Optimal control of quantum mechanical system with weighted energy cost functional

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Abstract

We have derived in this paper optimal control of quantum mechanical system with weighted energy cost function by representing the unitary operator in terms of the projection operators of the Hamiltonian of the control system. The admissible Hilbert space of controllers of the system is expressed as the direct sum of the Hilbert spaces corresponding to the weights of the controllers of the quantum mechanical system. The optimal control which steers the state of the quantum mechanical system from the initial state to a target state, minimizing the weighted energy, is formulated in terms of the controllability operator of the system.

1 Introduction

Stable operation is the fundamental prerequisite for proper functioning of any technological system [6, 7, 9]. The formulation of the quantum mechanical control system under this circumstances is seemed to be great challenge for the control theory. The wide perspectives of quantum mechanics are utilized in developing a new Emerging Field- Quantum Control System , a marriage of quantum physics and classical control theory, with applications to various branches of modern control theory. Quantum Control Theory is an Emerging Field with application to Modern Technology of Quantum Computer and Quantum Information Processing. In recent years, much attention has been focussed in designing and developing quantum control systems in Hilbert space [1, 2, 5].The problem of generating and controlling quantum beats (qbits) are important in developing high speed quantum computer and communication system.

In a recent paper [11], an abstract function space approach to system analysis for deriving the optimal control of multilevel quantum mechanical system with quadratic energy constraint has been outlined. The problems of existence and uniqueness of the minimum energy control of the system in infinite dimensional Hilbert space have been analyzed. The present paper is concerned with the synthesis of the optimal control of the quantum mechanical system in some more explicit form and a generalization of the abstract approach in solving the weighted energy problem of the system.

The paper is organized as follows. In section 2, we described the state equation of closed quantum system and multi-level quantum control system. In section 3, we formulated the optimal control problem. In section 4, we gave the solution of optimal control problem and described the minimum weighted energy control in terms of controllability Grammian operator. In section 5, we mention different directions in which our theory is applicable. The future direction of generalization of our method is also discussed.

2 Quantum Control System in Hilbert Space

In modelling a quantum mechanical control system, let us first consider the Schrödinger equation of state of a closed quantum system.

2.1 State Equation of Closed Quantum System

In absence of any external influence (control) the state vector $|\psi(t)\rangle$ of a closed quantum system changes smoothly in time t according to the time dependent Schrödinger equation[4]

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

where the Hamiltonian H is a self-adjoint operator in a Hilbert space $\mathcal{H}$.

The rigorous meaning of the differential equation is that, for any vector $|\phi\rangle \in \mathcal{H}$, the complex function $\langle\phi|\psi(t)\rangle$ satisfies the ordinary differential equation

$$i\hbar\frac{d}{dt}\langle\phi|\psi(t)\rangle = \langle\phi|H|\psi(t)\rangle \tag{2}$$

Let us assume that the Hamiltonian operator H has the discrete set of different eigenvalues $\{a_1, a_2, \ldots a_M\}$

with a_m a $d(m)$-fold degenerate eigenvalue of H having independent eigenvectors $u_{m1}, u_{m2}, \ldots u_{md(m)}$. Then H assumes the spectral representation [4, 10]

$$H = \sum_{m=1}^{M} \sum_{j=1}^{d(m)} a_m |u_{mj}\rangle\langle u_{mj}| = \sum_{m=1}^{M} a_m P_m \tag{3}$$

where

$$P_m = \sum_{j=1}^{d(m)} |u_{m_j}\rangle\langle u_{m_j}| \tag{4}$$

is the projection operator onto the subspace of eigenvectors of H with eigenvalue a_m.

The projection operators are pairwise orthogonal and P_n satisfies

$$\begin{array}{rcl} P_n P_m &=& \delta_{nm} P_n \\ \sum_{m=1}^{M} P_m &=& I \end{array} \tag{5}$$

The equation (2) can then be written as

$$i\hbar \frac{d}{dt} \langle\phi|\psi(t)\rangle = \sum_{m=1}^{M} a_m \langle\phi|P_m|\psi(t)\rangle \tag{6}$$

Now, since equation(6) is true for all $|\phi\rangle$, it is true, in particular, for vector of the form $P_n|\chi\rangle$ with $|\chi\rangle$ an arbitrary vector and hence

$$i\hbar \frac{d}{dt} \langle\chi|P_n|\psi(t)\rangle = \sum_{m=1}^{M} a_m \langle\chi|P_n P_m|\psi(t)\rangle \tag{7}$$

As the projectors P_n satisfy (5), the equation (7) yields the following system of ordinary differential equations

$$i\hbar \frac{d}{dt} \langle\chi|P_n|\psi(t)\rangle = a_n \langle\chi|P_n|\psi(t)\rangle \tag{8}$$

for $n = 1, 2, \ldots, M$ and for all $|\chi\rangle \in \mathcal{H}$.

