On optimum Hamiltonians for state transformations

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Abstract. For a prescribed pair of quantum states $|\psi_I\rangle$ and $|\psi_F\rangle$ we establish an elementary derivation of the optimum Hamiltonian, under constraints on its eigenvalues, that generates the unitary transformation $|\psi_I\rangle \to |\psi_F\rangle$ in the shortest duration. The derivation is geometric in character and does not rely on variational calculus.

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Recently Carlini, *et al.* [1] considered the following problem: What is the optimum choice of the Hamiltonian, under a given set of constraints, such that the transformation between a designated pair of quantum states is achieved in the shortest possible time? Evidently this question is of relevance to the implementation of various algorithms in quantum computation (see, e.g., [1, 2] and references cited therein). Two specific examples for the constraints on the Hamiltonian are considered in [1], and the optimum solutions are obtained using the method of variational calculus.

The purpose of this paper is to show that analogous results can be obtained more directly by use of the symmetry properties of the quantum state space, hence avoiding the use of variational calculus. Our approach is closely related to the idea considered in [3], where an elementary derivation is provided for the minimum time required to transform one quantum state into another for a given Hamiltonian. The idea here is to reverse the argument to find the optimum choice of the Hamiltonian that achieves the transformation in the minimum time.

Consider a Hilbert space $\mathcal{H}^{n+1}$ of dimension $n+1$, and assume that an arbitrary pair of initial and final states $|\psi_I\rangle$ and $|\psi_F\rangle$ are specified. The task is to find the Hamiltonian H on $\mathcal{H}^{n+1}$ that generates the unitary transformation $|\psi_I\rangle \to |\psi_F\rangle = \mathrm{e}^{\mathrm{i}H\tau/\hbar}|\psi_I\rangle$ in shortest possible time τ. Clearly, if the differences between the eigenvalues of the Hamiltonian are allowed to take large values, then the value of τ can be made very small. This is because the 'speed' of a unitary evolution is proportional to the energy uncertainty (the so-called Anandan-Aharonov relation [4]). As a consequence, if the differences between eigenvalues can be made large, the energy uncertainty can also be made large. Hence we impose the constraint that the difference of the largest and the smallest eigenvalues of H be bounded by a constant.

