Bounds for nonadiabatic transitions

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We discuss bounds for nonadiabatic transitions from the viewpoints of the adiabatic perturbation theory and the quantum speed limit. We show that the amount of nonadiabatic transitions from the $n$th level to the $m$th level is bounded by a function of the quantum geometric tensor for the $n$th level. We analyze this bound from the viewpoint of the adiabatic perturbation theory. In addition, this bound and the viewpoint of the quantum speed limit suggest nontrivial relationship between the dynamical transformation and the adiabatic transformation. We also derive a universal bound for any nonadiabatic transition. This bound is written in terms of the counterdiabatic Hamiltonian.

\section{I. INTRODUCTION}

Nonadiabatic transitions, which are transitions between different energy eigenstates due to fast change of Hamiltonians in time, have been studied since the dawn of quantum mechanics [1--5]. Generally, energy gap closing leads dynamics to critical slowing down, i.e., around critical points states are frozen and cannot follow change of energy eigenstates, and thus transitions between different energy eigenstates take place [6--10].

Evaluation of the amount of nonadiabatic transitions is of interest. Besides the traditional Landau-Zener formula [1--5] and the Kibble-Zurek formula [6--10], we can approximately calculate the amount of nonadiabatic transitions by using the adiabatic perturbation theory [11--13]. It was shown that the amount of nonadiabatic transitions after a quantum quench is expressed by the adiabatic gauge potential, and as the result by the quantum geometric tensor.

Not only approximate evaluation but also bounds for the amount of nonadiabatic transitions are also of great interest. As predicted from the adiabatic theorem [14--17], it is known that bounds are related to (minimal) energy gaps and change of energy eigenstates [18]. Quantum speed limits, which give typical time scale to achieve quantum processes [19--22], can be also used to quantify deviation of a dynamical state from an adiabatic state [23].

Recently, suppression of nonadiabatic transitions has been paid much attention due to development of adiabatic quantum computation [24--26] and quantum annealing [27, 28]. In particular, finite time processes are important not only to achieve fast operation but also to avoid decoherence. Quantum adiabatic brachistochrone is a promising approach for parameter scheduling to reduce the amount of nonadiabatic transitions [29, 30]. Use of shortcuts to adiabaticity is also remarkable strategy to suppress nonadiabatic transitions [31--34].

In this paper, we discuss bounds for nonadiabatic transitions in general quantum dynamics from the viewpoints of the adiabatic perturbation theory and the quantum speed limit. We find that the amount of nonadiabatic transitions is bounded by a function of the quantum geometric tensor, and thus our result is clearly consistent with an approximate calculation by the adiabatic perturbation theory [11--13]. Note that this bound is also related to quantum adiabatic brachistochrone [29, 30]. We also derive a universal bound for any nonadiabatic transition. This bound is written in terms of the counterdiabatic Hamiltonian.

\section{II. BOUNDS FOR NONADIABATIC TRANSITIONS}

We consider a quantum system described by the time-dependent Hamiltonian
\begin{equation}
\hat{H}(\lambda_t) = \sum_n E_n(\lambda_t) \hat{P}_n(\lambda_t),
\end{equation}
where $E_n(\lambda_t)$ is the energy eigenvalue and $\hat{P}_n(\lambda_t)$ is the associated projection operator. Here, this Hamiltonian depends on time through the time-dependent parameter $\lambda_t = \{\lambda_t(1), \lambda_t(2), \cdots\}$. Dynamics of this system is generated by the time evolution operator $\hat{U}_D(t)$ satisfying
\begin{equation}
i\hbar \frac{d}{dt} \hat{U}_D(t) = \hat{H}(\lambda_t) \hat{U}_D(t), \quad \hat{U}_D(0) = 1.
\end{equation}
Throughout this paper, the dot symbol represents time derivative.