The first order differential equation can be solved as

$$\langle\chi|P_n|\psi(t)\rangle = e^{-\frac{i}{\hbar} a_n (t-t_0)} \langle\chi|P_n|\psi(t_0)\rangle \tag{9}$$

Again, since $I = \sum_{m=1}^{M} P_m$ we have

$$\langle\chi|\psi(t)\rangle = \sum_{m=1}^{M} \langle\chi|P_m|\psi(t_0)\rangle \tag{10}$$

From (9) and (10) we have

$$\langle\chi|\psi(t)\rangle = \sum_{m=1}^{M} e^{-\frac{i}{\hbar} a_m (t-t_0)} \langle\chi|P_m|\psi(t_0)\rangle \tag{11}$$

The equation(11) holds for all $|\chi\rangle$. We thus get the explicit representation of the Schrödinger equation (1) of the state function as

$$|\psi(t)\rangle = \sum_{m=1}^{M} e^{-\frac{i}{\hbar} a_m (t-t_0)} P_m |\psi(t_0)\rangle \tag{12}$$

Applying the general theorem for an exponential function f of the operators as

$$f(H) = \sum_{m=1}^{M} f(a_m) P_m,$$

the state of the quantum system is represented in the usual form

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} H(t-t_0)} |\psi(t_0)\rangle \tag{13}$$

with the unitary operator

$$U(t-t_0) = e^{-\frac{i}{\hbar} H(t-t_0)} \tag{14}$$

2.2 State Space Representation of Quantum Mechanical Control System

Consider the forced (controlled) system represented by the state equation in Hilbert space $\mathcal{L}^2(\mathbb{C}^n)$

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H_A |\psi(t)\rangle + i\hbar B |u(t)\rangle \tag{15}$$

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

The matrix representation of the Hamiltonian operator has impact on quantum mechanics that solves quite successfully the basic problem of quantum system. A practical problem is afforded by the famous Pauli spin matrices [4], which should be regarded as the matrix representations of electron spin operators acting on two dimensional vector space $\mathbb{C}^2$ or Hilbert space $\mathcal{L}^2(\mathbb{C}^2)$. The operator B is used for distributing the input(control) signal. For example, the beam splitter is a quantum device and is used for distributing the optical (input) signal to QED system. Then the multi-level quantum system(15) may be viewed as the classical analogue of multi-variable control system.

Utilizing the rigorous treatment made in the previous subsection and applying the classical variational principle, the state vector of the quantum dynamical system (15) can be represented in the form as

$$|\psi(t)\rangle = U(t-t_0)|\psi(t_0\rangle + \int_{t_0}^{t} U(t-\tau) B |u(\tau)\rangle d\tau \tag{16}$$

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

Using the general formula (14) of the unitary operator we now represent the control system (16) in the following suitable form.

Let us assume, for simplicity, that $d(m) = 1$. That is, the eigenvalues $a_1, a_2, \ldots a_n$ of the system matrix operator H_A are distinct. Then the adjoint of the unitary operator $U(t)$ assumes the representation

$$U^{+}(t) = \sum_{r=1}^{n} e^{\frac{i}{\hbar} a_r t} P_r = \sum_{r=1}^{n} g_r(t) P_r \tag{17}$$

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

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

$$\begin{aligned} |\psi(t)\rangle &= U(t)\{|\psi(0)\rangle + \int_0^t \sum_{r=1}^n g_r(\tau) P_r B |u(\tau)\rangle d\tau\} \\ &= U(t)\{|\psi(0)\rangle + S_0 |W(t)\rangle\} \end{aligned} \tag{18}$$

where

$$S_0 = [P_1 B, P_2 B, \ldots, P_n B] \tag{19}$$

and

$$|W(t)\rangle = \begin{bmatrix} |w_1(t)\rangle \\ |w_2(t)\rangle \\ \vdots \\ |w_n(t)\rangle \end{bmatrix} \tag{20}$$

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

Definition. The operator S_0 formulated in (19)is defined to be quantum controllability operator of the quantum control system (15).

Remark: The operator S_0 may be compared with the controllability matrix $S_0 = [B, AB, \ldots, A^{n-1}B]$ of the well known [7, 8] linear classical control system represented by the vector matrix differential equation in R^n as $\dot{x}(t) = Ax(t) + Bu(t)$.

3 Formulation of the Weighted Energy Control Problem

Given a quantum mechanical control system described in subsection 2.2 in the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{C}^n)$ by the time evolution state vector as

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H_A|\psi(t)\rangle + i\hbar B|u(t)\rangle \tag{21}$$

the optimal control problem is to find the controller $|u(t)\rangle \in \mathcal{L}^2(\mathbb{C}^m)$ which steers the initial state $|\psi(0)\rangle$ to the final state $|\psi(t_f)\rangle$ in $\mathbb{C}^n$ and minimizes the energy cost functional over the time interval $0 \le t \le t_f$ prescribed by

$$J(u) = \int_0^{t_f} \langle u^+(t)|Q|u(t)\rangle dt \tag{22}$$

where $Q(t)$ is a positive definite self-adjoint operator in the Hilbert space $\mathcal{L}^2_Q(0, t_f, C^m)$ of the controller $|u(t)\rangle$.

