Optimal Control of One-Qubit Gates

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Abstract

We consider the problem of carrying an initial Bloch vector to a final Bloch vector in a specified amount of time under the action of three control fields (a vector control field). We show that this control problem is solvable and therefore it is possible to optimize the control. We choose the physically motivated criteria of minimum energy spent in the control, minimum magnitude of the rate of change of the control and a combination of both. We find exact analytical solutions.

1 Introduction

Recent advances in experimental physics allowing for manipulation and measurement of single quantum systems, have stimulated a flurry of investigations on the control of quantum systems, and more or less formal schemes have been advanced[1, 2, 3, 4]. The conditions under which a given quantum system is completely controllable have been explored [5, 6, 7] and some limits of quantum controllability [8] have been found. Quantum control theory have several important applications including quantum state engineering [9], control of chemical reactions [10, 11], laser cooling of molecular degrees of freedom [12, 13], quantum register initialization [14] and the fabrication of robust quantum memories [15].

A major application of the theory of quantum control is the subject of quantum computation. The physical implementation of a quantum computer is a major challenge and many proposals[20] including ion traps, optical cavities, and quantum dots have been advanced. Promising practical implementations should be scalable, facing the problem of heat dissipation which gets worse along with the shrinking of the size of the proposed physical system. In this work we address the problem of carrying an initial qubit (more precisely of an initial Bloch vector) to an specified final qubit in a given amount of time using the minimum amount of energy possible. This paper is organized as follows: first we review the controllability of Bloch vector, and then we formulate and solve the problem of optimal control under the criteria of minimum energy, minimum energy derivative and a combination of both.

Two level systems adequately model many physical systems (spin 1/2, photon polarization, atoms in (quase) monochromatic electromagnetic fields, etc), despite its simplicity. A general 1-qubit gate can be represented as a 2-level quantum system, and the most general Hamiltonian for such a system can be written as $H = h_0 I + \vec{h} \cdot \vec{\sigma}$, where $\vec{\sigma}$ are Pauli´s matrices, $h_0$ determines the zero energy reference, and $\vec{h}$ is a classical vector. Since we can use any $\vec{h}$ we want, and this is the field we use to control our system, here on we call $\vec{h}$ our vector control. We moreover assume $h_0 = 0$.

2 Bloch vector Controllability

All of the information of the quantum state of a two level system is completely determined by its density matrix $\rho$, or equivalently by its Bloch vector $\vec{s}(t) = \frac{1}{2} \text{Tr}(\rho \vec{\sigma})$. The dynamics of Bloch vector, given by well known Bloch equation $\dot{\vec{s}}(t) = \vec{b} \times \vec{s}$, where $\vec{b} = 2\vec{h}/\hbar$, can be put in the more explicit way $\dot{\vec{s}} = (b_x \mathcal{J}_x + b_y \mathcal{J}_y + b_z \mathcal{J}_z)\vec{s}$, where the $\mathcal{J}$s are the rotation generators. In this case we can formulate the problem of taking an initial state $\rho_i$ to a final state $\rho_f$ in a specified amount of time $T = t_f - t_i$. After rescaling, we take $t_i = 0, t_f = 1$. Remember that we assume that all three components of $\vec{h}$ (or of $\vec{b}$) are control fields. Thus, since we have all three rotation generators, the system is completely controllable in the sense that every rotation can be reached from the identity $\mathbb{I}$. In

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other words, any final vector can be reached from any other initial vector (of the same length, or the same degree of mixture) in any finite time, provided there are no constraints on the size of the control fields. Moreover, the motion equation can be inverted \[\mathbf{b} = \mathbf{s} \times \mathbf{s} s^{-2} - f(t)\mathbf{s},\] where \(f(t)\) is an arbitrary function, which shows that not only the control problem is solvable, but that it is solvable even when a path to realize such control is given. Moreover, even in this event the solution is not unique.

3 Optimal Control

As mentioned before, the larger the fields used for control the greater the amount of heat to be dissipated. Then, proved the complete controllability of the one qubit gate, it is meaningful asking which is the control vector field required to perform an arbitrary rotation operation with the minimum amount of energy spent. We address this problem an optimal “classical” control problem for the Bloch vector, that is we shall extremize the cost functional

\[
S = \int_{t_0}^{t_f} dt \left\{ \frac{1}{2a} \mathbf{b} \cdot \mathbf{b} + \lambda \cdot \left( \mathbf{s} \times \mathbf{b} \right) \right\},
\]

where \(\mathbf{b} = 2\hbar / \hbar,\) and \(\lambda\) is a (vector) Lagrange multiplier, and the momentum corresponding to \(\mathbf{s}\). Notice that the form of the cost functional above is not arbitrary: were the vector control field a magnetic field acting on a spin half system, or an electromagnetic field for a charged two level system, the (electro)magnetic energy would have had the assumed form. For the sake of simplicity we scale the variables to get the following cost functional

\[
S = \int_{0}^{1} dt \left\{ \frac{1}{2a} \mathbf{b} \cdot \mathbf{b} + \lambda \cdot \left( \mathbf{s} \times \mathbf{b} \right) \right\},
\]

where the constant \(a\) have been introduced to have \(s\) and \(\lambda\) in the same units.

