Energy Optimal Interpolation in Quantum Evolution

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Abstract
We introduce the concept of interpolation in quantum evolution and present a general framework to find the energy optimal Hamiltonian for a quantum system evolving among a given set of middle states using variational and geometric methods. The quantum brachistochrone problem is proved as a special case.

1 Introduction

Recently the Quantum Brachistochrone Problem (QBP) proposed by Carlini, et al. [1] has become a hot topic. The aim of QBP is to find the time optimal Hamiltonian under a given set of constraints for the quantum evolution between two given states.

In this paper we will consider a more general problem: energy optimal interpolation in quantum evolution, and prove that QBP is a special case.

The interpolation in quantum evolution can be described as follows: find a Hamiltonian in a given Hilbert space under proper constraints, so that the quantum state $|\psi(t)\rangle$ equals given states $|\psi_1\rangle, \ldots, |\psi_m\rangle$ at given times $t_1, \ldots, t_m$. The energy optimal interpolation (EOI) is to find the Hamiltonian in the solution space of the former problem such that

$$tr(|\hat{H}|^2) = \min.$$ (1)

For the case $m=2$, the solution to EOI is the same as the result in [2,3,4,5,6]. If $H$ is dependent on time, the evolution between $t_i$ and $t_{i+1}$ is reduced to the case $m=2$, then EOI turns trivial. In practical consideration, the quantum evolution is usually too

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1See, for example, [2,3,4,5,6].
2To be proved in section 3.
quick to control the Hamiltonian for corresponding changes. Thus we only consider time-independent Hamiltonians.

## 2 General Discussion

Write the interpolation conditions in Schrödinger equation:

$$\exp(-i\hat{H}t_i) |\psi_i\rangle = |\psi_i\rangle, \ i = 1, \ldots, m,$$

(2)

where we take $\hbar = 1$, $t_1 = 0$ for convenience.

A global phase factor will not alter the physical results, so (2) can be rewritten as:

$$\exp(-i\hat{H}t_i) |\psi_i\rangle = \exp(i\theta_i) |\psi_i\rangle, \ i = 1, \ldots, m,$$

(3)

where $\theta_i$ can be arbitrarily adjusted to fit the physical system.

Consider the Hilbert space of dimension $n$, in the eigenstate representation the Hamiltonian is diagonalized:

$$\hat{E} = \hat{T}\hat{H}\hat{T}^\dagger = \text{diag}(\varepsilon_1, \ldots, \varepsilon_n),$$

(4)

where $\hat{T}$ is the transformation matrix, $\hat{T}\hat{T}^\dagger = \hat{T}^\dagger\hat{T} = \hat{I}$, $\varepsilon_1, \ldots, \varepsilon_n$ are the eigenvalues of energy.

The state $|\psi_i\rangle$ now transforms to $|\psi_i'\rangle = e^{i\theta_i} \hat{T} |\psi_i\rangle$. Write $\hat{A}_{n \times m} = (|\psi_1'\rangle, \ldots, |\psi_m'\rangle)$, then (3) becomes:

$$(\lambda_k \exp(-i\varepsilon_k t_i))_{n \times m} = \hat{A},$$

(5)

where $(\lambda_1, \ldots, \lambda_n)^T = \hat{T} |\psi_1\rangle$, and normalization requires

$$\sum_{k=1}^n |\lambda_k|^2 = 1$$

(6)

Take the Hermitian adjoint of (5) and then multiply it by (5) we obtain:

$$\left(\sum_{k=1}^n |\lambda_k|^2 e^{i\varepsilon_k (t_i - t_j)}\right)_{m \times m} = \hat{A}^\dagger \hat{A} = (e^{i(\theta_j - \theta_i)} \langle \psi_i | \psi_j \rangle)_{m \times m},$$

(7)

or writing in component form

$$\sum_{k=1}^n |\lambda_k|^2 \exp(i\varepsilon_k (t_i - t_j) + i(\theta_i - \theta_j)) = \Delta_{ij}, \ 1 \leq j < i \leq m,$$

(8)

\(^3\text{In this paper we only concern Hermitian Hamiltonians.}\)
where $\Delta_{ij} = \langle \psi_i | \psi_j \rangle = \langle \psi_j | \psi_i \rangle^* = \Delta_{ji}^*$, so the case $i \leq j$ is trivial. This is the fundamental equation for interpolation.