In describing the specific control system, the operator $Q(t)$ is defined by a diagonal matrix of the form

$$Q(t) = \begin{bmatrix} q_1(t) & 0 & \ldots & 0 \\ 0 & q_2(t) & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & q_m(t) \end{bmatrix} \tag{23}$$

The cost functional (22) is then reduced to the form

$$J(u) = \int_0^{t_f} [q_1(t)\langle u_1(t)|u_1(t)\rangle| + \ldots + q_m(t)\langle u_m(t)|u_m(t)\rangle]dt \tag{24}$$

It follows that each controller $|u_r(t)\rangle \in \mathcal{L}^2_Q(0, t_f)$ is weighted by the positive function $q_r(t)$. It is known that the weight function $q_r(t)$ is used in system analysis to measure the efficiency of each controller $|u_r(t)\rangle$ of the dynamical system (21). Hence the admissible space of the controllers $|u(t)\rangle$ of the system is the Hilbert space expressed as the direct sum of the Hilbert spaces

$$\mathcal{L}^2_Q(0, t_f; C^m) = \bigoplus_{r=1}^m \mathcal{L}^2_{q_r}(0, t_f). \tag{25}$$

The inner product and norm of the Hilbert space $\mathcal{L}^2_{q_r}(0, t_f)$ are respectively defined by

$$\langle f|g\rangle_{q_r} = \int_0^{t_f} q_r(t)\langle f(t)|g(t)\rangle dt \tag{26}$$

and

$$\|f\|_{q_r} = (\int_0^{t_f} q_r(t)\langle f(t)|f(t)\rangle dt)^{1/2} \tag{27}$$

In view of the above notation, the cost functional $J(u)$ is then represented by the sum of square-norms on the Hilbert spaces as

$$J(u) = \||u\rangle\|^2_Q = \||u_1\rangle\|^2_{q_1} + \ldots + \||u_m\rangle\|^2_{q_m} \tag{28}$$

The optimal control problem of the quantum mechanical system (21) is to find the optimal controllers $|\hat{u}_r(t)\rangle \in \mathcal{L}^2_{q_r}(0, t_f)$ which steer the initial state $|\psi(0)\rangle$ to the final state $|\psi(t_f)\rangle$ in C^n and minimize the weighted energy functional defined in (28).

The existence and uniqueness of the optimal control of the system can be proved by generalizing Theorem-1 and Theorem-2 in paper [11]. The optimal control stated above can be shown to exist in a finite dimensional subspace of the Hilbert space $\mathcal{L}^2_Q(0, t_f; C^m)$.

4 Solution of the Optimal Control Problem

The analytical technique developed in paper [11] is now generalized to solve the weighted energy optimal control problem of the system.

In this general case, it follows from the state equations (18), (19) and (20) of the control system that all the eigenfunctions of the sequence $\{g_i(t)\}_1^n$ of the operator H_A of the system (21) are associated with each controller $|u_r(t)\rangle$. It also follows from the expression of the cost functional (28) that the controllers $|u_1(t)\rangle, \ldots, |u_m(t)\rangle$ belong to different Hilbert spaces. For instances, the controller $|u_r(t)\rangle$ weighted by the function $q_r(t)$ lies in the Hilbert space $\mathcal{L}^2_{q_r}(0, t_f)$.

As in section 4 of paper[11] we now construct m sequences of weighted orthonormal functions from the given sequence $\{g_i(t)\}_1^n$ as follows:

$$\{\theta_i^{q_1}\}_1^n, \{\theta_i^{q_2}\}_1^n, \ldots, \{\theta_i^{q_m}\}_1^n,$$

where $\{\theta_i^{q_r}\}_1^n$ is a finite sequence of functions orthonormal related to the weight function $q_r(t)$, and

$$g_i(t)=\sum_{k=1}^{i}\langle g_i,\theta_k^{q_r}(t)\rangle_{q_r}\theta_k^{q_r}(t) \tag{29}$$

with $i=1,2,\dots,n$ and $r=1,2,\dots,m$.

Let $M^2[0,T]$ be the linear manifold generated by the eigen functions $\{g_i(t), i=1,2,\dots n\}$ of the Hermitian operator H_A of the dynamical system in the Hilbert space $\mathcal{L}^2(\mathbb{C}^m)$.

We now construct an orthonormal basis $\{\theta_i^{q_r}\}_1^n$ corresponding to the weight function $q_r(t)$ of the linear manifold $M^2[0,T]$.

Using Gram-Schmidt orthogonalization process, let us construct an orthonormal functions $\{\theta_i^{q_r}(t), i=1,2\dots n\}$ as

$$\begin{array}{rcl}\beta_1 & = & g_1\\ \beta_i & = & g_i-\sum_{k=1}^{i-1}\langle g_i,\theta_k^{q_r}\rangle\theta_k^{q_r}\end{array} \tag{30}$$

where $\theta_1^{q_r}=\frac{\beta_1}{\|\beta_1\|}$ *and* $\theta_i^{q_r}=\frac{\beta_i}{\|\beta_i\|}$.

We elaborate the above in a few more steps:

$$\begin{array}{rcl}\beta_1 & = & g_1\\ \beta_2 & = & g_2-\langle g_2,\theta_1^{q_r}\rangle\theta_1^{q_r}\\ \beta_3 & = & g_3-\langle g_3,\theta_1^{q_r}\rangle\theta_1^{q_r}-\langle g_3,\theta_2^{q_r}\rangle\theta_2^{q_r}\\ \beta_4 & = & g_4-\langle g_4,\theta_1^{q_r}\rangle\theta_1^{q_r}-\langle g_4,\theta_2^{q_r}\rangle\theta_2^{q_r}-\langle g_4,\theta_3^{q_r}\rangle\theta_3^{q_r}\\ \dots & \dots & \dots\\ \beta_n & = & g_n-\langle g_n,\theta_1^{q_r}\rangle\theta_1^{q_r}-\langle g_n,\theta_2^{q_r}\rangle\theta_2^{q_r}-\langle g_n,\theta_3^{q_r}\rangle\theta_3^{q_r}\\ & & -\dots\langle g_n,\theta_{n-1}^{q_r}\rangle\theta_{n-1}^{q_r}\end{array}$$

with $\theta_1^{q_r}=\frac{\beta_1}{\|\beta_1\|}$, $\theta_2^{q_r}=\frac{\beta_2}{\|\beta_2\|}$, $\theta_3^{q_r}=\frac{\beta_3}{\|\beta_3\|}$ and so on $\theta_n^{q_r}=\frac{\beta_n}{\|\beta_n\|}$.

