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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 expended in the control, minimum magnitude of the rate of change of the control and a combination of both. We find exact analytical solutions, determine the fields for a general one-qubit gate, and use the *Y* gate as an example. We argue that in the case of less than three controls, only the physical intuition does not provide a straight reasonable solution, and solve the problem in the case of a unique control minimizing the energy consumption.

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1. Introduction

Recent advances in experimental physics in the field of manipulation and measurement of single quantum systems have stimulated a flurry of investigations into the control of quantum systems, and more or less formal schemes have been developed [1–5]. The conditions under which a given quantum system is completely controllable have been explored [6–10] and some limits of quantum controllability [12] have been found. Quantum control theory has several important applications including quantum state engineering [13], control of chemical reactions [14, 15], laser cooling of molecular degrees of freedom [16, 17] and quantum register initialization [18].

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 [21] including ion traps, optical cavities and quantum dots have been made. Promising practical implementations face the problem of heat dissipation which gets worse with the shrinking of the size of the proposed physical system. Thus it is desirable to find a set of energy efficient universal quantum gates, for example, general one-qubit gates and one-entangling two-qubit gates. In this paper we address the problem of carrying an initial qubit (more precisely of an initial Bloch vector) to a specified final qubit in a given amount of time, short enough to ignore decoherence effects, using the minimum amount of energy possible. The optimal problem for the propagator of two-level systems with cost quadratic in the control was addressed and solved in [24] using different techniques.

This paper is organized as follows: we review the controllability of the Bloch vector in section 2. In section 3 we formulate and solve the problem of optimal control under the criteria of minimum energy, minimum energy derivative and a combination of both with a three-component vector field, and apply it to a general one-qubit gate. Although most of the time we do not have three available controls, the optimization can show small surprises (the result in the second case is not of sine type as one would naively expect), and allows for a precise definition of a compromise between different criteria and for an easy generalization to more complex cases (for example, in the presence of dissipation/decoherence we can add terms proportional to the entropy). Finally, the problem of optimal control with a single control and minimum energy is considered, and applied to the Y gate.

Two-level systems adequately model many physical systems (spin-$\frac{1}{2}$, photon polarization, atoms in (quasi) monochromatic electromagnetic fields, etc), despite its simplicity. A general one-qubit gate can be represented as a two-level quantum system, and the most general Hamiltonian for such a system can be written as $H = h_0 I + \boldsymbol{h} \bullet \sigma$, where σ are Pauli's matrices, h_0 determines the zero energy reference, and $\boldsymbol{h}$ is a classical vector. Since we can use any $\boldsymbol{h}$ we want, and this is the field we use to control our system, from now we refer to $\boldsymbol{h}$ as our vector control. Moreover, we assume $h_0 = 0$.

2. Bloch vector controllability

All information regarding the quantum state of a two-level system is completely determined by its density matrix ρ, or equivalently by its Bloch vector $\boldsymbol{s}(t) = \mathrm{Tr}(\rho\sigma)$. The dynamics of the Bloch vector, given by the well-known Bloch equation $\dot{\boldsymbol{s}}(t) = \boldsymbol{b} \times \boldsymbol{s}$, where $\boldsymbol{b} = 2\boldsymbol{h}/\hbar$, can be put in the more explicit form $\dot{\boldsymbol{s}} = (b_x \mathcal{J}_x + b_y \mathcal{J}_y + b_z \mathcal{J}_z)\boldsymbol{s}$, where the $\mathcal{J}$ are the rotation generators. In this case we can formulate the problem of taking an initial state ρ_i to a final state ρ_f in a specified amount of time $T = t_f - t_i$. After rescaling, we take $t_i = 0, t_f = 1$. Note that we assume all three components of $\boldsymbol{h}$ (or of $\boldsymbol{b}$) 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 [8, 11]. In 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 [19] to give $\boldsymbol{b} = \boldsymbol{s} \times \dot{\boldsymbol{s}} s^{-2} - f(t)\boldsymbol{s}$, where $f(t)$ is an arbitrary function, which shows that the control problem is solvable, i.e. a suitable $b(t)$ can be found, even when a path $s(t)$ is prescribed. 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, proving the complete controllability of the one-qubit gate, it is meaningful to ask which control vector field is required to perform an arbitrary rotation operation with the minimum expenditure of energy. We address this problem as an optimal 'classical' control problem for the Bloch vector, that is we shall extremize the cost functional