From (8) we can immediately make the following observations:

* The solution to the interpolation problem is invariant under a unitary transformation applied to the given states. Hence two different sets of given states will yield the same result, if they are connected by a unitary transformation.

* If $(\varepsilon_1, \ldots, \varepsilon_n, \lambda_1, \ldots, \lambda_n, \theta_1, \ldots, \theta_n)$ is a solution set to the equations, then for arbitrary $\Delta \varepsilon$, $(\varepsilon_1 + \Delta \varepsilon, \ldots, \varepsilon_n + \Delta \varepsilon, \lambda_1, \ldots, \lambda_n, \theta_1 - \Delta \varepsilon t_1, \ldots, \theta_n - \Delta \varepsilon t_n)$ is also a solution set. The zero point of energy only cause a total phase change, thus we can always adjust the phases to adjust the zero point of energy without altering the solution.

* There are $m(m - 1)$ equations in (8) (consider the real and imaginary part separately). The unknowns are $\theta_i, |\lambda_k|$ and $\varepsilon_k$. So there are in general $m^2 - m$ equations and $2n + m$ unknowns in total.

The structure of the solution space is determined by the number of independent equations. When the number of equations exceeds that of unknowns, we can use methods like least squares to find a path optimal Hamiltonian. When the number of unknowns exceeds that of equations, we can introduce the energy optimal Hamiltonian using constraint (11).

As $\text{tr}(|E|^2) = \text{tr}(\hat{T} \hat{H}^\dagger \hat{T}^\dagger \hat{T} \hat{H} \hat{T}^\dagger) = \text{tr}(|\hat{H}|)^2$, (11) now becomes

$$\sum_{k=1}^{n} \varepsilon_k^2 = \min.$$  \hspace{1cm} (9)

View the $m(m - 1)$ equations in (8) as constraints, (6) gives another constraint. Introduce corresponding Lagrangian multipliers $\alpha_{ij}, \beta_{ij}, \gamma$, the variational function is defined as follows:

$$S = \sum_{k=1}^{n} \varepsilon_k^2 + \sum_{1 \leq j < i \leq m} [\alpha_{ij} (\sum_{k=1}^{n} |\lambda_k|^2 \cos(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j) - \Re \Delta_{ij}) + \beta_{ij} (\sum_{k=1}^{n} |\lambda_k|^2 \sin(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j) - \Im \Delta_{ij})] + \gamma (\sum_{k=1}^{n} |\lambda_k|^2 - 1)$$  \hspace{1cm} (10)

Variation with respect to $\varepsilon_k$ leads to:
\[
\frac{\partial S}{\partial \varepsilon_k} = 2 \varepsilon_k - \sum_{1 \leq j < i \leq m} |\lambda_k|^2 (t_i - t_j)\left[\alpha_{ij} \sin(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j) - \beta_{ij} \cos(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j)\right] = 0, \; k = 1, \ldots, n. \tag{11}
\]

Variation with respect to $|\lambda_k|$ leads to:
\[
\frac{\partial S}{\partial |\lambda_k|} = 2 \gamma |\lambda_k| + 2 |\lambda_k| \sum_{1 \leq j < i \leq m} \left[\alpha_{ij} \cos(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j) + \beta_{ij} \sin(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j)\right] = 0, \; k = 1, \ldots, n. \tag{12}
\]

Variation with respect to $\theta_i$ leads to:
\[
\frac{\partial S}{\partial \theta_i} = \sum_{j \neq i} \sum_{k=1}^n |\lambda_k|^2 \left[-\tilde{\alpha}_{ij} \sin(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j) + \tilde{\beta}_{ij} \cos(\varepsilon_k (t_i - t_j) + \theta_i - \theta_j)\right] = 0, \; i = 1, \ldots, m. \tag{13}
\]

where
\[
\tilde{\alpha}_{ij} = \begin{cases} 
\alpha_{ij} & i > j, \\
\alpha_{ji} & i < j,
\end{cases} \quad \tilde{\beta}_{ij} = \begin{cases} 
\beta_{ij} & i > j, \\
\beta_{ji} & i < j.
\end{cases}
\tag{14}
\]

Hence the fundamental equations for EOI are (8), (11), (12) and (13). The unknowns are $\varepsilon_k$, $|\lambda_k|$, $\theta_i$, $\alpha_{ij}$, $\beta_{ij}$ and $\gamma$. In total there are $m^2 + 2n + 1$ equations and $m^2 + 2n + 1$ unknowns, and can be solved in principle.