We now write the eigenfunctions $g_i(t)$ as

$$\begin{array}{rcl}g_1 & = & \langle g_1,\theta_1^{q_r}\rangle\theta_1^{q_r}\\ g_2 & = & \langle g_2,\theta_1^{q_r}\rangle\theta_1^{q_r}+\langle g_2,\theta_2^{q_r}\rangle\theta_2^{q_r}\\ g_3 & = & \langle g_3,\theta_1^{q_r}\rangle\theta_1^{q_r}+\langle g_3,\theta_2^{q_r}\rangle\theta_2^{q_r}+\langle g_3,\theta_3^{q_r}\rangle\theta_3^{q_r}\\ g_4 & = & \langle g_4,\theta_1^{q_r}\rangle\theta_1^{q_r}+\langle g_4,\theta_2^{q_r}\rangle\theta_2^{q_r}+\langle g_4,\theta_3^{q_r}\rangle\theta_3^{q_r}\\ & & +\langle g_4,\theta_4^{q_r}\rangle\theta_4^{q_r}\\ \dots & \dots & \dots\\ g_n & = & \langle g_n,\theta_1^{q_r}\rangle\theta_1^{q_r}+\langle g_n,\theta_2^{q_r}\rangle\theta_2^{q_r}+\langle g_n,\theta_3^{q_r}\rangle\theta_3^{q_r}+\\ & & +\langle g_n,\theta_4^{q_r}\rangle\theta_4^{q_r}+\dots+\langle g_n,\theta_n^{q_r}\rangle\theta_n^{q_r}\end{array}$$

In a compact form we have

$$\begin{array}{rcl}g_i(t) & = & \|\beta_i\|\theta_i^{q_r}(t)+\sum_{k=1}^{i}\langle g_i,\theta_k^{q_r}\rangle\theta_k^{q_r}(t)=\\ & = & \sum_{k=1}^{i}\langle g_i,\theta_k^{q_r}\rangle\theta_k^{q_r}(t),\ i=1,2,\dots n.\end{array} \tag{31}$$

Using the representations of the functions $g_i(t)$, $i=1,2,\dots n$ given in (31), the adjoint $U^+(t)$ operator defined in (17) can be represented in terms of the orthonormal functions $\theta_i^{q_r}(t), i=1,2,\dots n$

as

$$U^+(t)=\sum_{i=1}^{n}A_i\theta_i^{q_r}(t) \tag{32}$$

where

$$A_i=\langle g_i,\theta_i^{q_r}\rangle P_i+\langle g_{i+1},\theta_i^{q_r}\rangle P_{i+1}+\dots+\langle g_n,\theta_i^{q_r}\rangle P_n \tag{33}$$

With elaboration we have

$$\begin{array}{rl} & \sum_{i=1}^{n}g_i(t)P_i\\ = & g_1(t)P_1+g_2(t)P_2+g_3(t)P_3+g_4(t)P_4+\dots\\ & +g_n(t)P_n\\ = & \langle g_1,\theta_1^{q_r}\rangle\theta_1^{q_r}P_1\\ & +\langle g_2,\theta_1^{q_r}\rangle\theta_1^{q_r}P_2+\langle g_2,\theta_2^{q_r}\rangle\theta_2^{q_r}P_2\\ & +\langle g_3,\theta_1^{q_r}\rangle\theta_1^{q_r}P_3+\langle g_3,\theta_2^{q_r}\rangle\theta_2^{q_r}P_3+\langle g_3,\theta_3^{q_r}\rangle\theta_3^{q_r}P_3\\ & +\langle g_4,\theta_1^{q_r}\rangle\theta_1^{q_r}P_4+\langle g_4,\theta_2^{q_r}\rangle\theta_2^{q_r}P_4+\langle g_4,\theta_3^{q_r}\rangle\theta_3^{q_r}P_4\\ & +\langle g_4,\theta_4^{q_r}\rangle\theta_4^{q_r}P_4\\ & \dots\dots\dots\dots\\ & +\langle g_n,\theta_1^{q_r}\rangle\theta_1^{q_r}P_n+\langle g_n,\theta_2^{q_r}\rangle\theta_2^{q_r}P_n\\ & +\langle g_n,\theta_3^{q_r}\rangle\theta_3^{q_r}P_n+\dots\langle g_n,\theta_n^{q_r}\rangle\theta_n^{q_r}P_n\\ = & A_1\theta_1^{q_r}(t)+A_2\theta_2^{q_r}(t)+A_3\theta_3^{q_r}(t)+A_4\theta_4^{q_r}(t)\\ & +\dots+A_n\theta_n^{q_r}(t)\end{array} \tag{34}$$

