Unitary deformations of counterdiabatic driving

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We study a deformation of the counterdiabatic-driving Hamiltonian as a systematic strategy for an adiabatic control of quantum states. Using a unitary transformation, we design a convenient form of the driver Hamiltonian. We apply the method to a particle in a confining potential and discrete systems to find explicit forms of the Hamiltonian and discuss the general properties. The method is interpreted from the aspects of the quantum brachistochrone equation. We show the existence of a nontrivial dynamical invariant in the deformed system.

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I. INTRODUCTION

The method “shortcuts to adiabaticity” has attracted much attention recently. A state evolution by the adiabatic process is accelerated by applying the counterdiabatic Hamiltonian and many applications have been discussed [1–5]. From a more fundamental perspective, the method is understood as an optimized protocol [6, 7]. Furthermore, it has been shown to be useful in real experiments [8–11].

Some technical problems arise when we apply the method for a given adiabatic Hamiltonian. First, we need all eigenstates of the Hamiltonian to construct the counterdiabatic term. It is generally a difficult task except the case where the Hamiltonian takes a simple form in a small Hilbert space. Second, even if the counterdiabatic term is found, it involves operators which are difficult to implement in the laboratory.

These problems can be circumvented when we use the invariant-based engineering which is known to be equivalent essentially to the counterdiabatic driving [4]. To find an ideal control, we first specify the form of the invariant instead of preparing the adiabatic Hamiltonian. Thus, the initial setting is different in both the methods and the availability depends on the problem to consider. Therefore, it will be useful if we have other choices.

As possible solutions of the problems, various methods have been discussed intensively: approximations of the counterdiabatic term by a simple operator [12, 13], unitary transformations of the state [14, 15], modification of the formula using arbitrariness of the counterdiabatic term [16], and use of scale invariance [17, 19].

In this paper, we discuss a strategy for constructing a driver Hamiltonian. Using a unitary transformation, we design the counterdiabatic term in a convenient form. The same strategy was used in many works such as Refs. [14, 15, 17, 19]. We go further to obtain a convenient form of the driver Hamiltonian. There are some arbitrariness of choosing the driver Hamiltonian as discussed in Ref. [16] if we control a specific state. We exploit this arbitrariness to find the counterdiabatic potential.

We should also mention a similarity of our method to the fast-forward scaling [20–25] where the state evolution is fast-forwarded by using the time scaling. To find the fast-forward potential, a position-dependent phase is added to the wavefunction. It is important to notice that the point of the method is not in the scaling but in the addition of the phase. The phase is nothing but a unitary transformation to be discussed more generally in the present paper. Thus, the same idea is used by many works. Our aim is to combine the ideas used in many contexts and to clarify the general properties of the method.

The organization of the paper is as follows. In Sec. II the basic idea of our method is described. By applying the idea to a particle in a potential in Sec. III and discrete systems in Sec. IV, we discuss general properties of the method. In Sec. V we formulate the problem using the quantum brachistochrone equation to see the method from a different aspect. Finally, the summary is given in Sec. VI.

II. UNITARY DEFORMATION

We describe our basic idea of the unitary deformation. We start from the Schrödinger equation

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

For a given time-dependent Hamiltonian $\hat{H}(t)$ and an initial condition of state $|\psi(0)\rangle$, $|\psi(t)\rangle$ is obtained by solving the equation. In the method of counterdiabatic driving, the Hamiltonian is divided into two parts:

$$\hat{H}(t) = \hat{H}_{ad}(t) + \hat{H}_{cd}, \tag{2}$$

$$\hat{H}_{ad}(t) = \sum_{n} E_{n}(t) |n(t)\rangle\langle n(t)|, \tag{3}$$

$$\hat{H}_{cd}(t) = i \sum_{m,n \neq n} \langle m(t)|\langle m(t)|\hat{n}(t)|n(t)\rangle|n(t)\rangle, \tag{4}$$

where $E_{n}(t)$ is real and the dot denotes the time derivative as $|\dot{n}(t)\rangle = \frac{d}{dt} |n(t)\rangle$. The solution of the Schrödinger equation is given by a linear combination of the adiabatic
state of $\hat{H}_{\text{ad}}(t)$ defined as
\begin{equation}
|\psi_n(t)\rangle = \exp \left[ -i \int_0^t dt' \left( E_n(t') - i \langle n(t')|\hat{n}(t') \rangle \right) \right] |n(t)\rangle.
\end{equation}

This result is very convenient for the ideal control of the system since the deviation from the adiabatic state is prevented by the presence of the counterdiabatic term $\hat{H}_{\text{cd}}(t)$.