$$S = \int_{t_0}^{t_f} \mathrm{d}t \left\{ \frac{1}{2} \boldsymbol{b} \bullet \boldsymbol{b} + \boldsymbol{\lambda} \bullet (\dot{\boldsymbol{s}} - \boldsymbol{b} \times \boldsymbol{s}) \right\} \tag{1}$$

where $\boldsymbol{b} = 2\boldsymbol{h}/\hbar$, and $\boldsymbol{\lambda}$ is a (vector) Lagrange multiplier, and the momentum corresponding to $\boldsymbol{s}$. Note that this formulation is easy to generalize for more complex situations. For example, under dissipative conditions, it is possible to add a term proportional to the entropy of the two-level system, thus making possible a compromise between the energy spent and the entropy gained. Note too that the form of the cost functional above is not arbitrary: where the vector control field is a magnetic field acting on a spin-$\frac{1}{2}$ system, or an electromagnetic field for a charged two-level system, the (electro)magnetic energy would have the assumed form. For the sake of simplicity we scale the variables to get the following cost functional:

$$S = \int_{0}^{1} \mathrm{d}t \left\{ \frac{1}{2a} \boldsymbol{b} \bullet \boldsymbol{b} + \boldsymbol{\lambda} \bullet (\dot{\boldsymbol{s}} - \boldsymbol{b} \times \boldsymbol{s}) \right\} \tag{2}$$

where the constant a is introduced to have $\boldsymbol{s}$ and $\boldsymbol{\lambda}$ of the same length.

Not all of the resulting Euler–Lagrange equations

$$\boldsymbol{b} = a\boldsymbol{s} \times \boldsymbol{\lambda} \qquad \dot{\boldsymbol{s}} = \boldsymbol{b} \times \boldsymbol{s} \qquad \dot{\boldsymbol{\lambda}} = \boldsymbol{b} \times \boldsymbol{\lambda} \tag{3}$$

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 $s^2 = \boldsymbol{s} \bullet \boldsymbol{s}$, $\lambda^2 = \boldsymbol{\lambda} \bullet \boldsymbol{\lambda}$ and $\nu = \boldsymbol{\lambda} \bullet \boldsymbol{s} = \lambda s \cos(\theta)$, where θ is the angle between $\boldsymbol{\lambda}$ and $\boldsymbol{s}$. The equations of motion can be put in the equivalent form

$$\frac{\mathrm{d}}{\mathrm{d}[at]} \begin{pmatrix} \boldsymbol{s} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} -\boldsymbol{\lambda} \cdot \boldsymbol{s} & s^2 \\ -\lambda^2 & \boldsymbol{\lambda} \cdot \boldsymbol{s} \end{pmatrix} \begin{pmatrix} \boldsymbol{s} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} -\cos(\theta) & 1 \\ -1 & \cos(\theta) \end{pmatrix} \begin{pmatrix} \boldsymbol{s} \\ \boldsymbol{\lambda} \end{pmatrix} \tag{4}$$

whose solution reads

$$\begin{pmatrix} \boldsymbol{s} \\ \boldsymbol{\lambda} \end{pmatrix} = \frac{1}{\sin(\theta)} \begin{pmatrix} \sin(\theta - at\sin\theta) & \sin(at\sin\theta) \\ -\sin(at\sin\theta) & \sin(\theta + at\sin\theta) \end{pmatrix} \begin{pmatrix} \boldsymbol{s}(0) \\ \boldsymbol{\lambda}(0) \end{pmatrix}. \tag{5}$$

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

$$\boldsymbol{s}(t) = \frac{\sin(b(1-t))}{\sin(b)} \boldsymbol{s}_i + \frac{\sin(bt)}{\sin(b)} \boldsymbol{s}_f \tag{6}$$

where

$$\boldsymbol{b}(t) = \boldsymbol{b}(0) = \frac{\arcsin(\sin(\theta))}{\sin(\theta)} \boldsymbol{s}_i \times \boldsymbol{s}_f = (\theta + 2\pi n)\boldsymbol{s}_\perp = b_1(t; n)\boldsymbol{s}_\perp. \tag{7}$$