where

$$\begin{array}{rcl}A_1 & = & \langle g_1,\theta_1^{q_r}\rangle P_1+\langle g_2,\theta_1^{q_r}\rangle P_2+\langle g_3,\theta_1^{q_r}\rangle P_3\\ & & +\langle g_4,\theta_1^{q_r}\rangle P_4+\dots+\langle g_n,\theta_1^{q_r}\rangle P_n\\ A_2 & = & \langle g_2,\theta_2^{q_r}\rangle P_2+\langle g_3,\theta_2^{q_r}\rangle P_3+\langle g_4,\theta_2^{q_r}\rangle P_4\\ & & +\dots+\langle g_n,\theta_2^{q_r}\rangle P_n\\ A_3 & = & \langle g_3,\theta_3^{q_r}\rangle P_3+\langle g_4,\theta_3^{q_r}\rangle P_4+\dots+\langle g_n,\theta_3^{q_r}\rangle P_n\\ & & \dots\dots\dots\dots\\ A_n & = & \langle g_n,\theta_n^{q_r}\rangle P_n.\end{array} \tag{35}$$

Then using (32) the state vector $|\psi(t)\rangle$ described in (16) of the dynamical system(21) may be represented as

$$\begin{array}{rcl}|\psi(t)\rangle & = & U(t)|\psi(0)\rangle+\int_0^t U(t-\tau)B|u(\tau)\rangle d\tau\\ & = & U(t)|\psi(0)\rangle+U(t)\int_0^t U^+(\tau)B|u(\tau)\rangle d\tau\\ & = & U(t)\{|\psi(0)\rangle+\int_0^t U^+(\tau)B|u(\tau)\rangle d\tau\}\\ & = & U(t)\{|\psi(0)\rangle+\int_0^t\sum_{i=1}^{n}A_i\theta_i^{q_r}(\tau)B|u(\tau)\rangle d\tau\}\\ & = & U(t)\{|\psi(0)\rangle+\sum_{i=1}^{n}A_iB\int_0^t\theta_i^{q_r}(\tau)|u(\tau)\rangle d\tau\}\\ & = & U(t)\{|\psi(0)\rangle+S|V(t)\rangle\}\end{array} \tag{36}$$

where

$$S=[A_1B,A_2B,\dots A_nB] \tag{37}$$

and

$$|V(t)\rangle=\begin{bmatrix}|v_1(t)\rangle\\ |v_2(t)\rangle\\ \vdots\\ |v_n(t)\rangle\end{bmatrix},|v_i(t)\rangle=\int_0^t\theta_i^{q_r}(\tau)|u(\tau)\rangle d\tau \tag{38}$$

where $|u(\tau)\rangle$ is a $m\times 1$ column vector.

Putting the values of A_i's in (37) from (35) we get the algebraic relation

$$\begin{aligned}
& S \\
= {} & [A_1B, A_2B, \ldots, A_nB] \\
= {} & [\langle g_1, \theta_1^{q_r}\rangle P_1B + \ldots + \langle g_n, \theta_1^{q_r}\rangle P_nB, \ldots, \langle g_n, \theta_n^{q_r}\rangle P_nB] \\
= {} & [P_1B, P_2B, \ldots, P_nB]. \\
& \begin{pmatrix} \langle g_1, \theta_1^{q_r}\rangle I_m & 0 & \cdots & 0 \\ \langle g_2, \theta_1^{q_r}\rangle I_m & \langle g_2, \theta_2^{q_r}\rangle I_m & \cdots & 0 \\ \langle g_3, \theta_1^{q_r}\rangle I_m & \langle g_2, \theta_2^{q_r}\rangle I_m & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ \langle g_n, \theta_1^{q_r}\rangle I_m & \langle g_n, \theta_2^{q_r}\rangle I_m & \cdots & \langle g_n, \theta_n^{q_r}\rangle I_m \end{pmatrix} \\
= {} & S_0\triangle
\end{aligned} \tag{39}$$

where S_0 is given in (19) and $\triangle$ is a nonsingular lower triangular matrix given by

$$\triangle = \begin{bmatrix} \triangle_{11} & 0 & 0 & \ldots & 0 \\ \triangle_{21} & \triangle_{22} & 0 & \ldots & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \\ \triangle_{n1} & \triangle_{n2} & \triangle_{n3} & \ldots & \triangle_{nn} \end{bmatrix} \tag{40}$$

with $\triangle_{ik}$'s are the scalar matrices of order m expressed as

$$\triangle_{ik} = diag\{\langle g_i, \theta_k^{q_r}\rangle, \langle g_i, \theta_k^{q_r}\rangle, \ldots \langle g_i, \theta_k^{q_r}\rangle\},\ i \geq k \tag{41}$$

and $\triangle_{ik} = 0$, the null matrix of order m, for $i < k$.

Hence comparing the representation of the state function in (18) and (36) we get

$$W(t) = \triangle|V(t)\rangle. \tag{42}$$

Now we are in a position to solve the weighted optimal control problem.

Replacing the functions $g_i(t)$ from (29) we first calculate the components $|\omega_1(t)\rangle$, $|\omega_2(t)\rangle, |\omega_3(t)\rangle, \ldots, |\omega_n(t)\rangle$ of

$$|W(t)\rangle = [|w_1(t)\rangle, \ldots, |w_n(t)\rangle]^T \tag{43}$$

with $|w_i(t)\rangle = \int_0^t g_i(\tau)|u(\tau)\rangle d\tau$.