The assumption here is that the form of $\hat{H}_{\text{cd}}(t)$ becomes complicated and is hard to be realized. Although the counterdiabatic term is specified as in Eq. (4), its formal representation based on a spectral decomposition is not a useful one. We introduce a unitary transformation
\begin{equation}
|\tilde{\psi}(t)\rangle = \hat{U}_{\psi}(t)|\psi(t)\rangle.
\end{equation}
The Schrödinger equation takes the form
\begin{equation}
i \frac{d}{dt} |\tilde{\psi}(t)\rangle = \hat{H}_U(t)|\tilde{\psi}(t)\rangle,
\end{equation}
\begin{equation}
\hat{H}_U(t) = \hat{U}_{\psi}(t)\hat{H}(t)\hat{U}_{\psi}^\dagger(t) - i\hat{U}_{\psi}(t)\frac{d\hat{U}_{\psi}^\dagger(t)}{dt}.
\end{equation}

We want to find a convenient form of potential term $\hat{V}_{\psi}(t)$ such that the following relation is satisfied:
\begin{equation}
\hat{H}_U(t)|\tilde{\psi}(t)\rangle = (\hat{H}_{\text{ad}}(t) + \hat{V}_{\psi}(t))|\tilde{\psi}(t)\rangle.
\end{equation}

We note that the equality $\hat{H}_U(t) = \hat{H}_{\text{ad}}(t) + \hat{V}_{\psi}(t)$ is not necessarily satisfied. With the potential term, the state follows an adiabatic passage which is different from the original one although the adiabatic Hamiltonian is the same in both the evolutions.

There is of course a large amount of arbitrariness in the choice of the unitary transformation. Our aim is to establish the general strategy to determine the driving potential $\hat{V}_{\psi}(t)$. We note that the form of the potential $\hat{V}_{\psi}(t)$ crucially depends on the state $|\tilde{\psi}(t)\rangle$ to accelerate. If we change the state, the form will be changed accordingly. The original counterdiabatic driving is applied to any state. By abandoning such a universal property, we can use the convenient acceleration potential. However, we show in the following that the potential can be effectively independent of states in some special cases.

### III. A PARTICLE IN A POTENTIAL WELL

In this section, we study one-particle systems in a position-dependent potential. The adiabatic Hamiltonian is given by
\begin{equation}
\hat{H}_{\text{ad}}(t) = \frac{\hat{p}^2}{2m} + U(\hat{r}, t).
\end{equation}

A time dependence is present in the potential function $U$.

#### A. One-dimensional system

For one-dimensional bound states in a confining potential $U(\hat{x}, t)$, the wavefunction is real and one can simplify the formula of the potential. The adiabatic state corresponding to an eigenvalue $E_n(t)$ is represented as
\begin{equation}
\psi_n(x, t) = \exp \left( -i \int_0^t dt' E_n(t') \right) \varphi_n(x, t),
\end{equation}
where $\varphi_n(x, t)$ is real. We note that the geometric phase is zero since $\langle \varphi_n(t)|\varphi_n(t) \rangle = 0$.

In this system, the counterdiabatic term depends not only on the position operator $\hat{x}$ but also on the momentum operator $\hat{p}$, which is inconvenient in practical applications. We consider the unitary deformation to control the system by a local potential $V_n(\hat{x}, t)$. We define the new state
\begin{equation}
\tilde{\psi}_n(x, t) = e^{-i\phi_n(x, t)} \psi_n(x, t),
\end{equation}
where $\phi_n(x, t)$ is a real function. This new state satisfies the Schrödinger equation
\begin{equation}
i \frac{\partial}{\partial t} \tilde{\psi}_n(x, t) = \left( -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + U(x, t) + V_n(x, t) \right) \tilde{\psi}_n(x, t).
\end{equation}

Using the properties that $\psi_n$ is factorized as Eq. (11) and $\varphi_n(x, t)$ is real, we obtain
\begin{equation}
\frac{\partial \phi_n}{\partial t} + E_n = \frac{1}{2m} \left( \frac{\partial \phi_n}{\partial x} \right)^2 + U + V_n - \frac{1}{2m} \frac{\partial \phi_n}{\partial x} \frac{\partial \phi_n}{\partial x}.
\end{equation}

The first equation at the classical limit represents the Hamilton-Jacobi equation and the second one is the continuity equation. We note that the role of the additional phase $\phi_n(x, t)$ is to induce a current with the probability density unchanged. The current is exactly equal to zero in the original wavefunction, which is not appropriate to describe the present dynamical problem.