Equations (6) and (7) constitute the solution to the proposed problem and agree with the result of [20]. Observe that in the scaled variables that the magnitude of the field is essentially equal to the value of the angle between the initial and the final Bloch vectors. The solution, which corresponds to a rotation around $(-)\boldsymbol{s}_\perp$ at constant speed, from the initial Bloch vector to the final one, is not unique: due to the multivaluedness of the function arcsin, there is an infinite number of solutions. Each solution corresponds to a local minimum, the global minimum being the solution whose magnitude is equal to the angle between the initial and the final Bloch vector. The other solutions correspond to an integer number of turns followed by this angle, or to the case where the final Bloch vector is reached rotating the other way. Choices different from $\boldsymbol{\lambda}(0) = \boldsymbol{s}(1)$ are also meaningful, but should lie on the plane which contains the initial and final Bloch vectors. Observe that the solution breaks down when the initial and final vectors are antipodal. In this case there is an infinite number of solutions all of them expending 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 the minimum path on the Bloch sphere. The length l transversed by the tip of the Bloch vector is given by

$$l = \int_0^1 \left|\frac{\mathrm{d}\boldsymbol{s}}{\mathrm{d}t}\right| \mathrm{d}t = \int_0^1 |\boldsymbol{b} \times \boldsymbol{s}| \,\mathrm{d}t = s\int_0^1 b(t)|\sin(\theta(t))| \,\mathrm{d}t \leqslant s\int_0^1 b(t)\,\mathrm{d}t. \tag{8}$$

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 the Bloch vector, and if the Bloch vector transverses a longer path, it is necessary to have a larger average control field. This allows us to consider only vector controls pointing in the direction of $\boldsymbol{s}_i \times \boldsymbol{s}_f$. Making the ansatz

$$\boldsymbol{b}(t) = b(t)\boldsymbol{s}_\perp \tag{9}$$

after some algebra, we obtain

$$\boldsymbol{s}(t) = \frac{\sin\left(\theta - \int_0^t b(t')\,\mathrm{d}t'\right)}{\sin(\theta)}\boldsymbol{s}_i + \frac{\sin\left(\int_0^t b(t')\,\mathrm{d}t'\right)}{\sin(\theta)}\boldsymbol{s}_f \tag{10}$$

where b should satisfy the equality $\int_0^1 b(t)\,\mathrm{d}t = \theta$. 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 $\int_0^1 b^2(t)\,\mathrm{d}t = \theta^2 + \int_0^1 \delta^2(t)\,\mathrm{d}t$. Thus, the minimum is attained when the control vector field is constant from the initial until 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 $\boldsymbol{b} = \boldsymbol{s} \times \dot{\boldsymbol{s}} + f\boldsymbol{s}$, and the energy expended in the control $\int_0^1 b^2(t)\,\mathrm{d}t = \int_0^1 ((\dot{\boldsymbol{s}})^2 - (\boldsymbol{s}\cdot\dot{\boldsymbol{s}})^2 + f^2)\,\mathrm{d}t$. 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 equation (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 time necessary to perform a single quantum operation is generally short in low-dimensional condensed matter systems, which are the most promising candidates, one should also analyse possible limitations set by the rate at which control fields can be set. In particular, it is worth noting that the solution (7) 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

$$S = \int_0^1 \mathrm{d}t \left\{\frac{1}{2\Omega^2}\frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t} \bullet \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t} + \boldsymbol{\lambda} \bullet (\dot{\boldsymbol{s}} - \boldsymbol{b} \times \boldsymbol{s})\right\} \tag{11}$$

the solutions obtained above would also have been solutions of the new problem. In this case a whole set of new solutions arises, which are of constant magnitude but whose direction changes with time. It is easy to construct such solutions. If $\{\boldsymbol{b}(t), \boldsymbol{s}(t)\}$ is a solution of the Bloch equations, with a time dependent $b^2(t)$, then $\{\tilde{\boldsymbol{b}}(t) = \boldsymbol{b}(t) + f(t)\boldsymbol{s}, \boldsymbol{s}\}$ is also a solution, no matter how the function f is chosen. In particular, we can adjust f to obtain $\tilde{b}^2$ a constant, and make it also of minimum control field derivative. For instance, if we set