Before doing that we first write down the eigenfunction $g_i(t)$ with different weights $q_1, q_2, \ldots, q_m$ as

$$\begin{aligned}
g_1 &= \langle g_1, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1} \\
g_2 &= \langle g_2, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1} + \langle g_2, \theta_2^{q_1}\rangle_{q_1}\theta_2^{q_1} \\
g_3 &= \langle g_3, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1} + \langle g_3, \theta_2^{q_1}\rangle_{q_1}\theta_2^{q_1} + \langle g_3, \theta_3^{q_1}\rangle_{q_1}\theta_3^{q_1} \\
g_4 &= \langle g_4, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1} + \langle g_4, \theta_2^{q_1}\rangle_{q_1}\theta_2^{q_1} + \langle g_4, \theta_3^{q_1}\rangle_{q_1}\theta_3^{q_1} \\
&\quad + \langle g_4, \theta_4^{q_1}\rangle_{q_1}\theta_4^{q_1} \\
\cdots & \cdots \cdots \\
g_n &= \langle g_n, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1} + \langle g_n, \theta_2^{q_1}\rangle_{q_1}\theta_2^{q_1} + \langle g_n, \theta_3^{q_1}\rangle_{q_1}\theta_3^{q_1} + \\
&\quad + \langle g_n, \theta_4^{q_1}\rangle_{q_1}\theta_4^{q_1} + \ldots + \langle g_n, \theta_n^{q_1}\rangle_{q_1}\theta_n^{q_1}
\end{aligned}$$

with weight q_1 and then

$$\begin{aligned}
g_1 &= \langle g_1, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} \\
g_2 &= \langle g_2, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} + \langle g_2, \theta_2^{q_2}\rangle_{q_2}\theta_2^{q_2} \\
g_3 &= \langle g_3, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} + \langle g_3, \theta_2^{q_2}\rangle_{q_2}\theta_2^{q_2} + \langle g_3, \theta_3^{q_2}\rangle_{q_2}\theta_3^{q_2} \\
g_4 &= \langle g_4, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} + \langle g_4, \theta_2^{q_2}\rangle_{q_2}\theta_2^{q_2} + \langle g_4, \theta_3^{q_2}\rangle_{q_2}\theta_3^{q_2} \\
&\quad + \langle g_4, \theta_4^{q_2}\rangle_{q_2}\theta_4^{q_2} \\
\cdots & \cdots \cdots \\
g_n &= \langle g_n, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} + \langle g_n, \theta_2^{q_2}\rangle_{q_2}\theta_2^{q_2} + \langle g_n, \theta_3^{q_2}\rangle_{q_2}\theta_3^{q_2} + \\
&\quad + \langle g_n, \theta_4^{q_2}\rangle_{q_2}\theta_4^{q_2} + \ldots + \langle g_n, \theta_n^{q_2}\rangle_{q_2}\theta_n^{q_2}
\end{aligned}$$

with weight q_2 and so on with weight q_m

$$\begin{aligned}
g_1 &= \langle g_1, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m} \\
g_2 &= \langle g_2, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m} + \langle g_2, \theta_2^{q_m}\rangle_{q_m}\theta_2^{q_m} \\
g_3 &= \langle g_3, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m} + \langle g_3, \theta_2^{q_m}\rangle_{q_m}\theta_2^{q_m} + \langle g_3, \theta_3^{q_m}\rangle_{q_m}\theta_3^{q_m} \\
g_4 &= \langle g_4, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m} + \langle g_4, \theta_2^{q_m}\rangle_{q_m}\theta_2^{q_m} + \langle g_4, \theta_3^{q_m}\rangle_{q_m}\theta_3^{q_m} \\
&\quad + \langle g_4, \theta_4^{q_m}\rangle_{q_m}\theta_4^{q_m} \\
\cdots & \cdots \cdots \\
g_n &= \langle g_n, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m} + \langle g_n, \theta_2^{q_m}\rangle_{q_m}\theta_2^{q_m} + \langle g_n, \theta_3^{q_m}\rangle_{q_m}\theta_3^{q_m} + \\
&\quad + \langle g_n, \theta_4^{q_m}\rangle_{q_m}\theta_4^{q_m} + \ldots + \langle g_n, \theta_n^{q_m}\rangle_{q_m}\theta_n^{q_m}
\end{aligned}$$

$$\begin{aligned}
& |\omega_1(t)\rangle \\
= {} & \int_0^t g_1(\tau)|u(\tau)\rangle d\tau \\
= {} & \int_0^t [\langle g_1, \theta_1^{q_1}\rangle_{q_1}\theta_1^{q_1}, \langle g_1, \theta_1^{q_2}\rangle_{q_2}\theta_1^{q_2} \ldots, \langle g_1, \theta_1^{q_m}\rangle_{q_m}\theta_1^{q_m}]. \\
& \begin{bmatrix} |u_1(\tau)\rangle \\ |u_2(\tau)\rangle \\ \vdots \\ |u_m(\tau)\rangle \end{bmatrix} d\tau \\
= {} & \begin{bmatrix} \langle g_1, \theta_1^{q_1}\rangle_{q_1} & 0 & \ldots & 0 \\ 0 & \langle g_1, \theta_1^{q_2}\rangle_{q_2} & \ldots & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ 0 & 0 & \ldots & \langle g_1, \theta_1^{q_m}\rangle_{q_m} \end{bmatrix}. \\
& \begin{bmatrix} \int_0^t \theta_1^{q_1}|u_1(\tau)\rangle d\tau \\ \int_0^t \theta_1^{q_2}|u_2(\tau)\rangle d\tau \\ \vdots \\ \int_0^t \theta_1^{q_m}|u_m(\tau)\rangle d\tau \end{bmatrix} \\
= {} & c_{11}|v_1(t)\rangle.
\end{aligned} \tag{44}$$