### 3 Quantum Brachistochrone Problem

Constraint (11) is to minimize the module of $H$ while the evolution time keep fixed. From Anandan-Aharonov relation [7], which states that the ‘speed’ of quantum evolution is given by $2\Delta \hat{H}/\hbar$, $\Delta \hat{H}$ being the standard deviation of the Hamiltonian, we conclude the reversed constraint, viz.
\[
tr(|\hat{H}|^2) = \text{const. }, t = \text{min.}, \tag{15}
\]
should be equivalent to (11).

Carlini, et al. [1] used the constraint
\[
tr(|\hat{H}|^2) = tr(|\hat{H} - tr(\hat{H})/n|^2) = \text{const. }, t = \text{min.}, \tag{16}
\]
in solving QBP. The difference of $\hat{H}$ and $\hat{H}$ only lies in the choice of the zero point of energy.

From (8) we know the choice of the zero point of energy would not alter the solution, since $tr(|\hat{H}|^2) = tr(|\hat{H}|^2) - |tr(\hat{H})|^2/n \leq tr(|\hat{H}|^2)$, constraint (1) requires

$$tr(\hat{H}) = 0,$$

i.e. $tr(|\hat{H}|^2) = tr(|\hat{H}|^2)$. Hence (15) and (16) are equivalent. So the special case $m = 2$ for EOI should reduce to QBP. Now (8) and (11) become:

$$2\varepsilon_k = |\lambda_k|^2 t \left[ \alpha \sin(\varepsilon_k t + \theta) - \beta \cos(\varepsilon_k t + \theta) \right], k = 1, \ldots, n;$$

$$\sum_{k=1}^n |\lambda_k|^2 \exp(i(\varepsilon_k t + \theta)) = \Delta,$$

for convenience we set $t_1 = \theta_1 = 0$ and omit redundant subscripts. Treat $\theta_i$’s and $|\lambda_k|$’s as known parameters we can solve (18), then adjust the values of $\theta_i$’s and $|\lambda_k|$’s to minimize the energy cost.

To simplify (18), we shall now consider from the geometry viewpoint. The two given states $|\psi_i\rangle$ and $|\psi_f\rangle$ span a space of dimension 2. It’s natural that the time optimal evolution should be the geodesic in this space. So the Hamiltonian is of dimension 2.

From (17) we have

$$\sum_{k=1}^n \varepsilon_k = tr(\hat{E}) = tr(\hat{H}) = 0.$$ (19)

Thus

$$\varepsilon_1 = -\varepsilon_2 = \varepsilon. \quad \varepsilon_k = 0, k = 3, \ldots, n.$$ (20)

Then (18) reduce to:

$$2\varepsilon = |\lambda_1|^2 t \left[ \alpha \sin(\varepsilon t + \theta) - \beta \cos(\varepsilon t + \theta) \right];$$

$$-2\varepsilon = |\lambda_2|^2 t \left[ \alpha \sin(-\varepsilon t + \theta) - \beta \cos(-\varepsilon t + \theta) \right];$$

$$0 = |\lambda_k|^2 t \left[ \alpha \sin \theta - \beta \cos \theta \right], k = 3, \ldots, n;$$ (21)

$$\Delta e^{-i\theta} = |\lambda_1|^2 e^{i\varepsilon t} + |\lambda_2|^2 e^{-i\varepsilon t} + \sum_{k=3}^n |\lambda_k|^2.$$
The third eqn. of (21) yields $|\lambda_k| = 0, k \geq 3$. Substitute it into the forth eqn. we have:

$$\Lambda e^{i\tau} + (1 - \Lambda)e^{-i\tau} = \Delta e^{-i\theta},$$

(22)

where we have used (6) and write $|\lambda_1|^2 = \Lambda$ for convenience.