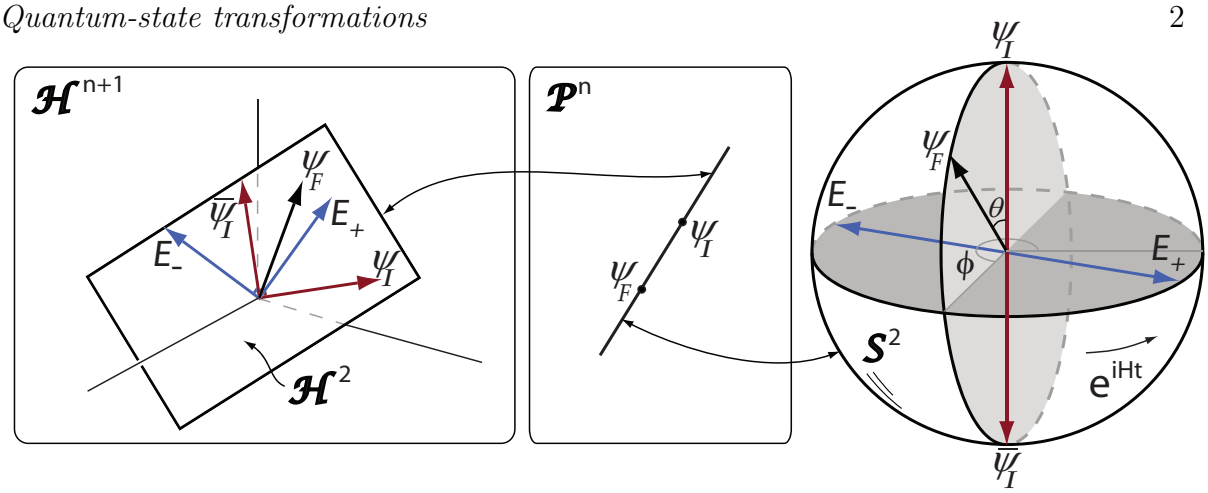

Figure 1. *Optimum state transformation.* In Hilbert space $\mathcal{H}^{n+1}$ one wishes to unitarily transform the initial state $|\psi_I\rangle$ into the final state $|\psi_F\rangle$ in the shortest possible time. In $\mathcal{H}^{n+1}$ there is a unique two-plane $\mathcal{H}^2$ that contains the two endpoints of the vectors $|\psi_I\rangle$ and $|\psi_F\rangle$, and the origin. In projective terms this plane corresponds to a complex projective line in the space $\mathcal{P}^n$ of pure states, and the two vectors $|\psi_I\rangle$ and $|\psi_F\rangle$ determine a pair of points on this line. The geodesic curve that joins these two points lies on this complex line, which in real terms is just a two-sphere S^2. Given a pair of points ψ_I and ψ_F on S^2 there is a unique great circle arc passing through these points. The most expedient transformation $|\psi_I\rangle \to |\psi_F\rangle$ is thus obtained by the rotation of S^2 around the axis that is orthogonal to the hemispherical plane containing ψ_I and ψ_F. The axis of rotation, in particular, corresponds to a pair of orthogonal states $|E_\pm\rangle$. The Hamiltonian that generates this rotation therefore takes the form $H = \lambda_+|E_+\rangle\langle E_+| + \lambda_-|E_-\rangle\langle E_-|$ for a pair of real parameters $\lambda_\pm$.

For the analysis of a problem of this kind it is useful to work directly with the space of rays through the origin of $\mathcal{H}^{n+1}$. This is just the complex projective space $\mathcal{P}^n$ of dimension n; each ray $|\varphi\rangle \in \mathcal{H}^{n+1}$ then corresponds to a point $\varphi \in \mathcal{P}^n$. Thus $\mathcal{P}^n$ can be thought of as the space of directions in $\mathcal{H}^{n+1}$. Now given a pair of points $\psi_I, \psi_F \in \mathcal{P}^n$ corresponding to the states $|\psi_I\rangle$ and $|\psi_F\rangle$ in $\mathcal{H}^{n+1}$ we can join these two points by a line. The points on this line correspond to all possible linear superpositions of the states $|\psi_I\rangle$ and $|\psi_F\rangle$. That is, the (complex) line in $\mathcal{P}^n$ corresponds to the two-dimensional subspace of $\mathcal{H}^{n+1}$ spanned by the two vectors $|\psi_I\rangle$ and $|\psi_F\rangle$ (see Figure 1). In real terms the complex line in $\mathcal{P}^n$ corresponds to a two-sphere (the so-called Bloch sphere) S^2, and the two states thus correspond to a pair of points on the surface of this two-sphere.

It is evident that there is a unique geodesic curve on S^2 that joins ψ_I and ψ_F; this is just the great circle arc passing through these two points (cf. [5, 6]). Therefore, the unitary transformation that takes the state $|\psi_I\rangle$ into $|\psi_F\rangle$ in the smallest possible time is achieved by a rotation of S^2 around the axis such that the geodesic curve joining ψ_I and ψ_F constitutes the equator associated with that axis. There are infinitely many other unitary transformations that achieve the transformation $|\psi_I\rangle \to |\psi_F\rangle$, however, all these transformations will require longer times to be realised because the corresponding trajectories are not geodesic curves.

We thus proceed to determine this axis of rotation. To this end let us write $|\bar{\psi}_I\rangle$ for the state orthogonal to the initial state $|\psi_I\rangle$ that is contained in the two-dimensional

span of the initial and final states in $\mathcal{H}^{n+1}$ (i.e. the antipodal point on S^2). Then the final state $|\psi_F\rangle$ can be written in the form

$$|\psi_F\rangle = \cos\tfrac{1}{2}\theta|\psi_I\rangle + \mathrm{e}^{\mathrm{i}(\phi+\pi/2)}\sin\tfrac{1}{2}\theta|\bar{\psi}_I\rangle. \tag{1}$$

