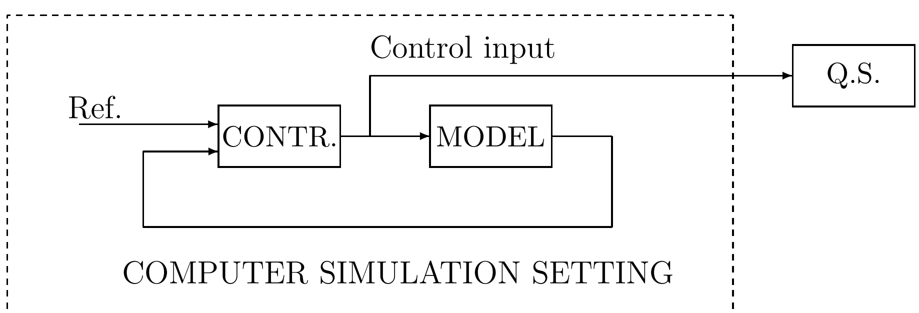

Figure 1: A model of the system is employed in a computer simulation to derive, by means of feedback control techniques, an open loop input for the actual physical quantum system Q.S.

journal paper [29] where, however, only finite-dimensional systems are considered.

Quantum mechanics associates to each physical system a complex Hilbert space $\mathcal{H}$. To every (pure) state of the system there corresponds an equivalence class of unit vectors $|\psi\rangle$ in $\mathcal{H}$ called a *ray*, where $|\psi\rangle$ and $|\varphi\rangle$ are called equivalent if $|\psi\rangle = a\,|\varphi\rangle$ for some complex number a of absolute value one. The evolution of the system is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \mathbf{H}(t) |\psi(t)\rangle , \tag{1.1}$$

where the *Hamiltonian operator* $\mathbf{H}(t)$ is a self-adjoint operator on $\mathcal{H}$ representing the energy of the system. The self-adjointness of $\mathbf{H}(t)$ implies that the evolution is unitary so that

$$|\psi(t)\rangle = \mathbf{U}(t) |\psi_0\rangle , \tag{1.2}$$

where $\{\mathbf{U}(t)\}_{t\geq 0}$ is a family of unitary operators on $\mathcal{H}$. The Hamiltonian operator $\mathbf{H}(t)$ is given as the sum of two self-adjoint operators $\mathbf{H}(t) = \mathbf{H}_0 + \mathbf{H}_c(t)$, where $\mathbf{H}_0$ is the unperturbed (internal) Hamiltonian and $\mathbf{H}_c(t)$ is the interaction (external) Hamiltonian.

2 Feedback control strategies for the steering problem

Let us consider the case where $\mathcal{H} = L^2_c(R^n)$, namely the space of square-integrable, complex-valued functions defined on R^n. Suppose that the internal and interaction Hamiltonians are given by

$$\mathbf{H}_0 = [-\frac{1}{2}\Delta \, + V_0(x)], \qquad \mathbf{H}_c(t) = V_c(x,t), \tag{2.3}$$

respectively, so that (1.1) takes the form

$$\frac{\partial \psi}{\partial t} = \frac{i}{2}\Delta \, \psi - i\, V(x,t)\psi, \tag{2.4}$$

where Δ is the Laplacian operator and ,as it is customary, we have chosen units so that $m = 1$ and $\hbar = 1$.