Since $\varphi_n(x, t)$ represents the eigenstate of the adiabatic Hamiltonian, we have the relation
\begin{equation}
E_n(t) = -\frac{1}{2m} \frac{\partial \varphi_n(x, t)}{\partial x} + U(x, t).
\end{equation}

Using this, we can write the potential as
\begin{equation}
V_n(x, t) = \frac{\partial \phi_n(x, t)}{\partial t} - \frac{1}{2m} \left( \frac{\partial \phi_n(x, t)}{\partial x} \right)^2.
\end{equation}

The phase $\phi_n(x, t)$ is determined from the continuity equation as
\begin{equation}
\phi_n(x, t) = m \int_x^t dz_1 \int_x^{z_1} dz_2 \frac{\partial \rho_n(z_2, t)}{\partial t},
\end{equation}
where
where \( x^* \) is a reference point and \( \rho_n(x,t) = \varphi_n^2(x,t) \) represents the probability density. Thus, once if we know the probability density of the adiabatic state, we can calculate the counterdiabatic potential. We note that it is not necessary to know the form of the counterdiabatic term to find the potential. Therefore, this formula can be a general strategy to obtain the counterdiabatic driving.

The form of the potential depends on the adiabatic state as it is labeled by the index \( n \). We show that it is independent of \( n \) for several typical situations. First, we consider the transport dynamics. The potential is given by

\[
U(x,t) = U_0(x - x_0(t)),
\]

where \( x_0(t) \) is a real function and describes the translation of the potential. The probability density takes the form

\[
\rho_n(x,t) = f_n(x - x_0(t)).
\]

In this case, the phase is obtained from the continuity equation as

\[
\phi_n(x,t) = -m\dot{x}_0(t)(x - x_0(t)) + m\dot{x}_0(t)(x^* - x_0(t)) + m\dot{x}_0(t)\int_x^{x^*} \frac{dx_1}{f_n(x_1 - x_0(t))}.
\]

The corresponding potential is calculated from Eq. (19). The result depends on the function \( f_n \), which means that the counterdiabatic potential is crucially depends on the state to accelerate. However, the last term in Eq. (21) can be neglected if we set \( f_n(x^* - x_0(t)) = 0 \). For bound states, we can set \( x^* = \infty \) or \( -\infty \). In this case, the second term in Eq. (21) is divergent but it is an irrelevant energy shift and does not affect the adiabatic state. We can use the phase

\[
\phi_n(x,t) = -m\dot{x}_0(t)(x - x_0(t)).
\]

The potential is given by

\[
V_n(x,t) = -m\dot{x}_0(t)(x - x_0(t)) + \frac{m}{2}\dot{x}_0^2(t)
= -m\dot{x}_0(t)x + c(t),
\]

where \( c(t) \) is an irrelevant function which is proportional to the identity operator. We can conclude that this counterdiabatic potential works for arbitrary bound states \( \varphi_n(x,t) \) in the present system with the potential [19] if we neglect the effect of energy shift.

Second, we consider the case where the potential is takes the form

\[
U(x,t) = \frac{1}{\xi^2(t)} U_0 \left( \frac{x}{\xi(t)} \right).
\]

A positive function \( \xi(t) \) represents the dilatation. With this potential, the probability density is given by

\[
\rho_n(x,t) = \frac{1}{\xi(t)} f_n \left( \frac{x}{\xi(t)} \right).
\]

where \( f \) is a positive function. Then, the phase is given by

\[
\phi_n(x,t) = -\frac{m}{2} \frac{\dot{\xi}(t)}{\xi^2(t)} (x^2 - x^*2)
+ m \dot{\xi}(t) x^* f_n \left( \frac{x^*}{\xi(t)} \right) \int_{x/x^*}^{x/\xi(t)} \frac{d\xi_1}{f_n(\xi_1)}.
\]

The last term is neglected if we set \( f_n(x/x^*\xi(t)) = 0 \). In that case, we obtain the corresponding counterdiabatic potential

\[
V_n(x,t) = -\frac{m}{2} \frac{\ddot{\xi}(t)}{\xi(t)} x^2 + c(t).
\]

The last term represents an irrelevant shift.

The same systems are analyzed in Refs. [17, 19] as the scale-invariant driving. A system in a moving harmonic potential is analyzed in Ref. [20]. Our results are consistent with their ones. However, we note that the potential depends on the adiabatic state in principle. The dependence can be included to an irrelevant term in principle but we can consider the state dependent potential by keeping the last term of Eqs. (21) and (26).

\[\text{B. Generalization}\]

It is a straightforward task to extend the method to systems in arbitrary dimensions. We write the original adiabatic state as

\[
\psi_n(r,t) = e^{-i\int_0^t dt' E_n(t') - i\phi_n^{(0)}(r,t)} \sqrt{\rho_n(r,t)}.
\]

Introducing the new state \( \tilde{\psi}_n(r,t) = e^{-i\phi_n(r,t)} \psi_n(r,t) \), we obtain the continuity equation

\[
\frac{\partial \rho_n}{\partial t} = \frac{1}{m} \nabla \cdot (\rho_n \nabla \phi_n),
\]

and the potential

\[
V_n = \dot{\phi}_n - \frac{1}{2m} (\nabla \phi_n)^2 + \phi_n^{(0)} - \frac{1}{m} \nabla \phi_n^{(0)} \cdot \nabla \phi_n.
\]

We note that the original adiabatic state satisfies the relation

\[
\nabla \cdot (\rho_n \nabla \phi_n^{(0)}) = 0,
\]

which means that the original current is in a form as \( j^{(0)} = \nabla \times \mathbf{A} \).