Not all of the resulting Euler–Lagrange equations

\[
\dot{s} = a\mathbf{s} \times \lambda, \quad \ddot{s} = b \times s, \quad \dot{\lambda} = -b \times \lambda,
\]

are true dynamical equations: the first equation is a constraint. A few simple calculations show that the system of equations \((3)\) possesses the following constants of motion

\[
s^2 = \mathbf{s} \cdot \mathbf{s}, \quad \lambda^2 = \mathbf{\lambda} \cdot \mathbf{\lambda} \quad \text{and} \quad \nu = \mathbf{\lambda} \cdot \mathbf{s} = \nu s \cos(\theta),
\]

where \(\theta\) is the angle between \(\mathbf{\lambda}\) and \(\mathbf{s}\). The equations of motion can be put in the equivalent form

\[
\frac{d}{d[\mathbf{at}]} \begin{pmatrix} \mathbf{s} \\ \lambda \end{pmatrix} = \begin{pmatrix} -\lambda & s^2 \\ -\nu & \lambda \end{pmatrix} \begin{pmatrix} \mathbf{s} \\ \lambda \end{pmatrix} = \begin{pmatrix} -\lambda \cos(\theta) & 1 \\ 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} \mathbf{s} \\ \lambda \end{pmatrix},
\]

whose solution reads

\[
\begin{pmatrix} \mathbf{s} \\ \lambda \end{pmatrix} = \frac{1}{\sin(\theta)} \begin{pmatrix} \sin(\theta - at \sin(\theta)) & \sin(at \sin(\theta)) \\ -\sin(\theta + at \sin(\theta)) & \sin(\theta + at \sin(\theta)) \end{pmatrix} \begin{pmatrix} \mathbf{s}(0) \\ \lambda(0) \end{pmatrix}.
\]

We have assumed that \(\mathbf{s}\) and \(\lambda\) are unitary vectors. Notice that we have obtained an orthogonal transformation. In fact this could have been anticipated by showing that \(\mathbf{b}\) is constant both in norm and direction. Let us see that the solution is valid for any value of \(\theta\), so we have freedom to choose \(\theta\) to our best convenience. For example, we can choose \(\lambda(0) = \mathbf{s}(1)\). It follows \(\cos(\theta) = \mathbf{s}(0) \cdot \mathbf{s}(1)\), and \(\sin(a \sin(\theta)) = \sin(\theta)\). This choice leads to the solution

\[
\mathbf{s}(t) = \frac{\sin(b(1-t))}{\sin(b)} \mathbf{s}_i + \frac{\sin(bt)}{\sin(b)} \mathbf{s}_f,
\]

where

\[
\mathbf{b}(t) = \mathbf{b}(0) = \frac{\text{ArcSin}(\sin(\theta))}{\sin(\theta)} \mathbf{s}_i \times \mathbf{s}_f = (\theta + 2\pi n) \mathbf{s}_\perp = b_1(t; n) \mathbf{s}_\perp.
\]
Finally, the other solutions correspond to reaching the final Bloch vector from the initial one but rotating the other way. Choices different to $\hat{\lambda}(0) = \hat{s}(1)$ are also meaningful, but should lie on the plane which contains the initial and final Bloch vectors. Let us see that the solution found breaks down when the initial and final vector are antipodal. In this case there are an infinite number of solutions all of them spending the same amount of energy. In this case the choice of an initial Lagrange multiplier vector which is not (anti)parallel to the initial Bloch vector leads to a particular solution.

