

Optimal Control of Two-level Quantum System with Energy Cost Functional

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1 Multi-level Quantum Control System

We consider a forced (controlled) system represented by the state equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H_A |\psi(t)\rangle + i\hbar B |u(t)\rangle \quad (1) \quad \text{where}$$

where the system Hamiltonian operators H_A and B are taken to be matrices of dimensions $n \times n$ and $n \times m$ respectively.

Applying the classical variational principle the state vector of the quantum dynamical system (1) can be represented in the form as

$$|\psi(t)\rangle = U(t-t_0) |\psi(t_0)\rangle + \int_{t_0}^t U(t-\tau) B |u(\tau)\rangle d\tau \quad (2)$$

where U is the unitary matrix operator corresponding to the Hamiltonian H_A .

We assume that the eigenvalues a_1, a_2, \dots, a_n of the system matrix operator H_A are distinct. Then the adjoint of the unitary operator $U(t)$ assumes the representation

$$U^+(t) = \sum_{r=1}^n e^{\frac{i}{\hbar} a_r t} P_r = \sum_{r=1}^n g_r(t) P_r \quad (3)$$

with $g_r(t) = e^{\frac{i}{\hbar} a_r t}$, $n = 1, 2, \dots, n$.

Then the system state is given by taking $t_0 = 0$ with initial state $|\psi(0)\rangle$,

$$\begin{aligned} & |\psi(t)\rangle \\ &= U(t) \{ |\psi(0)\rangle + \int_0^t \sum_{r=1}^n g_r(\tau) P_r B |u(\tau)\rangle d\tau \} \\ &= U(t) \{ |\psi(0)\rangle + S_0 |W(t)\rangle \} \end{aligned} \quad (4)$$

$$S_0 = [P_1 B, P_2 B, \dots, P_n B] \quad (5)$$

$$|W(t)\rangle = \begin{bmatrix} |w_1(t)\rangle \\ |w_2(t)\rangle \\ \vdots \\ |w_n(t)\rangle \end{bmatrix} \quad (6)$$

with $|w_r(t)\rangle = \int_0^t g_r(\tau) |u(\tau)\rangle d\tau$.

1.1 Formulation of the Optimal Control Problem

Given a quantum mechanical control system described in section-1 in the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathcal{C}^n)$ by the time evolution state vector as

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H_A |\psi(t)\rangle + i\hbar B |u(t)\rangle \quad (7)$$

the optimal control problem is to find the controller $|u(t)\rangle \in \mathcal{L}^2(\mathcal{C}^m)$ which steers the initial state $|\psi(0)\rangle$ to the final state $|\psi(T)\rangle$ in \mathcal{C}^n

and minimizes the energy cost functional over the time interval $0 \leq t \leq T$ prescribed by

$$J(u) = \int_0^T \langle u^+(t)|Q|u(t) \rangle dt \quad (8)$$

where Q is a positive definite self-adjoint operator in the respective Hilbert space of the controller $|u(t)\rangle$.

Without loss of generality the operator Q in (8) of the cost functional may be taken to be unity operator I . Because, for a positive definite self-adjoint operator Q there exists a nonsingular operator P such that $Q = P^+P$.

Now put $|v(t)\rangle = P|u(t)\rangle$. Then (8) becomes

$$J = \int_0^T \langle v^+(t)|v(t) \rangle dt = \|\|v\rangle\|^2 \quad (9)$$

the norm of the vector $|v(t)\rangle$ and in this case, we have to replace $|u(t)\rangle$ by $|v(t)\rangle$ and B by BP^{-1} in (1).

Hence, in general, we can take the cost functional (8) to be the norm functional as

$$J(u) = \|\|u(t)\rangle\|^2. \quad (10)$$

1.2 Solution of the optimal problem

The solution of the optimal control problem is given in the form of the following theorem where the notations in the theorem will be clear when we describe optimal control of quantum two-state system.