Once if we can find the original wavefunction, we can calculate the potential by solving the above equations. It is interesting to see that the problem of the level degeneracy does not exist in the present method. It was a serious problem of the counterdiabatic driving where the counterdiabatic term [18] goes to infinity at the degenerate point. Instead, the phase can be infinity when the probability density becomes zero at some point. This problem was recognized in the fast-forward method [21, 22, 23].

The form of the counterdiabatic potential depends on the adiabatic state in principle. The general properties of the present result is not clear and we study a specific system in the following.
C. $1/r$-potential

We study the potential for the hydrogen atom

$$U(r, t) = -\frac{1}{m\xi(t)|r - r_0(t)|}.$$  \hspace{1cm} (32)

$r_0(t)$ describes translation and $\xi(t)$ dilatation. The wave function of the ground state is real and we have $\phi^{(0)} = 0$. The probability density is given by

$$\rho(r, t) = \frac{1}{\pi \xi^3(t)} \exp\left( -\frac{2|r - r_0(t)|}{\xi(t)} \right).$$ \hspace{1cm} (33)

We first consider the case with $t$-independent $\xi$. Then, the phase $\phi$ becomes a function of $\phi(r(t))$ where $r(t) = |r - r_0(t)|$. Solving the continuity equation, we obtain

$$\frac{\partial \phi}{\partial r(t)} = m\dot{r}(t) \left( 1 + \frac{\xi}{r(t)} + \frac{\xi^2}{2r^2(t)} \right),$$ \hspace{1cm} (34)

where we take the reference point $r^*$ to be infinity. Correspondingly, the potential is

$$V = -\frac{m\xi^2}{2} \left( z - 1 - \frac{1}{2} \right),$$ \hspace{1cm} (35)

This result can be understood qualitatively. We need a strong attraction at $r = r_0(t)$ to avoid deviation from the trapped state in a moving potential.

In the case of $r_0(t) = 0$, $\phi$ is a function of $z(r, t) = r/\xi(t)$ and $t$. We obtain

$$\frac{\partial \phi}{\partial z} = -m\dot{\xi}(t) \left( z - 1 - \frac{1}{4z} \right),$$ \hspace{1cm} (36)

and

$$V = -\frac{m\xi^2}{2} \left( z^2 - z - \frac{1}{2} \right),$$ \hspace{1cm} (37)

These results show that the counterdiabatic potential depends on the form of the ground state wavefunction and takes a complicated form. There is no universal property in three dimensional systems as we found in the one-dimensional systems.

IV. DISCRETE SYSTEMS

We apply the unitary deformation to systems in a finite-dimensional Hilbert space.

A. General discussions

We consider the $N$-dimensional system. The adiabatic Hamiltonian is given by Eq. 3. The corresponding adiabatic state is written as

$$|\psi_n(t)\rangle = \exp \left[ -i \int_0^t dt' \left( E_n(t') - i \langle n(t')|\dot{n}(t') \rangle \right) \right] |n(t)\rangle.$$ \hspace{1cm} (38)

We consider the unitary transformation

$$\hat{U}_n(t) = \exp \left( -i \hat{\phi}^{(n)}(t) \right),$$ \hspace{1cm} (39)

where $\hat{\phi}^{(n)}(t)$ is a diagonal operator written as

$$\hat{\phi}^{(n)}(t) = \sum_{a=1}^N \phi^{(n)}_a(t) \hat{X}_a,$$ \hspace{1cm} (40)

Our goal is to find the potential in a diagonal form

$$\hat{V}_n(t) = \sum_{a=1}^N \nu^{(n)}_a(t) \hat{X}_a,$$ \hspace{1cm} (41)

The unitary-transformed state satisfies the Schrödinger equation

$$i\frac{d}{dt} |\psi_n(t)\rangle = \left( \hat{H}_{ad}(t) + \hat{V}_n(t) \right) |\psi_n(t)\rangle,$$ \hspace{1cm} (42)

where $|\psi_n(t)\rangle = \hat{U}_n(t) |\psi_n(t)\rangle$. This condition gives

$$\sum_{a=1}^N (\hat{\phi}^{(n)}_a - \nu^{(n)}_a) \hat{X}_a |n\rangle + i(1 - |n\rangle \langle n|) |\dot{n}\rangle$$

$$+ (E_n - c^{i\phi^{(n)}_a}) \hat{H}_{ad} e^{-i\phi^{(n)}_a}) |n\rangle = 0.$$ \hspace{1cm} (43)