Consider the following *transfer problem*: Let $\psi_0(x)$ be the initial state, and let $\psi_f(x)$ be a desired terminal state. We assume for simplicity that our target state is an eigenstate of the ambient Hamiltonian so that $\psi_f(x)$ satisfies the time-independent Schrödinger equation

$$\left[-\frac{1}{2}\Delta \, + V_0(x) - E\right]\psi_f = 0, \tag{2.5}$$

where E has the dimension of energy. We seek a control potential $V_c(x,t)$, $t \geq t_0$, in a suitable class such that the solution $\psi(x,t)$ of the controlled Schrödinger equation

$$\frac{\partial \psi}{\partial t} = \frac{i}{2}\Delta \, \psi - i\,[V_0(x,t) + V_c(x,t)]\psi, \qquad \psi(x,t_0) = \psi_0(x), \tag{2.6}$$

converges to the desired terminal state $\psi_f(x)$. A simple idea to determine suitable $V_c(x,t)$ functions is the following. We seek control potential functions $V_c(x,t)$ that will eventually force a decrease of the L^2 distance $||\psi(t) - \psi_f||_2$. To this end, notice that (2.6) and (2.5) yield

$$\frac{\partial}{\partial t}(\psi - \psi_f) = \frac{i}{2}\Delta(\psi - \psi_f) - iV_0(x)(\psi - \psi_f) - iV_c(x,t)\psi - iE\psi_f. \tag{2.7}$$

This, in turn, gives

$$\frac{d}{dt}\left[\frac{1}{2}||\psi(t)-\psi_f||_2^2\right]=\int_{R^n}\Re\left[\left(\frac{\partial}{\partial t}(\psi-\psi_f)\right)(\psi-\psi_f)^*\right]dx=$$

$$=\int_{R^n}\Re\left[\left(\frac{i}{2}\Delta(\psi-\psi_f)-iV_0(x)(\psi-\psi_f)-iV_c(x,t)\psi-iE\psi_f,\right)(\psi-\psi_f)^*\right]dx, \quad (2.8)$$

where $*$ denotes conjugation. Integrating by parts, and taking into account the "natural boundary condition", we get

$$\frac{d}{dt}\left[\frac{1}{2}||\psi(t)-\psi_f||^2\right]=-\int\left[V_c(x,t)+E\right]\psi_f(x)\Im\left(\psi(x,t)\right)dx. \quad (2.9)$$

At this point it is apparent that there are many control potentials guaranteeing

$$\frac{d}{dt}\left[\frac{1}{2}||\psi(t)-\psi_f||^2\right]\leq 0.$$

Two possible control strategies are the following:

$$V_c'(x,t)=-E+K\,\Im\left(\psi(x,t)\right),\quad K>0 \quad (2.10)$$

and

$$V_c''(x,t)=-E+K\,\mathrm{sign}[\Im\left(\psi(x,t)\right)],\quad K>0. \quad (2.11)$$

Clearly, neither strategy guarantees convergence of the solution of the Schrödinger equation to the target state. Nevertheless, plugging the functional form of the control (2.10) or (2.11) into equation (2.6), we get a nonlinear Schrödinger equation that may be numerically integrated. We may then check whether convergenge has occurred. In some preliminary simulation work in the case of a potential well ($V_0(x)=0$ if $|x|\leq a$, $V_0(x)=+\infty$ otherwise) convergence does occur.

In the next section we describe how this procedure can be adapted to a finite dimensional quantum system (spin system).

3 Steering for the propagator of an n-level system

In the finite-dimensional case, we may choose a basis $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle$ in $\mathcal{H}$. We can then identify $|\psi\rangle$ with the corresponding vector of coefficients $\bar{c}$ in $\mathbb{C}^n$, and the operators $\mathbf{H}(t)$, $\mathbf{H}_0$, $\mathbf{H}_c(t)$ with the corresponding Hermitian matrices. Similarly, we identify the *propagator* $\mathbf{U}(t)$ with the corresponding unitary matrix. In many applications (see [14]), the interaction Hamiltonian has the form

$$\mathbf{H}_c(t)=\sum_{i=1}^{m}\mathbf{H}_i u_i(t), \quad (3.12)$$

where the $\mathbf{H}_i$, $i = 1, ..., m$, are $n \times n$ Hermitian matrices, and the $u_i(t)$ are scalar real-valued control functions representing the applied electromagnetic fields. The Schrödinger equation (2.4) may then be replaced by

$$i\hbar\dot{\bar{c}}(t) = \left(\mathbf{H}_0 + \sum_{i=1}^{m} \mathbf{H}_i u_i(t)\right) \bar{c}(t). \tag{3.13}$$