Now, we remark that the minimum energy control corresponds to minimum path on the Bloch sphere. The length $l$ transversed by the tip of the Bloch vector is given by

$$l = \int_0^1 \left| \frac{d\bar{s}}{dt} \right| dt = \int_0^1 |\bar{b} \times \bar{s}| dt = s \int_0^1 b(t) |\sin(\theta(t))| dt \leq s \int_0^1 b(t) dt. \quad (8)$$

This means that, for a given magnitude of the control field, the transversed length is maximized when the control vector field makes a right angle with the Bloch vector. In other words, if we restrict to control fields that are perpendicular to Bloch vector, and if Bloch vector transverses a longer path, it is necessary to have a larger average control field. This remark allows us to restrict ourselves to consider the vector control to point out in the direction of $\hat{s}_i \times \hat{s}_f$. Making the Ansatz

$$\bar{b}(t) = b(t) \hat{s}_\perp, \quad (9)$$

after some algebra we obtain

$$\bar{s}(t) = \frac{\sin(\theta - \int_0^t b(t') dt')}{\sin(\theta)} \hat{s}_i + \frac{\sin(\int_0^t b(t') dt')}{\sin(\theta)} \hat{s}_f, \quad (10)$$

were $b_0$ should satisfy the equality $\int_0^1 b(t) dt = \theta$. If we write $b(t)$ as $\theta + \delta(t)$ we see that the average value of $\delta(t)$ over the unitary interval is zero and that $\int_0^1 b^2(t) dt = \theta^2 + \int_0^1 \delta^2(t) dt$. Thus, the minimum is attained when the control vector field is constant from the initial till the final time. It is possible to give an alternative argument which shows that the solution of minimum fluence is the same as the shortest geodesic. Inverting the Bloch equation we obtain the control field $\bar{b} = \bar{s} \times \bar{s} + f \hat{s}$, and the energy spent in the control $\int_0^1 b^2(t) dt = \int_0^1 \left( (\bar{s})^2 - (\bar{s} \cdot \bar{s})^2 + f^2 \right) dt$. Since the second subintegral term is identically zero, and the function $f(t)$ should be zero for the extrema, we see that the fluence minimization and geodesic minimization (see Eq. 8) are almost the same, and reach their extrema together. Had we chosen the squared length instead of the length, both expressions would have been identical.

Since the times to perform quantum computation are generally short in low dimensional condensed matter systems, which are the most promising candidates, one also should analyze possible limitations set by the rate at which control fields can be set. In particular, it is worth paying attention that the solution (9) is a discontinuous one, zero before the initial time, constant between the initial and final times, and zero again from the final time on. Had we used the square of the time derivative of the control field instead of the square of the field itself, defining the cost functional

$$S = \int_0^1 dt \left\{ \frac{1}{2} \bar{b} \cdot \frac{d\bar{b}}{dt} + \bar{s} \cdot \left( \frac{d\bar{s}}{dt} - \bar{b} \times \bar{s} \right) \right\}, \quad (11)$$

the solutions obtained above would have been also solutions of the new problem. In this case a whole set of new solutions arise, which are of constant magnitude but whose direction changes with time. It is easy to construct such a kind of solutions. Let $\{ \bar{b}(t), \bar{s}(t) \}$ a solution of the new problem, but with a time dependent $\bar{b}(t)$, then $\{ \bar{b}(t) = b(t) + f(t) \bar{s}_i, \bar{s}(t) \}$ is also a solution, no matter how the function $f$ is chosen. In particular, we can adjust $f$ to obtain $\bar{b}$ a constant. For instance, if we set $\bar{s}(t) = \cos(\phi(t)) \bar{s}_0(t) + \sin(\phi(t)) \bar{s}_\perp$, with $\bar{s}_0$ the solution for the problem of minimum fluence, and $\cos(\phi(t))$ a function with value 1 both at $t = 0$ and at $t = 1$, we have the control field $\bar{b}(t) = \theta \cos^2(\phi) \bar{s}_\perp - \hat{s} \hat{s}_\perp - \theta \sin(\phi) \cos(\phi) \bar{s}_0$ where $\bar{s}_\perp = \hat{s}_\perp \times \hat{s}_0$ is a unitary vector needed to define a time dependent right triade $\{ \bar{s}_0, \bar{s}_\perp, \bar{s}_\perp \}$. One can choose $f$ as $f = \pm \sqrt{B^2 - \theta^2 \cos^2(\phi) - \hat{\phi}^2}$, with $B^2$ the maximum value of $b^2$, so at instants where the maximum is attained, $f$ vanishes. For the sake of definiteness we use $\phi(t) = \theta \mu t (1 - t)$ which yields $f^2 = \theta^2 (\sin^2(\mu t) + \mu^2 t (2 - t))$, and produces a new constant norm vector control $\bar{b}$ with magnitude $\theta \sqrt{1 + \mu^2}$. This solution, of course, spends more energy than the found before to perform the same control.