Since both $|\psi_I\rangle$ and $|\psi_F\rangle$ are prespecified, the values of the two parameters θ, ϕ are known. Our objective now is to find the axis defined by a pair of antipodal points on S^2 for which $|\psi_I\rangle$ and $|\psi_F\rangle$ lie on the equator (see Figure 1). Since $|\psi_I\rangle$ and $|\bar{\psi}_I\rangle$ lie on the equator associated with the (E_+, E_-)-axis, conversely the two states $|E_+\rangle, |E_-\rangle$ lie on the equator associated with the $(\psi_I, \bar{\psi}_I)$-axis. Hence these states can be expressed as equal superpositions of $|\psi_I\rangle$ and $|\bar{\psi}_I\rangle$:

$$|E_+\rangle = \tfrac{1}{\sqrt{2}}\left(|\psi_I\rangle + \mathrm{e}^{\mathrm{i}\phi}|\bar{\psi}_I\rangle\right) \quad \text{and} \quad |E_-\rangle = \tfrac{1}{\sqrt{2}}\left(|\psi_I\rangle - \mathrm{e}^{\mathrm{i}\phi}|\bar{\psi}_I\rangle\right). \tag{2}$$

Solving (1) for $|\bar{\psi}_I\rangle$ and substituting the result into (2) we obtain

$$|E_+\rangle = \frac{1}{\sqrt{2}}\left[\left(1 + \mathrm{i}\frac{\cos\frac{1}{2}\theta}{\sin\frac{1}{2}\theta}\right)|\psi_I\rangle - \frac{\mathrm{i}}{\sin\frac{1}{2}\theta}|\psi_F\rangle\right] \tag{3}$$

and

$$|E_-\rangle = \frac{1}{\sqrt{2}}\left[\left(1 - \mathrm{i}\frac{\cos\frac{1}{2}\theta}{\sin\frac{1}{2}\theta}\right)|\psi_I\rangle + \frac{\mathrm{i}}{\sin\frac{1}{2}\theta}|\psi_F\rangle\right]. \tag{4}$$

These states thus determine the axis of rotation that we are seeking.

Now the unitary rotation that gives rise to the rotation of the two sphere about the axis $|E_+\rangle$ and $|E_-\rangle$ is generated by the Hamiltonian

$$H = \lambda_+|E_+\rangle\langle E_+| + \lambda_-|E_-\rangle\langle E_-| \tag{5}$$

for some choice of real parameters $\lambda_+ \neq \lambda_-$. Substituting (3) and (4) into (5) we can express this Hamiltonian in terms of the two input states:

$$\begin{aligned} H = {} & \frac{\lambda_+ + \lambda_-}{2\sin^2\frac{1}{2}\theta}\Big(|\psi_I\rangle\langle\psi_I| + |\psi_F\rangle\langle\psi_F|\Big) \\ & + \left[\frac{\lambda_+}{2}\left(\mathrm{i}\frac{1}{\sin\frac{1}{2}\theta} - \frac{\cos\frac{1}{2}\theta}{\sin^2\frac{1}{2}\theta}\right) - \frac{\lambda_-}{2}\left(\mathrm{i}\frac{1}{\sin\frac{1}{2}\theta} + \frac{\cos\frac{1}{2}\theta}{\sin^2\frac{1}{2}\theta}\right)\right]|\psi_I\rangle\langle\psi_F| \\ & + \left[\frac{\lambda_+}{2}\left(-\mathrm{i}\frac{1}{\sin\frac{1}{2}\theta} - \frac{\cos\frac{1}{2}\theta}{\sin^2\frac{1}{2}\theta}\right) - \frac{\lambda_-}{2}\left(-\mathrm{i}\frac{1}{\sin\frac{1}{2}\theta} + \frac{\cos\frac{1}{2}\theta}{\sin^2\frac{1}{2}\theta}\right)\right]|\psi_F\rangle\langle\psi_I|. \end{aligned} \tag{6}$$