We consider the case where the adiabatic Hamiltonian is a real symmetric matrix in the present representation. Then, the eigenstate can be represented by a real vector and we can decompose the above equation into the real and imaginary parts as we did in the previous section. We obtain

$$\langle a| \hat{H}_{ad} |b\rangle \cos(\phi^{(n)}_a - \phi^{(n)}_b) |b| n\rangle = 0,$$ \hspace{1cm} (44)

$$\langle a| \hat{H}_{ad} |b\rangle \sin(\phi^{(n)}_a - \phi^{(n)}_b) |b| n\rangle = 0.$$ \hspace{1cm} (45)

where $|a| n\rangle$ denotes the $a$-th component of the vector $|n\rangle$ and $\langle a| \hat{H} |b\rangle$ the $(a, b)$ component of the matrix $\hat{H}$. $a$ takes integers between 1 and $N$. We note that $\langle n| \dot{n}\rangle = 0$. These equations represent the Hamilton-Jacobi equation and the continuity equation respectively. Since we consider the discrete systems, the equations are not written by differential ones. We can obtain the phase $\phi^{(n)}_a$ from the second equation and the potential $\nu^{(n)}_a$ from the first.

Before considering examples, we study the state dependence of the potential. We assume that $\phi^{(n)}_a$ and $\nu^{(n)}_a$ are independent of $n$. Then, using the completeness relation, we obtain

$$\langle \phi^{(n)}_a - \nu^{(n)}_a \rangle \delta_{ab} + \langle a| \hat{H}_{ad} |b\rangle (1 - \cos(\phi^{(n)}_a - \phi^{(n)}_b)) = 0,$$ \hspace{1cm} (46)

$$-i \langle a| \hat{H}_{ad} |b\rangle - (a| \hat{H}_{ad} |b\rangle \sin(\phi^{(n)}_a - \phi^{(n)}_b) = 0.$$ \hspace{1cm} (47)
where the counterdiabatic Hamiltonian is written as
\[
\hat{H}_{cd} = i \sum_n (1 - |n\rangle \langle n|) \dot{|n\rangle \langle n|} = i \sum_n |\dot{n}\rangle \langle n|.
\] (48)

These equations give \( v_a = \dot{\phi}_a \) and \( \langle a | \hat{H}_{cd} | b \rangle = 0 \). Thus, the present assumption only describes a trivial situation where the counterdiabatic Hamiltonian is zero. We conclude that the potential \( V_n(t) \) crucially depends on the state \( n \). However, we can expect that the dependence appears only at the irrelevant energy shift for simple systems. We study this property in the following simple example.

**B. Two-level systems**

As an example, we study the two-level systems described by the Hamiltonian
\[
\hat{H}_{ad}(t) = \frac{h(t)}{2} \begin{pmatrix}
\cos \theta(t) & \sin \theta(t) \\
\sin \theta(t) & -\cos \theta(t)
\end{pmatrix},
\] (49)

The eigenvalues of \( \hat{H}_{ad}(t) \) are given by \( \pm h(t)/2 \). Each adiabatic state is given respectively by
\[
|\psi_1(t)\rangle = e^{-i \int_0^t dt' h(t')/2} \begin{pmatrix}
\cos \theta(t)/2 \\
\sin \theta(t)/2
\end{pmatrix},
\] (50)
\[
|\psi_2(t)\rangle = e^{i \int_0^t dt' h(t')/2} \begin{pmatrix}
\sin \theta(t)/2 \\
-\cos \theta(t)/2
\end{pmatrix}.
\] (51)

Equation (47) is written as
\[
\dot{\theta} + h \sin \theta \sin (\phi_1^{(n)} - \phi_2^{(n)}) = 0,
\] (52)
which means that the difference of the phases \( \phi_1^{(n)} - \phi_2^{(n)} \) is independent of \( n \). The same is true for the potential and we have from Eq. (46)
\[
v_1^{(n)} - v_2^{(n)} = \dot{\phi}_1^{(n)} - \dot{\phi}_2^{(n)} - h(1 - \cos (\phi_1^{(n)} - \phi_2^{(n)})) \cos \theta.
\] (53)

We obtain the form of the potential
\[
\dot{V}_n(t) = \frac{1}{2} v(t) \sigma^z + \frac{1}{2} (v_1^{(n)}(t) + v_2^{(n)}(t)),
\] (54)

where \( v(t) = v_1^{(n)}(t) - v_2^{(n)}(t) \). By applying this potential, we can realize the time evolution of the state along an adiabatic passage. In the two dimensional case, the state dependence of the potential only appears in the energy shift.

