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Explicit Generation of States in Quantum Control

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Abstract

In this paper an approach to the problem of generating unitary operators (and thus states) of a finite-dimensional quantum system is discussed. The method consists of decomposing the given unitary matrix into a product of ones with a special structure. This special structure is dependent on any approximation being used or laboratory constraints (and the control which respects both) and is chosen beforehand.

1 Introduction

Several problems in chemistry, nuclear magnetic resonance, optics, quantum information processing call for the creation of a prescribed unitary matrix from the evolution of a controlled quantum system. The applications in chemistry (specifically molecular control) are discussed in the survey paper [10]. Nuclear magnetic resonance applications of this control theoretic problem were addressed in talks in this conference. Likewise, in quantum computing an important problem is the creation of the unitary matrix which will serve as a particular logic gate. Several other novel applications, such as lasing without population inversion call for the preparation of a certain coherent superposition of states.

These problems may be described mathematically as either of the two following problems. First, create a desired final state $x_f \in S$ (S is the unit sphere in C^M) from the evolution of the following controlled bilinear system:

$$\dot{x} = Ax + Bxu(t); x(0) = x_0 \qquad (1)$$

The second problem is analogous, but is posed at the level of the invariant system on $U(M)$ which describes the evolution of the unitary generator corresponding to the system (1). Create a desired unitary matrix U_f from the evolution of the following system:

$$\dot{U} = AU + BUu(t); U(0) = I_M \qquad (2)$$

In both (1) and (2) the matrices A and B, which are $M \times M$ skew-Hermitian matrices, are matrix representations of the internal Hamiltonian and the external coupling to the control $u(t)$ respectively. Note that other applications lead to modified versions of the above two equations. For instance, in nuclear magnetic resonance experiments the system of interest is an affine inhomogeneous system with two inputs. The text [1] has some driftless systems as one of its models.

Remark 1 i) It is customary to start with Schrödinger's equation, $\dot{\psi} = (H_0 + V(x))\psi + H_{ext}\psi$, where $H_0 + V(x)$ is the internal Hamiltonian and H_{ext} is the external Hamiltonian. One example of H_{ext} is $-\mu(x)(t)$ in the control of molecular dynamics via electromagnetic radiation. Here $\mu(x)$ is the dipole and $u(t)$ is the electromagnetic radiation. One then obtains equation (1) from it via one or more of the approximations from physics (e.g; the Born-Oppenheimer approximation in chemical physics, the finite-level approximation used to describe lasers, molecular dynamics and control problems, ...). Some of the approximations and their limitations have been analyzed mathematically. However, scientists from various disciplines who use these approximations have a very good understanding of their range of applicability. Many of the spectacular theoretical predictions of qunatum mechanics and their experimental confirmations are based on such approximate models, and thus (1) is frequently a good starting point for further considerations. To give an extreme illustration of this principle, we point out that whilst the passage from quantum to classical still has its mathematical mysteries, no engineer would hesitate in using classical equations of motion in arriving at control designs for macroscopic systems. Furthermore, the discussion below on state steering will be based on the existence of known specific functional forms for the control $u(t)$. These forms are known to the respective scientists to respect the approximations used in arriving at (1) or its variants. It is also of interest to note that while A and B may be thought to be the matrix elements of the internal and external Hamitonians respectively, they are frequently obtained from experimental data (such as spectroscopic data). A thorough discussion of this and related issues may be found in [2].

ii) The state space for (1) is the unit sphere S in C^M. In quantum computing applications C^M is usually the tensor product of several copies (the number of copies is the same as the number of qubits) of C^2. This corresponds to the multi-particle picture of the implementation of quantum gates (such as ions in a trap). This picture is, of course, in keeping with the classical view of bits and is also driven by the structure of the algorithms such as Shor's algorithm. However, there is some interest in viewing these qubits as pairs of levels of a single particle. One reason is that single particles are more immune to the effects of decoherence than are several particles in tandem.

Since the unitary group and several other subgroups thereof act transitively on the unit sphere S, the problem of final state preparation of (1) can be subsumed by the final state preparation problem for (2). In fact, since the isotropy group corresponding to these transitive group actions are known, one can explicitly parametrize those matrices $V \in U_M$ such that $Vx_0 = x_f$. Thus obtaining x_f starting from x_0 can be (constructively) reduced to the problem of preparing any one of these V's starting from the identity matrix I_M. Thus our subsequent discussion will be confined to the latter problem. In [7] a measurement scheme is discussed which can be cast as the problem of the preparation of specific unitary matrices. Thus, in certain applications, even state readout amounts to final state preparation for (2).