Solutions with vanishing magnitude at the initial and final instants of time also exist. Observe that in this case the equation for $\bar{b}$ is

$$\ddot{\bar{b}} = -\Omega^2 \bar{s} \times \bar{\lambda} \quad (12)$$
which is a true dynamical equation. This allows for some extra flexibility: now we can add initial and final conditions on the value of the control field. From the point of view of the energy injected to the system, the most physically sensible conditions are those of vanishing control field both at the initial and the final times. We observe that in this case the solution should follow the shortest geodesic between the initial and the final Bloch vectors. In fact, since the control field begins and ends with a vanishing value, it should grow and decrease as slowly as possible but fast enough as to reach the maximum value necessary to have an average magnitude of at least $\theta$. If it had grown to a greater value it would have grown at a larger pace, so it would have been not the minimum solution sought.

Differentiating the equation $\frac{d^2\vec{s}}{dt^2} = \vec{b} \times \frac{d\vec{s}}{dt} - \Omega^2 \vec{s} \times \vec{s}_f$, we proceed to discuss the more general physical criterion in which one is interested on energy saving but with a limited rate of change of the control fields or a linear combination of both. We have found control given amount of time, using an optimal control scheme which minimizes the energy spent by the control fields, or the magnitude of the rate of change of the control fields or a linear combination of both. We have formulated and solved in an analytic way, the problem of rotation of the Bloch vector (which characterizes completely the state of a two level system) from a prescribed initial vector to a prescribed final vector, in a physically sensible conditions are those of vanishing control field both at the initial and the final times. We observe that in this case the solution should follow the shortest geodesic between the initial and the final Bloch vectors. In fact, since the control field begins and ends with a vanishing value, it should grow and decrease as slowly as possible but fast enough as to reach the maximum value necessary to have an average magnitude of at least $\theta$. If it had grown to a greater value it would have grown at a larger pace, so it would have been not the minimum solution sought.

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\[
S = \int_0^1 dt \left\{ \frac{1}{2a} \left( \vec{b} \cdot \vec{b} + \frac{1}{\omega^2} \frac{db}{dt} \cdot \frac{db}{dt} \right) + \vec{\Lambda} \cdot \left( \vec{s} - \vec{b} \times \vec{s}_f \right) \right\}. 
\]

The experience gained with the previous examples shows that the solution control field should point (anti)parallel to $\vec{s}_f$. Some algebra leads to the solution

\[
\vec{b}(t) = a |\sin(\theta)| \left( 1 - \frac{\cosh(\omega(t - \frac{1}{2}))}{\cosh(\frac{\omega}{2})} \right) \vec{s}_f = b_3(t) \vec{s}_f.
\]

We notice that all of the solutions so far found have the form of equation (9) and therefore have the solution (10). We only have to take care of the final value of $\vec{s}$. This leads to the following more explicit forms for $b(t)$

\[
b_2(t; n) = 6(\theta + 2\pi n) t(1-t), \quad b_3(t; n) = \frac{\theta + 2\pi n}{1 - \tanh(\omega/2)} (1 - \frac{\cosh(\omega(t - \frac{1}{2}))}{\cosh(\frac{\omega}{2})}).
\]

For the second case considered, the intuitive choice, $b = \pi \theta \sin(\pi t)/2$ produces a value of the cost functional only 1.5% above that of the optimal solution. Finally, for control fields of the form of equation (9) the cost functional can be written in purely geometric terms. If we set $\phi(t) = b(t)$, $\phi(0) = 0$, then $S$ can be expressed as

\[
S = \frac{1}{2a} \int_0^\phi \frac{b(\phi)}{1 + \left( \frac{1}{\omega} \frac{db}{d\phi} \right)^2} d\phi,
\]

where $\vec{b}$ is the average magnitude of the control field, and $\phi$ the accumulated angle (or the arc length) transversed by the Bloch vector. Equation (15), just like equation (13), contains the other two cases: the first in the limit $1/\omega \rightarrow 0$, and the second in the limit $1/a \rightarrow 0$ but with $\omega^2 = \Omega^2$ fixed. Of course, $b_1(t; n) = \lim_{1/\omega \rightarrow 0} b_3(t; n)$ and $b_2(t; n) = \lim_{1/a \rightarrow 0, \omega^2 = \Omega^2} b_3(t; n)$.

We have formulated and solved in an analytic way, the problem of rotation of the Bloch vector (which characterizes completely the state of a two level system) from a prescribed initial vector to a prescribed final vector, in a given amount of time, using an optimal control scheme which minimizes the energy spent by the control fields, or the magnitude of the rate of change of the control fields or a linear combination of both. We have found control fields perpendicular to both the initial and final Bloch vectors, and multiple local minima corresponding to arrival from the initial to the final Bloch vector in one or other senses or after one or more complete turns.

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