Theorem

If the rank of controllability matrix S_0 defined by (5) of the system (7) is n , then the optimal control $|\hat{u}(t)\rangle$ minimizing the energy cost functional (10) which transfer the state of the system from the initial state $|\psi(0)\rangle$ to the target state $|\psi(T)\rangle$ can be formulated as

$$\begin{aligned} |\hat{u}(t)\rangle &= K(t)|Y\rangle \\ |Y\rangle &= U^{-1}(T)|\psi(T)\rangle - |\psi(0)\rangle, \quad 0 \leq t \leq T \end{aligned} \quad (11)$$

where $U^+(T)$ is given by (3) for $t = T$ and $K(t)$ is an $m \times n$ matrix function of $t(0 \leq t \leq T)$

written as

$$K(t) = F(t)S_0^+(S_0DS_0^+)^{-1} \quad (12)$$

with

$$F(t) = [I_m(g_1), I_m(g_2), \dots, I_m(g_n)],$$

and $I_m(g_r)$ is a scalar matrix as

$$I_m(g_r) = \begin{bmatrix} g_r(t) & 0 & \dots & 0 \\ 0 & g_r(t) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & g_r(t) \end{bmatrix}$$

1.2.1 Electron spin:Quantum two-state system

The spin state of an electron is represented on \mathcal{P}^2 in the basis formed by the eigenstates of the spin operator

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (13)$$

The control system is defined by

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = S_x |\psi(t)\rangle + i\hbar\alpha |u(t)\rangle \quad (14)$$

The eigenvalues of S_x are $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$. The eigenvectors are given by $|\uparrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and

$|\downarrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. The projection operators,

for $a_1 = \frac{\hbar}{2}$ and $a_2 = -\frac{\hbar}{2}$, are $P_{|\uparrow\rangle} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

and $P_{|\downarrow\rangle} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ respectively.

The adjoint of unitary operator $U(t)$ is

$$U^+(t) = e^{\frac{i}{\hbar} S_x t} = e^{ia_1 t} P_{|\uparrow\rangle} + e^{ia_2 t} P_{|\downarrow\rangle}.$$

The optimal control of the system can then be synthesized using the explicit formula

$$|\hat{u}(t)\rangle = K(t)|Y\rangle \quad (15)$$

$$K(t) = F(t)S_0^+(S_0DS_0^+)^{-1} \quad (16)$$

and

$$|Y\rangle = U^{-1}(T)|\psi(T)\rangle = -|\psi(0)\rangle \quad (17)$$

Now

$$S_0 = [P_1B, P_2B] = \alpha[P_1, P_2] \quad (18)$$

Then

$$S_0^+ = \alpha \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \quad (19)$$

Also

$$F(t) = [g_1(t)I, g_2(t)I] \quad (20)$$

Now we have

$$\begin{aligned} & F(t)S_0^+ \\ &= [g_1(t)I, g_2(t)I]\alpha \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \\ &= \alpha[g_1(t)P_1 + g_2(t)P_2] \end{aligned} \quad (21)$$

Again

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} \quad (22)$$

where

$$D_{11} = \begin{bmatrix} \langle g_1g_1 \rangle & 0 \\ 0 & \langle g_1g_1 \rangle \end{bmatrix} \quad (23)$$

and similarly

$$\begin{aligned} D_{12} &= \langle g_1(t)g_2(t) \rangle I, \\ D_{21} &= \langle g_2(t)g_1(t) \rangle I, \\ D_{22} &= \langle g_2(t)g_2(t) \rangle I. \end{aligned}$$

We then at once obtain

$$S_0DS_0^+ = \alpha^2(TP_1 + TP_2) = \alpha^2T. \quad (24)$$

Hence

$$(S_0DS_0^+)^{-1} = (\alpha^2T)^{-1} = \frac{1}{\alpha^2T}. \quad (25)$$

Now

$$\begin{aligned} K(t) &= F(t)S_0^+(S_0DS_0^+)^{-1} \\ &= \alpha[g_1(t)P_1 + g_2(t)P_2] \frac{1}{\alpha^2T} \\ &= \frac{1}{\alpha T}[g_1(t)P_1 + g_2(t)P_2] \end{aligned} \quad (26)$$

In special case, let us try to find $|\hat{u}(t)\rangle$ for which the system is transferred from $|\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ to the state $|\psi(T)\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. Then

$$\begin{aligned} |Y\rangle &= \left(e^{\frac{iT}{2}}P_1 + e^{-\frac{iT}{2}}P_1 \right) \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ &= \left(\frac{e^{\frac{iT}{2}}}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{e^{-\frac{iT}{2}}}{2} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \right) - \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{aligned} \quad (27)$$

Thus the optimal control of the two-level Pauli spin system minimizing the system is given by

$$\begin{aligned} |\hat{u}(t)\rangle &= \frac{1}{\alpha T}[g_1(t)P_1 + g_2(t)P_2]|Y\rangle \\ &= \frac{1}{\sqrt{2}} \left\{ e^{\frac{i(t+T)}{2}}|\uparrow\rangle + e^{-\frac{i(t+T)}{2}}|\downarrow\rangle \right\} - |\psi(0)\rangle \end{aligned} \quad (28)$$

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