We note that the adiabatic passage is different from the original one. The Bloch vector of the unitary-transformed state is not in the \( z \)-plane. The initial and final states of \( \hat{\psi}(t) \) should be the same as those of the original state \( \hat{\psi}(t) \). We demand that the potential goes to zero at initial and final times. This is achieved when \( \phi_1 - \phi_2 = 0 \) and \( \dot{\phi}_1 - \dot{\phi}_2 = 0 \) at those times. From the condition (52), we obtain \( \theta = 0 \) and \( \dot{\theta} = 0 \), which means that

![FIG. 1. Potential \( v(t) = v_1(t) - v_2(t) \) in Eq. (53). The phase difference \( \phi_1 - \phi_2 \) is determined from Eqs. (50) and (51).](image)

the potential should be turned on and off very slowly. It would be interesting to understand the relation with the analysis of Ref. 27 where the same condition is obtained for improving the adiabatic approximation.

As a simple example, we consider
\[
\hat{H}_{ad}(t) = \frac{1}{2} h(t) \cdot \hat{\sigma} = \frac{1}{2} h(t) n(t) \cdot \hat{\sigma},
\] (55)
\[
h(t) = \begin{pmatrix}
\Gamma & 0 \\
0 & h_z(t)
\end{pmatrix}.
\] (56)

\( \theta(t) \) is represented as
\[
\cos \theta(t) = \frac{h_z(t)}{h(t)},
\] (57)
where \( h(t) = \sqrt{\Gamma^2 + h_z(t)^2} \). The Bloch vector \( n(t) \) is parametrized as
\[
n(t) = (\sin \theta(t), 0, \cos \theta(t)).
\] (58)

We impose the condition \( \theta(0) = \pi/2 \) and \( \theta(\infty) = 0 \), which means that the Bloch vector moves from \((1,0,0)\) to \((0,0,1)\) in the \( zx \)-plane.

In the unitary-deformed evolution, the Bloch vector is not in the plane. Equation (52) is written as
\[
\sin (\phi_1 - \phi_2) = \frac{\dot{h}_z(t)}{h_z(t)^3}.
\] (59)

To satisfy the condition that \( \phi_1 - \phi_2 \) and \( \dot{\phi}_1 - \dot{\phi}_2 \) go to zero at \( t = 0 \) and \( \infty \), we take the magnetic field in \( z \) direction as
\[
h_z(t) = ct^3,
\] (60)
where \( c \) is a constant. The potential \( v(t) \) obtained from (53) is plotted in Fig. 1. For comparison, we plot the
potential $v$ and the counterdiabatic field $h_y = \dot{\theta}$ in Fig. 2. We note that the counterdiabatic field is given by

$$\hat{H}_{cd}(t) = \frac{1}{2}(\hat{n}(t) \times \dot{\hat{n}}(t)) \cdot \sigma = \frac{1}{2}\dot{\theta}(t)\sigma_y.$$  \hspace{1cm} (61)

To see that the adiabatic passage of the unitary-deformed state is different from that of the original state, we plot the original Bloch vector $\hat{n}(t)$ and the vector after the deformation

$$\dot{\hat{n}}(t) = (\sin \theta(t) \cos \phi(t), \sin \theta(t) \sin \phi(t), \cos \theta(t)).$$  \hspace{1cm} (62)

They are plotted in Fig. 3.

V. QUANTUM BRACHISTOCHRONOME EQUATION

In the previous section, we have formulated the unitary deformation of the counterdiabatic driving. Here we formulate the problem using the quantum brachistochrone equation. This formulation allows us to understand what quantity characterizes the deformed system.

A. Formulation of the problem

We consider the Schrödinger equation in [1] with

$$i\frac{d}{dt}|\psi(t)\rangle = (\hat{H}_{ad}(t) + \hat{V}(t))|\psi(t)\rangle.$$  \hspace{1cm} (63)

The potential $\hat{V}(t)$ is diagonal in a specific basis. In the $N$-dimensional Hilbert space, the number of independent traceless diagonal operators are $N - 1$. Their basis operators commute with each other:

$$[\hat{X}_a, \hat{X}_b] = 0 \quad (a, b = 1, 2, \ldots, N - 1).$$  \hspace{1cm} (64)

They satisfy the orthonormal relations

$$\text{Tr} \hat{X}_a \hat{X}_b = \delta_{ab}.$$  \hspace{1cm} (65)

Using these operators, we can generally write

$$\hat{V}(t) = \sum_{a=1}^{N-1} v_a(t) \hat{X}_a,$$  \hspace{1cm} (66)

where

$$v_a(t) = \text{Tr} \hat{V}(t) \hat{X}_a.$$  \hspace{1cm} (67)

The original state $|\psi(t)\rangle$ is changed by the unitary deformation to a deformed state $|\tilde{\psi}(t)\rangle$. They are related by the constraints

$$|\langle \sigma |\psi(t)\rangle| = |\langle \sigma |\tilde{\psi}(t)\rangle|,$$  \hspace{1cm} (68)

where $|\sigma\rangle$ with $\sigma = 1, 2, \ldots, N$ represents a diagonal basis. This condition implies that the deformed state is written as

$$|\tilde{\psi}(t)\rangle = \hat{U}(t)|\psi(t)\rangle,$$  \hspace{1cm} (69)

where the unitary operator is written in terms of diagonal operators

$$\hat{U}(t) = \exp \left(-i\phi_0(t) - i \sum_{a=1}^{N-1} \phi_a(t) \hat{X}_a \right).$$  \hspace{1cm} (70)

Using this setting we consider the optimization of the potential.