It now follows from (3.13) and (1.2)), that the propagator satisfies the same equation as $\bar{c}$ $\mathbf{U}(t)$ (see Eq. (1.2)):

$$i\hbar\dot{\mathbf{U}}(t) = \left(\mathbf{H}_0 + \sum_{i=1}^{m} \mathbf{H}_i u_i(t)\right) \mathbf{U}(t), \quad \mathbf{U}(0) = I. \tag{3.14}$$

In quantum computation, steering the propagator to a given terminal condition $\mathbf{U}_f$ corresponds to implementating a specific logic gate, see [4]. As in the previous section, we seek control functions $u_i(t)$ that will eventually force a decrease of the distance

$$\|\mathbf{U}(t) - \mathbf{U}_f\|_{tr},$$

$\|\cdot\|_{tr}$ denoting the trace norm. By (3.14), setting $\hbar = 1$, we get

$$\begin{aligned}
\frac{d}{dt}\left[\frac{1}{2}\|\mathbf{U}(t) - \mathbf{U}_f\|_{tr}^2\right] &= \frac{1}{2}\mathrm{tr}\ \left[(\mathbf{U}^*(t) - \mathbf{U}_f^*)\dot{\mathbf{U}}(t) + \dot{\mathbf{U}}^*(t)(\mathbf{U}(t) - \mathbf{U}_f)\right] \\
&= \Re\left\{\mathrm{tr}\ \left[i\mathbf{U}^*(t)\left(\mathbf{H}_0 + \sum_{i=1}^{m}\mathbf{H}_i u_i(t)\right)(\mathbf{U}(t) - \mathbf{U}_f)\right]\right\} \\
&= -\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\left(\mathbf{H}_0 + \sum_{i=1}^{m}\mathbf{H}_i u_i(t)\right)\mathbf{U}_f\right]\right\}, \\
&= -\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\mathbf{H}(t)\mathbf{U}_f\right]\right\} \\
&= -\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\mathbf{H}_0\mathbf{U}_f\right]\right\} - \sum_{i=1}^{m} u_i(t)\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\mathbf{H}_i\mathbf{U}_f\right]\right\}
\end{aligned} \tag{3.15}$$

The first term in the right hand side does not depend explicitly on the control functions $u_i(t)$. It is therefore natural to look for control functions that make the second term nonpositive. Among all such strategies, the simplest appears to be the following

$$u_i(t) = K_i \text{ sign } \left\{\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\mathbf{H}_i\mathbf{U}_f\right]\right\}\right\}, \quad K_i > 0, \quad i = 1, 2, \ldots, m, \tag{3.16}$$

where the control function $u_i(t)$ only takes the values $\pm K_i$. Plugging (3.16) into (3.14), we get the nonlinear initial value problem

$$\begin{aligned}
i\dot{\mathbf{U}}(t) &= \left(\mathbf{H}_0 + \sum_{i=1}^{m}\mathbf{H}_i K_i \text{ sign } \left\{\Im\left\{\mathrm{tr}\ \left[\mathbf{U}^*(t)\mathbf{H}_i\mathbf{U}_f\right]\right\}\right\}\right)\mathbf{U}(t), && (3.17) \\
\mathbf{U}(0) &= I. && (3.18)
\end{aligned}$$

If, integrating (3.17), we find that indeed $\mathbf{U}(t)$ converges to $\mathbf{U}_f$, we can determine the control functions $\{u_i(t); 0 \leq t \leq T, i = 1, \ldots, m\}$ through (3.16). These controls can then be applied to the physical system in open loop.

Again, although convergence is not guaranteed, we may get satisfactory results in some specific applications. In the next section, we present a case study.