Time evolution of the projection operators is isometrically generated by the adiabatic transformation $\hat{U}_A(t)$ as
\begin{equation}
\hat{P}_n(\lambda_t) = \hat{U}_A(t) \hat{P}_n(\lambda_0) \hat{U}_A^\dagger(t),
\end{equation}
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\end{equation}
where
for all $n$. According to the theory of shortcuts to adiabaticity [34], the adiabatic transformation satisfies

$$i\hbar \dot{U}_A(t) = [\tilde{\mathcal{H}}(\lambda_t) + \mathcal{H}_{cd}(t)]U_A(t), \quad \dot{U}_A(0) = 1,$$

where $\mathcal{H}_{cd}(t)$ is the counterdiabatic Hamiltonian given by

$$\mathcal{H}_{cd}(t) = \frac{i\hbar}{2} \sum_n [\dot{\mathcal{P}}_n(\lambda_t), \mathcal{P}_n(\lambda_t)].$$

One may use the adiabatic Hamiltonian [15] (the reduced counterdiabatic Hamiltonian [35])

$$\tilde{\mathcal{H}}_{cd}^{(n)}(t) = i\hbar[\dot{\mathcal{P}}_n(\lambda_t), \mathcal{P}_n(\lambda_t)],$$

instead of the counterdiabatic Hamiltonian (5). In this case, only a single projection operator $\mathcal{P}_n(\lambda_t)$ is transformed as Eq. (3), but others $\dot{\mathcal{P}}_m(\lambda_t)$ ($m \neq n$) are not [14].

We introduce the transition rate from the $n$th level to the $m$th level

$$p_{nm}(t) = \|\mathcal{P}_m(\lambda_t)\tilde{U}_D(t)\mathcal{P}_n(\lambda_0)\tilde{U}^\dagger_D(t)\mathcal{P}_m(\lambda_0)\|^2$$

$$= \|\mathcal{P}_m(\lambda_t)\tilde{U}_D(t)\mathcal{P}_n(\lambda_0)\|^2$$

$$= \|\mathcal{P}_m(\lambda_0)\tilde{U}^\dagger_A(t)\tilde{U}_D(t)\mathcal{P}_n(\lambda_0)\|^2.$$ (7)

Here, $\| \cdot \|$ is the operator norm. Throughout this paper, we only consider bounded operators, and thus $\|A\| = \|A^\dagger\|$ holds. For non-degenerate eigenstates $\{ |n(\lambda_t)\rangle \}$, this quantity is nothing but the transition probability from the $n$th energy eigenstate to the $m$th energy eigenstate

$$p_{nm}(t) = |\langle m(\lambda_t)|\tilde{U}_D(t)|n(\lambda_0)\rangle|^2.$$ (8)

For degenerate eigenstates $\{ |n, \nu_n(\lambda_t)\rangle \}$, this quantity is the maximum transition probability from an energy eigenstate in the $n$th level to the $m$th level

$$p_{nm}(t) = \max_{|\nu_m(\lambda_t)\rangle} \sum_{\mu_m} |\langle m, \mu_m(\lambda_t)|\tilde{U}_D(t)|\psi_n(\lambda_0)\rangle|^2,$$ (9)

where $|\psi_n(\lambda_t)\rangle$ is an $n$th energy eigenstate, which is linear combination of $\{ |n, \nu_n(\lambda_t)\rangle \}$.

From the differential equation

$$i\hbar \frac{d}{dt} [\tilde{U}^\dagger_A(t)\tilde{U}_D(t)] = -\tilde{U}^\dagger_A(t)\mathcal{H}_{cd}(t)\tilde{U}_D(t),$$

we obtain

$$\tilde{U}^\dagger_A(t)\tilde{U}_D(t) = 1 - \frac{1}{i\hbar} \int_0^t dt' \tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t').$$ (11)

Note that $\tilde{U}^\dagger_A(t)\tilde{U}_D(t)$ is unitary, i.e.,

$$1 = \tilde{U}^\dagger_A(t)\tilde{U}_D(t)\tilde{U}^\dagger_A(t)\tilde{U}_D(t) = \left( 1 - \frac{1}{i\hbar} \int_0^t dt' \tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t') \right) \times \left( 1 + \frac{1}{i\hbar} \int_0^t dt' \tilde{U}^\dagger_D(t')\mathcal{H}_{cd}(t')\tilde{U}_A(t') \right)$$ (12)

holds, and thus the equality

$$0 = \frac{1}{i\hbar} \int_0^t dt' [\tilde{U}^\dagger_D(t')\mathcal{H}_{cd}(t')\tilde{U}_A(t') - \tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t')]$$

$$+ \frac{1}{i\hbar} \int_0^t dt' \tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t') \int_0^t dt'' \tilde{U}^\dagger_D(t'')\mathcal{H}_{cd}(t'')\tilde{U}_A(t''),$$ (13)

must be satisfied.