B. Action

The optimization problem is formulated by defining the action to be minimized. It consists of four parts:

$$S = \int dt (L_T + L_S + L_{c1} + L_{c2}).$$  \hspace{1cm} (71)
The first term represents the time duration \[ L_T = \sqrt{\frac{\langle \dot{\psi}|(1 - |\psi\rangle\langle\psi|)\dot{\psi}\rangle}{\langle\psi|(\hat{H}_{ad} + V)^2|\psi\rangle - \langle\psi|\hat{H}_{ad} + V|\psi\rangle^2}}, \] which means the Fubini-Study distance divided by the velocity based on the Anandan-Aharonov relation. The other terms represent constraints. The second term is for the Schrödinger equation:

\[ L_S = \langle \phi \left( i\frac{d}{dt} - (\hat{H}_{ad} + \hat{V}) \right) |\dot{\psi}\rangle + \text{(h.c.)}, \]

where \(|\phi\rangle = |\phi(t)\rangle\) plays the role of a multiplier function. The third term is constraints for the potential:

\[ L_{C1} = \lambda_0 \text{Tr} \hat{V} + \sum_{b=1}^{N^2-N} \lambda_b \text{Tr} \hat{V} \hat{Y}_b, \]

where \({\hat{Y}_b}\) are traceless offdiagonal operators. They are the complements of diagonal operators \({\hat{X}_a}\) and satisfy

\[ \text{Tr} \hat{X}_a \hat{Y}_b = 0, \]

for arbitrary \(a\) and \(b\). \(L_{C1}\) makes the trace and offdiagonal elements of the potential zero. The last term of the action represents constraints for the state \(|\dot{\psi}\rangle\). We write

\[ L_{C2} = \sum_{\sigma=1}^{N} \lambda_{\sigma} \left( |\langle\sigma|\dot{\psi}\rangle|^2 - |\langle\sigma|\psi\rangle|^2 \right). \]

We note that the last term \(L_{C2}\) is not present in the original formulation. The constraint for the state has not been studied before.

### C. Quantum brachistochrone equation

Now that the action is defined, we can derive the quantum brachistochrone equation from the extremized condition. The extremization is performed on the potential and the state. We have

\[ 0 = \frac{\delta S}{\delta \dot{\psi}} = i \frac{d}{dt} \left[ \frac{\hat{H}_{ad} + \hat{V} - \langle \dot{\psi}|(\hat{H}_{ad} + \hat{V})|\psi\rangle}{2\Delta E^2} - \sum_{\sigma} \lambda_{\sigma} |\langle\sigma|\dot{\psi}\rangle|^2 - \sum_{\sigma} \lambda_{\sigma} |\langle\sigma|\psi\rangle|^2 \right], \]

\[ 0 = \frac{\delta S}{\delta \dot{\psi}} = \frac{1}{2\Delta E^2} \left[ \hat{H}_{ad} + \hat{V} \right] \dot{\psi} + \hat{P} \left[ \hat{H}_{ad} + \hat{V} \right] \dot{\psi} - 2\langle \dot{\psi}|(\hat{H}_{ad} + \hat{V})|\psi\rangle \dot{\psi} - \left( |\dot{\psi}\rangle\langle\dot{\psi}| + |\phi\rangle\langle\phi| \right) + F. \]

We use the following notations:

\[ \hat{P} = |\psi\rangle\langle\psi|, \]

\[ \Delta E^2 = \langle \dot{\psi}|(\hat{H}_{ad} + \hat{V})^2|\psi\rangle - \langle \dot{\psi}|(\hat{H}_{ad} + \hat{V})|\psi\rangle^2, \]

\[ \hat{F} = \sum_{b=0}^{N^2-N} \lambda_b \hat{Y}_b. \]

These are time-dependent functions. Equation (77) is for \(|\phi\rangle\) and is written as

\[ i \frac{d}{dt} |\phi\rangle = \left( \hat{H}_{ad} + \hat{V} \right) |\phi\rangle - \frac{d \hat{D}}{dt} |\psi\rangle - \sum_{\sigma} \lambda_{\sigma} |\sigma\rangle \langle\sigma| \dot{\psi}, \]

\[ \dot{\hat{D}} = \frac{\hat{H}_{ad} + \hat{V} - \langle \psi|\dot{\psi}\rangle}{2\Delta E^2}. \]