4 Controlling a spin 1/2 particle by one electro-magnetic field

In order to illustrate the effectiveness of our control strategies, we consider here the simple case of a spin 1/2 particle controlled by varying only one component of the electromagnetic field. Assuming that we can only vary the external field in the y direction, the propagator evolution (setting $\hbar = 1$) is

$$i\dot{\mathbf{U}}(t) = \sigma_z \mathbf{U}(t) + \sigma_y \mathbf{U}(t) u(t), \quad \mathbf{U}(0) = I, \tag{4.19}$$

with $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. We seek a command input $u(t)$ that will drive (4.19) to the unitary matrix

$$\mathbf{U}_f = \begin{pmatrix} 0 & -\exp(-i\varphi) \\ \exp(i\varphi) & 0 \end{pmatrix}, \tag{4.20}$$

for some phase factor φ. The same case study has been discussed by D. D'Alessandro and M. Dahleh in [14] in the context of a general theory of optimal control of two-level quantum systems. We now apply the simple feedback control (3.16) to this problem. Since $\mathbf{U}(t)$ is *special unitary* (determinant equal to one), it has the form [31]

$$\mathbf{U}(t) = \begin{pmatrix} x_1(t) & x_2(t) \\ -\bar{x}_2(t) & \bar{x}_1(t) \end{pmatrix}. \tag{4.21}$$

We compute tr $[\mathbf{U}^*(t)\sigma_y \mathbf{U}_f]$ and get

$$\text{tr } [\mathbf{U}^*(t)\sigma_y \mathbf{U}_f] = -i\left[x_1(t)\exp(-i\varphi) + \bar{x}_1(t)\exp(i\varphi)\right].$$

Thus, the control (3.16) has the form

$$\begin{aligned} u(t) &= 2K \operatorname{sign} \left\{\Re\left[x_1(t)\exp(-i\varphi)\right]\right\} \\ &= 2K \operatorname{sign} \left\{\Re\left[x_1(t)\right]\cos\varphi + \Im\left[x_1(t)\right]\sin\varphi\right\}, \quad K > 0. \end{aligned} \tag{4.22}$$

Notice that at this stage we still have one degree of freedom: the parameter φ may be chosen in order to get the best performance. In Figure 2, we show the evolution of the elements of $\mathbf{U}(t)$ corresponding to the control (4.22) with $2K = 1$ and $\varphi = 0$.

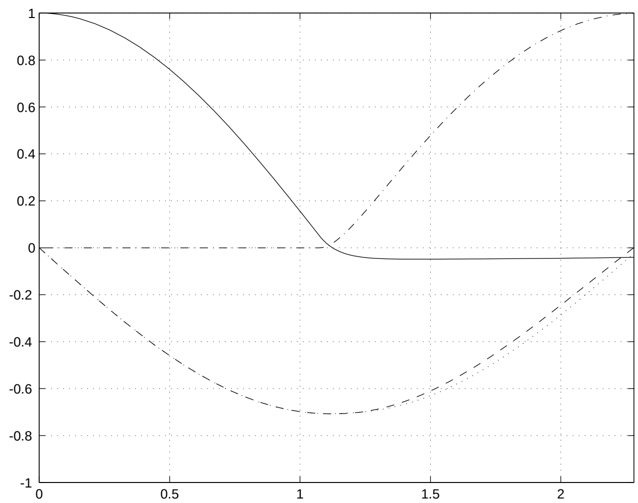

Figure 2: Time evolution of $\Re[x_1(t)]$, (solid line) $\Im[x_1(t)]$, (dashed line) $\Re[x_2(t)]$, (dotted line) and $\Im[x_2(t)]$ (dashdot line) with $2K = 1$ and $\varphi = 0$.

Under the action of this control function, the propagator reaches (with a very good approximation) a matrix of the form (4.20) at approximately the same time $T = \pi/\sqrt{2}$ imposed in [14]. For further details, see [29].

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