$\boldsymbol{s}(t) = \cos(\phi(t))\boldsymbol{s}_0(t) + \sin(\phi(t))\boldsymbol{s}_\perp$, where $\boldsymbol{s}_0$ is 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 $\boldsymbol{b}(t) = \theta\cos^2(\phi)\boldsymbol{s}_\perp - \dot\phi\boldsymbol{s}_\tau - \theta\sin(\phi)\cos(\phi)\boldsymbol{s}_0$ where $\boldsymbol{s}_\tau = \boldsymbol{s}_\perp \times \boldsymbol{s}_0$ is a unitary vector needed to define a time-dependent right triad $\{\boldsymbol{s}_0, \boldsymbol{s}_\tau, \boldsymbol{s}_\perp\}$. One can choose f as $f = \pm\sqrt{B^2 - \theta^2\cos^2(\phi) - \dot\phi^2}$, 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 $f^2 = \theta^2(\sin^2(\phi(t)) + \mu^2 t(2-t))$, and produces a new constant norm vector control $\tilde{\boldsymbol{b}}$ with magnitude $\theta\sqrt{1+\mu^2}$. This solution, of course, expends more energy than that previously found 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 $\boldsymbol{b}$ is

$$\ddot{\boldsymbol{b}} = -\Omega^2 \boldsymbol{s} \times \boldsymbol{\lambda} \tag{12}$$

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 into 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 to reach the maximum value necessary to have an average magnitude of at least θ. If the geodesic is not taken, the field should grow to a larger value and therefore, given that the time is fixed, it should grow at a faster pace so that it could not be the minimum solution sought.

Differentiating the equation (12) we obtain $\frac{\mathrm{d}^3\boldsymbol{b}}{\mathrm{d}t^3} = \boldsymbol{b} \times \frac{\mathrm{d}^2\boldsymbol{b}}{\mathrm{d}t^2}$, which immediately tells us that the second derivative of the vector control has constant norm. The first integral of this third-order equation, $\frac{\mathrm{d}^2\boldsymbol{b}}{\mathrm{d}t^2} = \boldsymbol{b} \times \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t} - \Omega^2\boldsymbol{s}_i \times \boldsymbol{s}_f$, where we have assumed $\boldsymbol{\lambda}(0) = \boldsymbol{s}_f$, can be solved under the assumption that the control vector is a second degree polynomial in t, with the result $\boldsymbol{b}(t) = \frac{\Omega^2|\sin(\theta)|}{2}t(1-t)\boldsymbol{s}_\perp = b_2(t)\boldsymbol{s}_\perp$. Numerical solution of these equations, without the ansatz made above, also leads to the same solutions. Before expressing $\boldsymbol{b}$ completely in terms of $\boldsymbol{s}_i$ and $\boldsymbol{s}_f$, we proceed to discuss the more general physical criterion in which one is interested in energy saving but with a limited rate of change of the vector control, through the cost functional

$$S = \int_0^1 \mathrm{d}t \left\{ \frac{1}{2a}\left(\boldsymbol{b} \bullet \boldsymbol{b} + \frac{1}{\omega^2}\frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t}\cdot\frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}t}\right) + \boldsymbol{\lambda} \bullet (\dot{\boldsymbol{s}} - \boldsymbol{b} \times \boldsymbol{s})\right\}. \tag{13}$$

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

$$\boldsymbol{b}(t) = a|\sin(\theta)|\left(1 - \frac{\cosh\omega\left(t-\frac{1}{2}\right)}{\cosh\left(\frac{\omega}{2}\right)}\right)\boldsymbol{s}_\perp = b_3(t)\boldsymbol{s}_\perp.$$

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

$$\begin{aligned} b_2(t;n) &= 6(\theta + 2\pi n)t(1-t) \\ b_3(t;n) &= \frac{\theta + 2\pi n}{1 - \frac{\tanh(\omega/2)}{\omega/2}}\left(1 - \frac{\cosh\left(\omega\left(t-\frac{1}{2}\right)\right)}{\cosh\left(\frac{\omega}{2}\right)}\right). \end{aligned} \tag{14}$$