Take module on both sides of (22):

$$\varepsilon t|\Delta|^2 = 1 - 4\Lambda(1 - \Lambda)\sin(\varepsilon t)^2.$$  

(23)

Thus $\varepsilon = \arcsin \sqrt{1 - |\Delta|^2} / t$, to minimize $\varepsilon$, we take $\Lambda = 1/2$. So

$$\varepsilon = \arcsin \sqrt{1 - |\Delta|^2} / t = \arccos |\Delta| / t,$$

(24)

$$tr(|\hat{H}|^2) = \sum_{k=1}^{n} \varepsilon_k^2 = 2(\arccos |\Delta| / t)^2.$$  

(25)

In the eigenstate representation, $\hat{H} = \text{diag}(\varepsilon, -\varepsilon, 0, \ldots, 0)$, $|\psi_1\rangle = (\lambda_1, \lambda_2, 0, \ldots, 0)^T$, $|\psi_2\rangle = \exp(-i\hat{H}t) |\psi_1\rangle = (\lambda_1 \exp(-i\varepsilon t), \lambda_2 \exp(i\varepsilon t), 0, \ldots, 0)^T$. The Gram-Schmidt orthonormalized state $|\psi'_2\rangle = (|\psi_2\rangle - \cos \varepsilon t |\psi_1\rangle) / \sin \varepsilon t = (-i\lambda_1, i\lambda_2, 0, \ldots, 0)^T$, so

$$i\varepsilon (|\psi'_2\rangle \langle \psi_1| - |\psi_1\rangle \langle \psi'_2|) = \text{diag}(\varepsilon, -\varepsilon, 0, \ldots, 0) = \hat{H}.$$  

(26)

At arbitrary time $\tau$,

$$|\psi(\tau)\rangle = (\lambda_1 \exp(-i\varepsilon \tau), \lambda_2 \exp(i\varepsilon \tau), 0, \ldots, 0)^T = \cos \varepsilon \tau |\psi_1\rangle + \sin \varepsilon \tau |\psi'_2\rangle.$$  

(27)

(25), (26) and (27) are the same as the main results in [1] which take $tr(|\hat{H}|^2)/2 = \omega^2$.

Substitute the results back into (21) we have:

$$|\Delta| = \Delta e^{-i\theta},$$

(28)

thus $\langle \psi_2| \psi_1\rangle = \Delta e^{-i\theta}$ is real. The global phases of $\psi_1$ and $\psi_2$ are adjusted to make $\langle \psi_2| \psi_1\rangle$ be a real number at optimal solution.

4 Case $\Delta_{ij} = \delta_{ij}, t_i = (i - 1)t$

Now we consider the special case when the given states are orthogonal and the given times are evenly spaced, viz.

$$\Delta_{ij} = \delta_{ij}, t_i = (i - 1)t.$$  

(29)
Since the given $|\psi_i\rangle$’s are lineal independent. We have:

\[ m \leq n \]  \hspace{1cm} (30)

Now (8) reduces to:

\[ \sum_{k=1}^{n} |\lambda_k|^2 \exp(i(l\varepsilon_k t + \theta_i)) = 0, \ l = i - j = 1, 2, \ldots, m - 1. \]  \hspace{1cm} (31)

In section 3 we concluded that the global phases $\theta_i$ are adjusted to make $\Delta_{ij}$ real at optimal solution. This conclusion is supposed to be still valid here. Thus we have $\theta_i = 0$.

When $l = 1$ a special solution can be easily found: the $n$ vectors $\exp(i\varepsilon_k t)(k = 1, \ldots, n)$ distribute uniformly on the unit circle, i.e.

\[ \varepsilon_k t = \frac{2k\pi}{n} + \theta_0, \ |\lambda_k|^2 = 1/n, \]  \hspace{1cm} (32)

If $n$ is prime, for any $l < n$, $\exp(il\varepsilon_k t)$ are still $n$ vectors distributing uniformly on the unit circle. If $n$ is not prime, when $l$ is a factor of $n$, $\exp(il\varepsilon_k t)$ are $n/l$ vectors distributing uniformly on the unit circle. In both cases we still have (31). But if $l = n$, (31) no longer holds, this is consistent with (30).

The result is a special solution to the quantum interpolation, whether it is the solution to EOI depends on whether it is consistent with (11), (12) and (13), which remains unproved.

## 5 Conclusion and Discussion

We have educed the fundamental equations for the quantum interpolation and EOI. The general behavior of its solutions are preliminarily studied. QBP is discussed in detail as a special case. Another simple case for quantum interpolation is also considered.

As future developments, the fundamental equations for EOI remains to be thoroughly investigated, and this framework can be extended to mixed states and non-Hermitian Hamiltonians. The behavior of path optimal Hamiltonian is also worth studying. Meanwhile applications in quantum computation are probable.

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6See page 3, probably defined via methods such as least squares.
Acknowledgments

The idea of this paper was inspired by the seminar on quantum mechanics by Prof. Zhuang, Pengfei. And we would like to thank Huang, Xuguang, our teaching assistant, for informative discussions.

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