2 A Constructive Scheme

In this section we will discuss the constructive procedure referred to in the abstract. Let us first make a couple of observations which are relevant. First, viewing (2) as an invariant system on a compact Lie group one can determine whether (2) is completely controllable. This can be found in [6] and it makes essential use of the results of [3]. However, this system has drift and thus there are no constructive techniques for path planning, as opposed to the case of systems without drift [4, 9]. While it is possible to make use of the structure of the drift term to come up with heuristics for path planning, these typically lead to complicated inputs. Thus we will use a different approach. First, a prescribed functional form for the input with a few floating parameters serving as our knobs will be imposed. This functional form is typically a consequence of both technological limitations and the use of an approximation which is respected by this input. These approximations enable us to more completely describe the response of the system to the given input. A typical example is the use of a sequence of monochromatic pulses (with predetermined frequencies) with the pulse area and phase as knobs together with the rotating wave approximation, [8]. The second observation consists in observing that any $U_f \in U(M)$ is $e^{C\phi}$ times a special unitary matrix. Since the $e^{C\phi}$ factor cannot be experimentally observed, any well posed state preparation problem should be susceptible to the case when U_f is special unitary. We will assume that this is so from now on.

Bearing these remarks in mind the constructive procedure consists of the following steps:

1. Assume that the underlying physical system can be controlled by addressing pairs of states at a time. One situation where this condition is met is that of a finite-level atom with wide separation (i.e., no resonances or near resonances) between the differences in energy levels of the atom, and which is further that if state i and j cannot be directly accessed from one another due to selection rules then there exist other states forming a ladder between i and j which enable us to access i from j and vice-versa.

2. Choose a functional form for the input such that both i) the response to the two-dimensional subsystem can be explictly computed via perhaps an approximation; and ii)the functional form, along with possible bounds for the parameters in the functional form, respect any approximation that was chosen. An example of this is the case of a sequence of monochromatic inputs with known bounds on the pulse area which will respect the fact the finite number of levels approximation.

3. Compute explicitly the matrix in $SU(2)$ (parametrized by the knobs) which results in response to this input. This parametrized form is the special structure referred to before. For that purpose the following proposition which computes explictly the exponential of an arbitrary linear (time-varying) combination of Pauli matrices is useful, [7]:

   Proposition 1 *Let* $\sigma_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ *and* $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ *be the Pauli matrices. Then we have*

   $$exp(i\alpha(t)\sigma_x+\beta(t)\sigma_y+\gamma(t)\sigma_z) = cos(\frac{\sqrt{\lambda(t)}}{2})I_2+i\frac{2}{\sqrt{\lambda(t)}}sin($$

   where $\alpha(t), \beta(t)$ *and* $\gamma(t)$ *are real valued functions of time, and*

   $$\lambda(t) = (\alpha(t)^2 + \beta(t)^2 + \gamma(t)^2)$$

4. Show that any matrix in $SU(2)$ can be written as a product of matrices in $SU(2)$ which have the special structure obtained in the step above. In this regard we note that this can always be done provided the logarithm of this special structure lies in the span of any two of $i\sigma_x$, $i\sigma_y$ or $i\sigma_z$. This is essentially a

controllability argument since the Lie algebra generated by any two of these matrices is all of $su(2)$, the Lie algebra of $SU(2)$. Doing so constructively and respecting any parameter bounds imposed by laboratory considerations requires extra effort. One such instance is described in [7].

5. Show that any matrix $V_f \in SU(M)$ can be written as the product of a sequence of matrices which are tensor products of I_{M-2} (the $(M-2)\times(M-2)$ identity matrix) and a 2×2 block with the special structure obtained in step 3. If no special structure is required and no selection rule type constraints are present, then a procedure for this is well known, [5]. Essentially one reduces each column of V_f to a unit vector in C^M by taking subvector of length two at a time and then premultiplying by a matrix in $SU(2)$ which results in one of the components being zero. That there is at least one such matrix is a consequence of the fact that $SU(2)$ acts transitively on spheres (of a given radius) in C^2. The presence of selection rules introduces some extra complications. The special structure requirement means, in conjunction with step 4, that more than one premultiplication by matrices in $SU(2)$ may be required.

It is worth noting that the matrices which enter into the product decompositions of V_f can be completely described by V_f and the selection of the parameters which enters the functional form of the control input can be determined, in view of step 3, from these factors in the product expansion of V_f by solving simple transcendental equations.

We believe that this methodology could be profitably applied to the control of various systems arising in quantum mechnaics. This should also extend to approximate path planning for invariant systems on compact Lie groups, if one can identify conditions which lead to weak coupling between susbsystems of the full system.

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