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), perpendicular to the initial and final Bloch vectors, the cost functional can be written in purely geometric terms. If we set $\dot{\phi}(t) = b(t)$, $\phi(0) = 0$, then S can be expressed as

$$S = \frac{1}{2a}\int_0^{\bar{b}} b(\phi)\left(1 + \left(\frac{1}{\omega}\frac{\mathrm{d}b}{\mathrm{d}\phi}\right)^2\right)\mathrm{d}\phi \tag{15}$$

where $\bar{b}$ is the average magnitude of the control field, and ϕ the accumulated angle (or the arc length) traversed by the Bloch vector. Equation (15), just like equation (13), contains the other two cases: the first in the limit $1/\omega \to 0$, and the second in the limit $1/a \to 0$ but with $a\omega^2 = \Omega^2$ fixed. Of course, $b_1(t; n) = \lim_{1/\omega\to 0} b_3(t; n)$ and $b_2(t; n) = \lim_{1/a\to 0, a\omega^2=\Omega^2} b_3(t; n)$. The parameter ω can be used to define, in a precise way, the relative importance of the energy and the energy derivative terms.

Now we can use these results for a general one-qubit gate, which can be described by the unitary matrix [23]

$$U = \mathrm{e}^{\mathrm{i}\alpha} R_{\hat{n}}(\theta) = \mathrm{e}^{\mathrm{i}\alpha}\,\mathrm{e}^{-\mathrm{i}\theta\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}/2}, \tag{16}$$

where α is an unimportant phase and $R_{\hat{n}}(\theta)$ is a matrix which rotates Bloch vectors for an angle θ around the direction give by $\hat{\boldsymbol{n}}$. Thus the optimal field for the general one-qubit gate is given by

$$\boldsymbol{b}(t) = b_i(t)\hat{\boldsymbol{n}}$$

where the subscript refers to the particular optimization criterion. We illustrate this solution in the case of a Y gate, where the upper level is transformed in $(-|+\rangle + |-\rangle)/2$, which expressed in terms of Bloch vectors corresponds to the transformation $\boldsymbol{k} \to -\boldsymbol{i}$. Using the expressions found above we have the control fields

$$\boldsymbol{b}_1(t) = -\frac{\pi}{2}\boldsymbol{j} \qquad \boldsymbol{b}_2(t) = -3\pi t(1-t)\boldsymbol{j} \qquad \boldsymbol{b}_3(t) = -\frac{\omega\pi}{2(\omega - 2\tanh(\omega/2))}\boldsymbol{j}$$

obtained using the criteria of minimum energy, minimum average rate of the magnitude of the control and a combination of both, respectively. Although the minimum energy result is expected, and the second and third results are also intuitively clear, precise results can be found within the optimal formulation used here.

4. Single control field

Typical physical realizations of quantum bits are such that the Hamiltonian is given by $H = \hbar(b_x\sigma_x + b_y\sigma_y + b_z\sigma_z)/2$ or $H = \hbar(b_x\sigma_x + b_z\sigma_z)/2$, where b_z is a constant and b_x and b_y are classical control fields. Since we have at least two rotation generators, it is possible to generate any rotation. However, since b_z is a constant over which we do not have any control, intuition is no longer as good. Thus, even when two controls allow the alignment of the total classical field $\boldsymbol{b}$ along $\hat{\boldsymbol{n}}$, its magnitude cannot be changed, and we are no longer free to choose the time to realize the rotation. Moreover, we have no hints about the choice of control fields to make some compromise between energy consumption and growth rate of the control. A single control only worsens things. We can still generate any rotation, for example, using the $SU(2)$ decomposition

$$\mathrm{e}^{-\mathrm{i}b_z t_1\sigma_z}\,\mathrm{e}^{-\mathrm{i}\beta\sigma_x}\,\mathrm{e}^{-\mathrm{i}b_z(1-t_1)\sigma_z}. \tag{17}$$

Note, however, that this decomposition is useful if the second rotation by β is performed in a very short time interval, that is, with big fields and big field gradients, exactly what we want to avoid. Also, given a b_z and a gate, there is a minimum time which allows for the realization of the gate, which means that any rotation can be realized only if enough time is given (see [24]). In fact, in the absence of the control field, the Bloch vector precesses at the rate b_z around the z-axis. That is, if the given interval of time is normalized to one, Bloch vectors lying on meridians set apart for an angle greater than b_z, measured in the sense in which the Bloch vector precesses, cannot be reached. Thus, even when it exists, the solution is not trivial, unless we use large fields and gradients, and renounce any attempt to control the time interval in which the rotation is performed. Alternatively, we can write a decomposition like (17) with time-dependent coefficients, derive and set up a system of three ordinary differential equations, which is not simpler than the optimization approach (and a condition such as minimum energy should be added *a posteriori*).