For $m \neq n$, the transition rate (7) becomes

$$p_{nm}(t) = \left| \frac{1}{i\hbar} \int_0^t dt' \tilde{P}_m(\lambda_0)\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t')\tilde{P}_n(\lambda_0) \right|^2.$$ (14)

In general, calculation of time evolution operator $\tilde{U}_D(t)$ is hard, and thus we omit it by using the properties of the operator norm as

$$p_{nm}(t) \leq \left[ \frac{1}{i\hbar} \int_0^t dt' \| \tilde{P}_m(\lambda_0)\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{U}_D(t')\tilde{P}_n(\lambda_0) \| \right]^2$$

$$\leq \left[ \frac{1}{i\hbar} \int_0^t dt' \| \tilde{P}_m(\lambda_0)\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\| \|\tilde{U}_D(t')\tilde{P}_n(\lambda_0)\| \right]^2$$

$$= \left[ \frac{1}{i\hbar} \int_0^t dt' \| \tilde{P}_m(\lambda_0)\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\| \right]^2$$

$$= \left[ \int_0^t dt' \| (1 - \tilde{P}_m(\lambda_0))\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{P}_m(\lambda_0) \| \right]^2.$$ (15)

Here, for the last line of the equality, we use Eq. (5).

For non-degenerate eigenstates $\{ |n(\lambda_t)\rangle \}$, the integrand of Eq. (15) is nothing but the Abelian quantum geometric tensor for the $m$th energy eigenstate

$$\| (1 - \tilde{P}_m(\lambda_0))\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{P}_m(\lambda_0) \|^2 = \langle \dot{\tilde{m}}(\lambda_0) | (1 - |m(\lambda_t)\rangle \langle m(\lambda_0)\| \dot{\tilde{m}}(\lambda_0) \rangle,$$ (16)

and for degenerate eigenstates $\{ |n, \nu_n(\lambda_t)\rangle \}$, it is the maximum expectation value of the non-Abelian quantum geometric tensor for the $m$th level

$$\| (1 - \tilde{P}_m(\lambda_0))\tilde{U}^\dagger_A(t')\mathcal{H}_{cd}(t')\tilde{P}_m(\lambda_0) \|^2$$

$$= \max_{|\psi_m(\lambda_t)\rangle} \sum_{\mu_m} \langle \psi_m(\lambda_t)|m, \mu_m(\lambda_t) \rangle \langle m, \mu_m(\lambda_t)\rangle |$$(17)

× (1 - $\sum_{\nu_m} |m, \nu_m(\lambda_t)\rangle \langle m, \nu_m(\lambda_t)\|$)

× $\sum_{\mu'_m} |m, \mu'_m(\lambda_t)\rangle \langle m, \mu'_m(\lambda_t)| \psi_m(\lambda_t)\rangle,$

(for the Abelian and the non-Abelian quantum geometric tensors, see, Ref. [36]). This result implies that nonadiabatic transitions are affected by geometry of excited states.
Next, we will consider the remaining rate, i.e., the transition rate (7) for $m = n$. In this case, by using Eq. (13), we find

$$p_{nn}(t) = \left\| \dot{P}_n(\lambda_0) \left( 1 - \frac{1}{\hbar} \int_0^t dt' \hat{U}_A^{-1}(t') \hat{H}_{cd}(t') \hat{U}_A(t') \right) P_n(\lambda_0) \right\|$$

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Finally we find similar quantity to the bound (15) by using the adiabatic perturbation theory, and thus this bound is a physically natural. Note that this bound is related to the energy cost of counterdiabatic driving [37, 38].