Similarly

$|\omega_2(t)\rangle = c_{21}|v_1(t)\rangle + c_{22}|v_2(t)\rangle$,

$|\omega_3(t)\rangle = c_{31}|v_1(t)\rangle + c_{32}|v_2(t)\rangle + c_{33}|v_3(t)\rangle$,

$|\omega_n(t)\rangle =$
$c_{n1}|v_1(t)\rangle + c_{n2}|v_2(t)\rangle + c_{n3}|v_3(t)\rangle \ldots c_{nn}|v_n(t)\rangle$.

Hence

$$\begin{aligned}
& |W(t)\rangle \\
= {} & \begin{bmatrix} c_{11}|v_1(t)\rangle \\ c_{21}|v_1(t)\rangle + c_{22}|v_2(t)\rangle \\ c_{31}|v_1(t)\rangle + c_{32}|v_2(t)\rangle + c_{33}|v_3(t)\rangle \\ c_{n1}|v_1(t)\rangle + c_{n2}|v_2(t)\rangle + c_{n3}|v_3(t)\rangle \ldots c_{nn}|v_n(t)\rangle \end{bmatrix}
\end{aligned} \tag{45}$$

Thus

$$\begin{aligned}
|W(t)\rangle &= \begin{bmatrix} c_{11} & 0 & 0 & \ldots & 0 \\ c_{21} & c_{22} & 0 & \ldots & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \\ c_{n1} & c_{n2} & c_{n3} & \ldots & c_{nn} \end{bmatrix} \begin{bmatrix} |v_1(\tau)\rangle \\ |v_2(\tau)\rangle \\ \vdots \\ |v_n(\tau)\rangle \end{bmatrix} \\
&= \triangle_Q|V_Q(t)\rangle,
\end{aligned} \tag{46}$$

Δ_Q being a lower triangular matrix defined by

$$\triangle_Q = \begin{bmatrix} C_{11} & 0 & 0 & \ldots & 0 \\ C_{21} & C_{22} & 0 & \ldots & 0 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots & \\ C_{n1} & C_{n2} & C_{n3} & \ldots & C_{nn} \end{bmatrix} \tag{47}$$

in which C_{ij}'s are the diagonal submatrices described as

$$C_{ij} = \begin{bmatrix} \langle g_i, \theta_j^{q_1} \rangle_{q_1} & 0 & 0 & \dots & 0 \\ 0 & \langle g_i, \theta_j^{q_2} \rangle_{q_2} & 0 & \dots & 0 \\ \dots\dots & \dots\dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \langle g_i, \theta_j^{q_m} \rangle_{q_m} \end{bmatrix} \tag{48}$$

Hence we get

$$\begin{aligned} |\psi(t)\rangle &= U(t)\{|\psi(0)\rangle + S_0|W(t)\rangle\} \\ &= U(t)\{|\psi(0)\rangle + S_0\triangle_Q|V_Q(t)\rangle\} \\ &= U(t)\{|\psi(0)\rangle + S_Q|V_Q(t)\rangle\} \end{aligned} \tag{49}$$

with

$$S_Q = S_0\Delta_Q. \tag{50}$$

Under the above transformation, the dynamical problem stated in section 3 is thus transformed into the following algebraic problem of norm minimization as follows:

When the state norm $|\psi(t)\rangle$ of the dynamical system (21) is transformed from the initial state $|\psi(0)\rangle$ to the state $|\psi(t_f)\rangle$ after time t_f, then putting $t = t_f$ in (49) we get

$$S_Q|V_Q(t_f)\rangle = |Y_f\rangle \tag{51}$$

where

$$|Y_f\rangle = U^\dagger(t_f)|\psi(t_f)\rangle - |\psi(0)\rangle. \tag{52}$$

The optimal solution of the algebraic problem is described by the pseudo-inverse S_Q^* of the operator S_Q as [5]

$$|\hat{V}_Q\rangle = S_Q^*|Y_f\rangle \tag{53}$$

where $S_Q^* = S_Q^\dagger(S_Q S_Q^\dagger)^{-1}$ with $\min\|V_Q\| = \min\|\hat{u}_Q\|$ which follows from the property of orthonormal functions.

The optimal control $|\hat{u}(t)\rangle$ is now described immediately as follows:

Lemma -1.

If the rank of controllability operator S_0 given in (9) of the dynamical system (5) be n, then the operator S_Q is of rank n.

Proof.

The proof follows from the relation $S_Q = S_0\Delta_Q$ and the fact that the triangular matrix Δ_Q is nonsingular.

Lemma-2.