Assuming the particular problem is solvable, we proceed to write an adequate cost functional,

$$S = \int_0^1 \mathrm{d}t \left(p\dot{q} - b_x p - b_z\sqrt{1-p^2}\sin(q) + \frac{1}{2a} b_x^2 \right)$$

where we have parametrized the Bloch vector according to $\boldsymbol{s} = (p, \sqrt{1-p^2}\cos(q), \sqrt{1-p^2}\sin(q))$, and written a classical Hamiltonian $H_{cl}(p,q) = \boldsymbol{s} \bullet \boldsymbol{b}$, with canonically conjugated variables p, q [25, 26]. Note also the appearance of a term proportional to the control energy spent. The equations of motion, equivalent to $\dot{\boldsymbol{s}} = \boldsymbol{b} \times \boldsymbol{s}$, are supplemented by the condition $b_x = ap = as_x$. When this constraint is used on the equations of motion

$$\dot{s}_x = -b_z s_y \qquad \dot{s}_y = b_z s_x - b_x s_z \qquad \dot{s}_z = b_x s_y$$

we get

$$\dot{s}_x = -b_z s_y \qquad \dot{s}_y = b_z s_x - a s_x s_z \qquad \dot{s}_z = a s_x s_y$$

from which we identify the constant of motion $as_x^2 + 2b_z s_z$. Using this constant of motion we obtain the equations

$$\dot{s}_x = -b_z s_y \qquad \dot{s}_y = \left(b_z - \frac{a^2}{2b_z} s_x^2(0) - a s_z(0) \right) s_x + \frac{a^2}{2b_z} s_x^3.$$

These equations, of Duffing type, resemble those of [24] for the optimal control variables and possess the constant of motion

$$\frac{b_z}{2} s_y^2 - \frac{1}{2} \left(\frac{a^2}{2b_z} s_x^2(0) - a s_z(0) - b_z \right) s_x^2 + \frac{a^2}{8b_z} s_x^4.$$

This last constant of motion allows us to derive

$$\dot{s}_x = -b_z s_y = \mp b_z \sqrt{A + B s_x^2 - C s_x^4},$$

with $A = s_x^2(0) + s_y^2(0) - a^2 s_x^4(0)/4 + ab_z s_z(0) s_x^2(0)$, $B = as_x^2(0)/2 - ab_z s_z(0) - b_z^2$, and $C = a/4$, which can be solved in terms of elliptic functions. In the case of the Y gate the motion equation is

$$\frac{\mathrm{d}s_x}{\mathrm{d}\tau} = \mp\sqrt{1 - \alpha^2 - (1 - 2\alpha^2)s_x^2 - \alpha^2 s_x^4} = \mp\sqrt{\left(1 - s_x^2\right)\left(1 - \alpha^2\left(1 - s_x^2\right)\right)},$$

where we have set $\tau = b_z t$ and $\alpha = a/(2b_z)$. Now we use the change of variables defined by

$$s_x = -\cos(y) \qquad \mathrm{d}s_x = \sin(y)\,\mathrm{d}y \qquad 1 - s_x^2 = \sin(y)$$

to obtain

$$\frac{\mathrm{d}y}{\mathrm{d}\tau} = \mp\sqrt{1 - \alpha^2 \sin^2(y)}.$$

Since $y(\tau = 0) = 0$ we get

$$s_x(\tau) = \pm cn(\alpha^2, \tau) \qquad s_x(t) = -cn\left(\left(\frac{a}{2b_z}\right)^2, b_z t\right).$$

The parameter a is chosen to have

$$s_x(1) = -cn\left(\left(\frac{a}{2b_z}\right)^2, b_z\right) = 0.$$

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 expended 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 the arrival from the initial to the final Bloch vector in one or other senses or after one or more complete turns. Finally, we applied the results to the general one-qubit gate and extended them to the case of a single control field minimizing the control energy, where physical intuition alone does not provide a reasonable solution.

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