III. ADIABATIC PERTURBATION THEORY VIEWPOINT

We discuss our results from the viewpoint of the adiabatic perturbation theory [11–13]. A quantum quench at time $t$ changes the $m$th projection operator as

$$\hat{P}_m(\lambda_{t+\delta t}) \approx \hat{P}_m(\lambda_t) + \delta t \dot{\hat{P}}_m(\lambda_t),$$

where $\delta t$ is a small time interval. Then, we find that a quantum quench causes nonadiabatic transitions from the $n$th level to the $m$th level as

$$\hat{P}_m(\lambda_{t+\delta t}) \hat{P}_n(\lambda_t) \hat{P}_m(\lambda_{t+\delta t}) \approx \delta t^2 \dot{\hat{P}}_m(\lambda_t) \hat{P}_n(\lambda_t) \dot{\hat{P}}_m(\lambda_t),$$

that is, the instantaneous transition rate at time $t$ for a quantum quench is given by

$$\Delta \rho_{nm}^{APT}(t) = \left\| \hat{P}_m(\lambda_{t+\delta t}) \hat{P}_n(\lambda_t) \hat{P}_m(\lambda_{t+\delta t}) \right\|$$

$$\approx \delta t^2 \| \hat{P}_n(\lambda_t) \dot{\hat{P}}_m(\lambda_t) \|^2.$$  

In the last inequality and the equality, we use similar calculations to Eq. (15).

We can also derive a universal bound for any nonadiabatic transition. By using the inequality

$$\| \hat{P}_m(\lambda_t) \hat{H}_{cd}(t) \| \leq \| \hat{H}_{cd}(t) \|,$$

we immediately find a universal bound for the transition rate

$$p_{nn}(t) \leq \left[ \frac{1}{\hbar} \int_0^t dt' \| \hat{H}_{cd}(t') \| \right]^2,$$

and similarly a universal bound for the remaining rate

$$p_{nn}(t) \geq 1 - \left[ \frac{1}{\hbar} \int_0^t dt' \| \hat{H}_{cd}(t') \| \right]^2.$$  

The small counterdiabatic Hamiltonian implies that small perturbation is enough to be adiabatic, and thus this bound is a physically natural. Note that this bound is related to the energy cost of counterdiabatic driving [37, 38].

IV. QUANTUM SPEED LIMIT VIEWPOINT

In the quantum speed limit [19–22], we introduce the distance between two quantum states, $\hat{\rho}_i$ and $\hat{\rho}_f$, by the Bures angle [39, 40]

$$L(\hat{\rho}_i, \hat{\rho}_f) = \arccos F(\hat{\rho}_i, \hat{\rho}_f),$$

where $F(\hat{\rho}_i, \hat{\rho}_f)$ is the Uhlmann fidelity [41]

$$F(\hat{\rho}_i, \hat{\rho}_f) = \left( \text{Tr} \sqrt{\sqrt{\hat{\rho}_i} \hat{\rho}_f \sqrt{\hat{\rho}_i}} \right)^2.$$
We consider time evolution governed by
\[ i\hbar \dot{\rho}(t) = [\hat{H}(\lambda), \rho(t)], \]
satisfying \( \dot{\rho}(0) = \dot{\rho}_i \) and \( \dot{\rho}(\tau) = \dot{\rho}_f \). It can be shown that this distance is bounded as
\[ L(\dot{\rho}_i, \dot{\rho}_f) \leq \frac{1}{\hbar} \int_0^\tau dt (\Delta \hat{H})_{\dot{\rho}_i}, \]
where \((\Delta \hat{H})_{\dot{\rho}_i}\) is the standard deviation of the Hamiltonian \( \hat{H}(\lambda_t) \) with a state \( \dot{\rho}(t) \) \([42, 43]\). This bound means that a quantum process between large distant states requires large energy cost or long operation time.

Here we consider a state in the mth level \( \dot{\rho}_m(0) = \hat{P}_m(\lambda_0)\dot{\rho}_m(0)\hat{P}_m(\lambda_0) \) and its adiabatic transformation \( \hat{P}_m(\lambda_0)\dot{\rho}_m(t)\hat{P}_m(\lambda_0) = \hat{U}_A(t)\dot{\rho}_m(0)\hat{U}_A^\dagger(t) \). For this adiabatic transformation, the quantum speed limit becomes \([44]\)
\[ L(\dot{\rho}_m(0), \dot{\rho}_m(t)) \leq \frac{1}{\hbar} \int_0^t dt' (\Delta \hat{H}_{\text{cd}})_{\dot{\rho}_m} . \]