The solution is written in the form

\[ |\phi(t)\rangle = \hat{T}(t) \left[ |\phi(0)\rangle - \left( \hat{T}^\dagger(t) \hat{D}(t) \hat{T}(t) - \hat{D}(0) \right) |\psi(0)\rangle \right] + i \sum_{\sigma} \int_0^t dt' \lambda_{\sigma}(t') \hat{T}^\dagger(t') |\sigma\rangle \hat{T}(t') |\psi(0)\rangle, \]

where \(\hat{T}(t)\) is the time-evolution operator of the Hamiltonian \(\hat{H}_{ad} + \hat{V}\) with the initial condition \(\hat{T}(0) = 1\). Inserting this expression to the second equation (78), we obtain

\[ \hat{F}(t) = |\psi(t)\rangle\langle\phi(t)| + |\phi(t)\rangle\langle\psi(t)| + \hat{D}(t) |\psi(t)\rangle\langle\dot{\psi}(t)| + |\dot{\psi}(t)\rangle\langle\dot{\psi}(t)| \dot{\hat{D}}(t) = \hat{T}(t) \left[ |\phi(0)\rangle\langle\psi(0)| + |\psi(0)\rangle\langle\phi(0)| \right] + i \left[ \hat{Z}(t), \hat{P}(0) \right] \dot{\hat{T}}(t), \]

where

\[ |\phi(0)\rangle = |\phi(0)\rangle + \hat{D}(0) |\psi(0)\rangle, \]

\[ \dot{\hat{Z}}(t) = \sum_{\sigma} \int_0^t dt' \lambda_{\sigma}(t') \hat{T}^\dagger(t') |\sigma\rangle \hat{T}(t'). \]

The operator \(\hat{F}(t)\) satisfies the differential equation

\[ i \frac{d\hat{F}(t)}{dt} = \left[ \hat{H}_{ad}(t) + \hat{V}(t), \hat{F}(t) \right] - \sum_{\sigma} \lambda_{\sigma}(t) \left[ |\sigma\rangle \langle\sigma|, \hat{P}(t) \right]. \]

If the second term of the right hand side is absent, this equation indicates that \(\hat{F}(t)\) is a dynamical invariant quantity. The presence of the state-constraint term changes this standard interpretation.

At \(t = 0\), \(\hat{F}\) is written as

\[ \hat{F}(0) = |\phi(0)\rangle\langle\psi(0)| + |\psi(0)\rangle\langle\phi(0)|, \]
where $\tilde{\psi}(0)$ is an arbitrary vector. We assume that the initial state is one of the eigenstates of $\hat{H}_{ad}(0)$ and the potential is absent at $t = 0$. Thus, we choose

$$\vec{F}(0) = |\tilde{\psi}(0)\rangle \langle \tilde{\psi}(0)|. \tag{90}$$

Then,

$$\vec{F}(t) = \vec{P}(t) + i \vec{T}(t) |\tilde{Z}(t), \vec{P}(0)\rangle \langle \tilde{Z}(t)|. \tag{91}$$

This equation shows that the operator defined as

$$\vec{I}(t) = \vec{F}(t) - i \vec{T}(t) |\tilde{Z}(t), \vec{P}(0)\rangle \langle \tilde{Z}(t)|, \tag{92}$$

represents the dynamical invariant in the unitary-deformed evolution. This operator satisfies the equation for the invariant

$$i \frac{d\vec{I}(t)}{dt} = \left[ \hat{H}_{ad}(t) + \tilde{V}(t), \vec{I}(t) \right]. \tag{93}$$

In conclusion of this section, the quantum brachistochrone equation shows that the unitary-deformed system is characterized by a dynamical invariant. It is different from the invariant of the original state before the deformation. The formulation using the invariant was done in Ref. [19] for scale-invariant systems. Our result implies that the method of the unitary-deformation is equivalent with the invariant-based method and can be applied to general systems.

VI. SUMMARY

We have formulated the method of unitary deformation. The counterdiabatic Hamiltonian which supports the adiabatic state evolution is represented by a local potential. The main results are presented in Eqs. (29) and (30) for potential systems and Eqs. (53) and (52) for discrete systems. The advantage of this method is that the counterdiabatic potential is constructed from the single adiabatic state. It is not necessary to know all eigenstates of the adiabatic Hamiltonian. The form of the potential is written immediately once if we specify the adiabatic state. Instead of this property, the form of the potential is dependent on the state to accelerate. However, for several cases such as two-level systems and one-dimensional systems with the scale invariance, the dependence can be included to the irrelevant energy shift.

The potential is not unique in principle. For example, by keeping the last term in Eq. (21), we can find a different form of the potential. There exist possibilities to find a more convenient form of the potential, which can be an interesting problem in future studies.

From the analysis of the quantum brachistochrone equation, we find that our method can be formulated by using the dynamical invariant as was done in other works. Our formulation is not useful to find the explicit form of the invariant. Rather, it is important to notice that we have derived the method from a general principle. We expect that the present analysis enhances the applicability of the method of shortcuts to adiabaticity to more various systems.

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