Let Δ_Q be a lower triangular matrix defined by (36). Then the product $\Delta_Q\Delta_Q^\dagger = D_Q$ is a nonsingular symmetric matrix described by

$$D_Q = \begin{bmatrix} D_{11} & D_{12} & D_{13} & \dots & D_{1n} \\ D_{21} & D_{22} & D_{23} & \dots & D_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ D_{n1} & D_{n2} & D_{n3} & \dots & D_{nn} \end{bmatrix} \tag{54}$$

where D_{ij}'s are diagonal matrices

$$D_{ij} = \begin{bmatrix} \langle g_i, g_j \rangle_{q_1} & 0 & 0 & \dots & 0 \\ 0 & \langle g_i, g_j \rangle_{q_2} & 0 & \dots & 0 \\ \dots\dots & \dots\dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & \langle g_i, g_j \rangle_{q_m} \end{bmatrix} \tag{55}$$

Proof.

The proof of the lemma is similar to that of Lemma - 1. In this case the relations in (29) and (50) are used in finding the product $\Delta_Q\Delta_Q^\dagger$.

We can now formulate the optimal solution of the weighted energy problem in terms of the generalized pseudo- inverse of the controllability operator S_Q by the following theorem:

Theorem - 1. If the dynamical system(21) is controllable, then there exists a unique optimal control $|\hat{u}_Q(t)\rangle \in \mathcal{L}_Q^2(0, t_f; C^m)$ which minimizes the cost functional $J(u)$ defined in (28) at $|u(t)\rangle = |\hat{u}_Q(t)\rangle$ and steers the state $|\psi(t)\rangle$ of the system from $|\psi(0)\rangle$ to $|\psi(t_f)\rangle$ in time t_f. The optimal control can be formulated as

$$|\hat{u}_Q(t)\rangle = G_Q(t)|\hat{V}_Q\rangle \tag{56}$$

where $G_Q(t) = [G_1(t) \vdots G_2(t) \vdots \dots \vdots G_n(t)]$ in which

$$G_i(t) = \begin{bmatrix} \theta_i^{q_1}(t) & 0 & \dots & 0 \\ 0 & \theta_i^{q_2}(t) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \theta_i^{q_m}(t) \end{bmatrix} \tag{57}$$

and

$$\begin{aligned} |\hat{V}_Q\rangle &= S_Q^*|Y_f\rangle \\ |Y_f\rangle &= U^\dagger(t_f)|\psi_{t_f}\rangle - |\psi_0\rangle, \end{aligned} \tag{58}$$

S_Q^* being the generalized inverse of the matrix S_Q described as [11]

$$S_Q^* = S_Q^\dagger(S_Q S_Q^\dagger)^{-1} \tag{59}$$

Proof.

The proof follows immediately when one considers the Fourier generalized expansion of $|u_r(t)\rangle$ in terms of the orthonormal functions

$$\theta_1^{q_r}(t), \dots, \theta_n^{q_r}(t) \tag{60}$$

and uses the state equation given in (49).

Corollary.

The optimal control described by (56) is formulated in explicit form in terms of the eigenfunctions $g_1(t), g_2(t), \dots g_m(t)$ of the system operator H_A of the dynamical system (21) as

$$|\hat{u}_Q(t)\rangle = K_Q(t)|Y_f\rangle \tag{61}$$

where

$$K_Q(t) = F(t)S_0^\dagger(S_0 D_Q S_0^\dagger)^{-1} \tag{62}$$

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

$$I_m(g_r(t)) = \begin{bmatrix} g_r(t) & 0 & \dots & 0 \\ 0 & g_r(t) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & g_r(t) \end{bmatrix} \tag{63}$$

Proof.

The proof of the corollary follows when one uses the relations defined in (29) and (38) and Lemma - 2.

Remark.

The matrix D_Q is a generalized Grammian matrix of the set of functions $\{g_i(t)\}_1^n$ with respect to the weight functions $q_1(t), q_2(t), \ldots, q_m(t)$ of the controllers of the dynamical system (21). The matrix $S_0 D_Q S_0^\dagger$ is an equivalent form of controllability Grammian matrix of the system. Again, the analytical procedure described in this section can be utilized to choose the weight functions of the controllers of a control process.

5 Conclusion

The optimal control of a quantum mechanical system has been reduced to an optimal problem of algebraic system and the optimal vector of the minimum norm has been solved by the method of pseudo-inverse. The importance of this study lies in the fact that the optimal control with minimum weighted energy has been expressed in terms of the eigenstates of the multilevel quantum system. It may be pointed out that the eigenstates of the Hamiltonian operator of the system play important role in quantum computing. The formulation of the optimal control in terms of controllability[6, 7, 9] Grammian operator $S_0 D S_0^+$ of the quantum mechanical system has been discussed. The formulation of the quantum field require in steering the quantum particles such as electron spin$\frac{1}{2}$ and photons from one state to another state is receiving much attention in recent years of solving computational problems of quantum computer. The optimal control vector $|\hat{u}\rangle$ is also useful in computing the special energy operator $\hat{J}_{\hat{u}} = |\hat{u}(t)\rangle\langle\hat{u}(t)|$ of the quantum control system. A generalization of the direct method outlined in this paper in solving the weighted energy minimization problem of time dependent quantum system and their applications in quantum domain can be studied. The technology that we have developed can also be used in laser pulse design and molecular dynamics phenomena.

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