Here, following the inequality holds:
\[ \frac{1}{\hbar} (\Delta \hat{H}_{\text{cd}})_{\dot{\rho}_m} = \frac{1}{\hbar} \sqrt{\text{Tr}[[\hat{H}_{\text{cd}}(t)]^2\dot{\rho}_m(t)] - \text{Tr}[[\hat{H}_{\text{cd}}(t)\dot{\rho}_m(t)]]^2}
= \frac{1}{\hbar} \sqrt{\text{Tr}[[\hat{H}_{\text{cd}}(t)]^2\dot{\rho}_m(t)]}
\leq \frac{1}{\hbar} \| \hat{H}_{\text{cd}}(t)\dot{P}_m(\lambda_t) \|
= \| [(1 - \hat{P}_m(\lambda_0))\dot{\rho}_m(\lambda_t)] \| . \]

In particular, nondegenerate eigenstates satisfies equality. Finally, the following bound exists:
\[ [L(\dot{\rho}_m(0), \dot{\rho}_m(t))]^2 \leq \int_0^t dt' \| [(1 - \hat{P}_m(\lambda_{t'}))\dot{\rho}_m(\lambda_{t'})] \|^2 . \]

Therefore, nonadiabatic transitions to the mth level caused by the dynamical transformation shares the identical upper bound with the quantum speed limit of the adiabatic transformation for the mth level.

Suppose that the bound \((15)\) \([33]\) is small, which is of interest. From the viewpoint of the quantum speed limit, it implies that the adiabatic transformation from \( \dot{\rho}_m(0) \) to \( \dot{\rho}_m(t) \) can be implemented without requiring large energy cost or long operation time. At the same time, the bound \((15)\) implies that the amount of nonadiabatic transitions to mth level is small. This result can be interpreted as follows: The distance between \( \dot{\rho}_m(0) \) and \( \dot{\rho}_m(t) \) is small. From the definition, the distance between \( \dot{\rho}_m(0) \) and \( \dot{\rho}_m(0) \) is large. Therefore, the distance between \( \dot{\rho}_n(0) \) and \( \dot{\rho}_m(t) \) is large, and thus nonadiabatic transitions do not take place that much.

V. SUMMARY AND DISCUSSION

In this paper, we discussed the bounds for nonadiabatic transitions from the viewpoints of the adiabatic perturbation theory and the quantum speed limit. From Eq. \((15)\), we found that the amount of nonadiabatic transitions from the nth level to the mth level is bounded by the function of the quantum geometric tensor for the mth level. This bound does not depend on n, but it might be natural because we have to accumulate all the paths of instantaneous nonadiabatic transitions as discussed from the viewpoint of the adiabatic perturbation theory. The viewpoint of the quantum speed limit provides us with nontrivial relationship between the quantum speed limit of the adiabatic transformation for the mth level and nonadiabatic transitions to the mth level caused by the dynamical transformation. We also derived the universal bound for any nonadiabatic transition written in terms of the counterdiabatic Hamiltonian.

In quantum adiabatic brachistochrone, we reduce nonadiabatic transitions by minimizing cost functions related to adiabaticity \([29, 30, 45]\). We note that the bound \((15)\) for nondegenerate eigenstates is the square of a cost function used in Ref. \([30]\). We have many choice for cost functions in quantum adiabatic brachistochrone \([29, 30, 45]\), but the present result suggests that the cost function used in Ref. \([30]\) is physically natural. Note that physically natural choice does not imply the best choice. From this relationship, we can easily find an optimal schedule of parameter \( \lambda_t \) minimizing the transition rate \( p_m(t) \) by using quantum adiabatic brachistochrone. Success of quantum adiabatic brachistochrone in adiabatic state preparation reported in literature \([45, 46]\) also supports effectiveness of the bound \((15)\).

Finally, we will explain that the universal bound \((20)\) may be more useful than the bound \((15)\) in some situations, while the universal bound \((20)\) is looser than the bound \((15)\). Both of the bounds \((15)\) and \((20)\) in principle requires knowledge of energy eigenstates, and this requirement makes it hard to obtain these bounds for general quantum systems. However, it is possible to construct counterdiabatic terms without knowing energy eigenstates of a system by using a variational approach \([47]\), i.e., we can estimate the value of the bound \((20)\). Furthermore, this can be systematically performed by calculating the nested commutators \([\hat{H}(\lambda_t), [\hat{H}(\lambda_t), [\cdots, [\hat{H}(\lambda_t), \cdots]] \cdots]] [48].

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