Because the Hamiltonian in standard quantum mechanics is defined up to an overall additive constant, without loss of generality we may set $\lambda_+ - \lambda_- = \xi$, and hence, $\lambda_+ = -\lambda_- = \xi/2$, for some real parameter ξ. It then follows at once from (6) that

$$H = \mathrm{i}\xi\frac{1}{2\sin\frac{1}{2}\theta}|\psi_I\rangle\langle\psi_F| - \mathrm{i}\xi\frac{1}{2\sin\frac{1}{2}\theta}|\psi_F\rangle\langle\psi_I|. \tag{7}$$

Finally we shall impose the constraint that the difference of the largest and the smallest eigenvalues (here there are only two) of the Hamiltonian be given by 2ω. Since the eigenvalues of H in (7) are $\pm\xi/2\sin\frac{1}{2}\theta$ we have $\omega = \xi/2\sin\frac{1}{2}\theta$.

More generally, we may consider time dependent Hamiltonians. However, because of the constraint on the difference of the eigenvalues, the parameter ω cannot vary in

time. As a consequence the only time-dependence that can be introduced here is that associated with the overall magnitude of the Hamiltonian, which in itself does not affect the dynamics. Letting $h(t)$ denote this gauge term and $\mathbf{1}$ denote the identity operator, the optimum choice for the Hamiltonian can thus be written as

$$H = \mathrm{i}\omega|\psi_I\rangle\langle\psi_F| - \mathrm{i}\omega|\psi_F\rangle\langle\psi_I| + h(t)\mathbf{1}. \tag{8}$$

This is the main result obtained in [1]. We emphasise that this result is obtained here from the symmetry properties of the quantum state space, essentially only requiring the use of elementary trigonometry.

As noted above, the time it takes to achieve the transformation $|\psi_I\rangle \to |\psi_F\rangle$, under the unitary evolution generated by the Hamiltonian (8), can be determined from the Anandan-Aharonov relation [4], which states that the 'speed' of the evolution of a given quantum state is given by $2\hbar^{-1}\Delta H$, where ΔH is the standard deviation of the Hamiltonian. Note that the energy variance is a constant of motion. Therefore, calculating the standard deviation of (8) in the state, say, $|\psi_I\rangle$, we deduce that

$$\Delta H = \omega \sin\frac{1}{2}\theta. \tag{9}$$

On the other hand, the separation of the two states $|\psi_I\rangle$ and $|\psi_F\rangle$ is just the angle θ. We thus find that

$$\tau = \frac{\hbar\theta}{2\omega\sin\frac{1}{2}\theta}. \tag{10}$$

Alternatively, the time required for achieving the transformation can be determined more explicitly as follows. We take the Hamiltonian (8) and use it to calculate the time-dependence of the state explicitly as

$$\begin{aligned}|\psi(t)\rangle = & \left[\cos\left(\hbar^{-1}\omega t\sin\tfrac{1}{2}\theta\right) - \frac{\cos\frac{1}{2}\theta}{\sin\frac{1}{2}\theta}\sin\left(\hbar^{-1}\omega t\sin\tfrac{1}{2}\theta\right)\right]|\psi_I\rangle \\ & + \frac{1}{\sin\frac{1}{2}\theta}\sin\left(\hbar^{-1}\omega t\sin\tfrac{1}{2}\theta\right)|\psi_F\rangle,\end{aligned} \tag{11}$$

where $|\psi(0)\rangle = |\psi_I\rangle$. Evidently the coefficient of $|\psi_I\rangle$ in the state $|\psi(t)\rangle$ first vanishes at time $t = \hbar\theta/2\omega\sin\frac{1}{2}\theta$, while at that time the coefficient of $|\psi_F\rangle$ becomes unity.

In the foregoing material we have considered the case for which there is only one constraint on the Hamiltonian, namely, that the difference of the largest and the smallest eigenvalues be a constant. In a more realistic setup, however, there can be further constraints to limit the allowable operations. Although the use of variational calculus suggested in [1] is quite effective in general, it should be evident that within a given context, the determination of the optimum Hamiltonian that achieves the desired transformation simplifies considerably by taking into account the symmetries of the relevant state space.

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