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Interpolation approach to Hamiltonian-varying quantum systems and the adiabatic theorem

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Abstract

Quantum control could be implemented by varying the system Hamiltonian. According to adiabatic theorem, a slowly changing Hamiltonian can approximately keep the system at the ground state during the evolution if the initial state is a ground state. In this paper we consider this process as an interpolation between the initial and final Hamiltonians. We use the mean value of a single operator to measure the distance between the final state and the ideal ground state. This measure resembles the excitation energy or excess work performed in thermodynamics, which can be taken as the error of adiabatic approximation. We prove that under certain conditions, this error can be estimated for an arbitrarily given interpolating function. This error estimation could be used as guideline to induce adiabatic evolution. According to our calculation, the adiabatic approximation error is not linearly proportional to the average speed of the variation of the system Hamiltonian and the inverse of the energy gaps in many cases. In particular, we apply this analysis to an example in which the applicability of the adiabatic theorem is questionable.

Keywords: quantum control; adiabatic theorem; interpolation of Hamiltonian

1 Introduction

Adiabatic process is aimed at stabilizing a parameter-varying quantum system at its eigenstate. This process has many applications in the engineering of quantum systems [1–5], and in particular plays the fundamental role in adiabatic quantum computation (AQC) [6–8]. The adiabatic theorem [9, 10] states that a system will undergo adiabatic evolution given that the system parameter varies slowly.

Quantifying the applicability of adiabatic approximations is an interesting topic of current research efforts. On the one hand, this kind of research has been spurred by so-called shortcuts to adiabaticity [11], and on the other hand recent insights from thermodynamics haven put adiabatic processes back into focus [12, 13]. In particular, the validity of the adiabatic theorem has been under intensive studies both theoretically and experimentally since it was proposed, and much of these efforts were devoted to the rigorous description of the sufficient quantitative conditions of adiabatic theorem, and the estimation of the error accumulated over a long time [10, 14–16]. Once the exact knowledge on the adiabatic process is available, it is straightforward to apply the results to the optimal design of adiabatic control on specific systems [17, 18]. The most interesting progress is that the validity of the adiabatic theorem itself has been challenged in the recent decade [19–27], both by strict analysis and counter-examples. According to these findings, the errors induced by the adiabatic approximation could accumulate over time despite certain quantitative condition is satisfied [19–21, 24, 25], e.g., when there exists an additional perturbation or driving that is resonant with the system. Particularly as indicated in [24], it is not new that resonant driving can cause population transfer between eigenstates. Also, a proof can be found in [25] stating that only a resonant perturbation whose amplitude gradually decays to zero can result in a violation of a well-known sufficient condition.

In this paper we consider the following process: the process starts at $t = 0$. The system Hamiltonian at $t = 0$ is H_1, and the system Hamiltonian at $t = T$ is $H_2 = H_1 + \lambda\Delta H$, $\lambda > 0$. λ is a dimensionless quantity. ΔH is a fixed operator and so the direction of the variation is fixed. We assume H_1, H_2, and ΔH are bounded operators throughout this paper. T is the evolution time. The transition of the system from H_1 to H_2 can be described using an interpolating function $f(t)$ so that

$$H(t) = H_1 + f(t)(H_2 - H_1) = H_1 + \lambda f(t)\Delta H, \tag{1}$$

with $f(0) = 0$ and $f(T) = 1$. We work under the condition that a valid perturbative analysis of the system evolution is available. This often means λ should be smaller than a threshold value. It is worth mentioning that the classical adiabatic theorem was proved also using a perturbative analysis, which cannot be applied directly to a large variation of Hamiltonian. Therefore, our analysis in this paper is not concerned with the adiabatic evolution for a large variation of Hamiltonian. However, our analysis provides a rigorous estimation of the error accumulated during this small-variation evolution for an arbitrarily given interpolation.

Our work is different from the previous works in two ways. First, instead of studying the evolution of the eigenstates and their corresponding probability amplitudes, the mean value of a Hermitian operator is defined as a measure of the error. For example, in the context of adiabatic quantum computation where one wants to prepare the ground state of a target Hamiltonian $\hat{H}_2 \geq 0$ whose ground-state energy is 0, $\epsilon = \langle \hat{H}_2 \rangle_{\rho_t}$ serves as a good measure of the distance between the real-time state ρ_t and the ground state. This measure resembles the excitation energy or excess work performed during the process, as studied in thermodynamics [12]. In this paper we only consider the error accumulated over the entire process, which means we are only interested in $\epsilon = \langle \hat{H}_2 \rangle_{\rho_T}$. The second difference is that the error, or the excitation energy or excess work performed during the process, can be estimated with a sufficient precision for arbitrarily given interpolating functions. As a result, the parameters which are related to the suppression of the error can be easily identified. For example, we have $\epsilon = O(\frac{\lambda^2}{T^2\lambda_2^3})$ as $\lambda \to 0$ in the case of linear interpolation. Here λ_2 is the energy gap between the ground and first-excited states of the initial Hamiltonian. However for the interpolation in the counterexample [19, 25], the scaling of ϵ is not so simple.

This paper is organized as follows. In Section 2, we introduce the model of this paper. In Section 3, we give the estimation of the error for linear interpolation. In Section 4, we present the general algorithm to estimate the error for an arbitrarily given interpolating function. We discuss three examples in Section 5. Conclusion is given in Section 6.

2 Definitions and preliminaries

The system is defined on an N-dimensional Hilbert space. We set Dirac constant $\hbar = 1$. $\|\cdot\|$ denotes the matrix norm. Two real functions $f_1(x)$ and $f_2(x)$ can be denoted as $f_1(x) = O(f_2(x))$, $x \to \infty$, if and only if there exists a positive real number M and a real number x_0 such that $|f_1(x)| \le M|f_2(x)|$, $x \ge x_0$, where $|\cdot|$ denotes the absolute value.

Let $\{\omega_i : i = 1, 2, \ldots, N\}$ be the monotonically increasing sequence of eigenvalues of H_1, so that $\omega_i \ge \omega_j$ when $i > j$, and $\{|i\rangle\}$ be the corresponding eigenstates. We denote the energy gap between the ith eigenstate and the ground state as $\lambda_i = \omega_i - \omega_1$. Similarly, we define the increasing sequence of eigenvalues of H_2, $\{\omega'_i : i = 1, 2, \ldots, N\}$ and $\{\lambda'_i\}$, $\{|i'\rangle\}$ correspondingly.

For convenience, we also introduce two offset Hamiltonians, $\hat{H}_1$ and $\hat{H}_2$. The Hamiltonian $\hat{H}_1$ is defined as $\hat{H}_1 = H_1 - \omega_1$, i.e., by offsetting the Hamiltonian of the system at $t = 0$ by a constant operator ω_1 so that $\hat{H}_1 \ge 0$. By $\hat{H}_1 \ge 0$ we mean $\hat{H}_1$ is positive semidefinite and its the smallest eigenvalue of $\hat{H}_1$ is zero. Similarly, we define $\hat{H}_2 = H_2 - \omega'_1 \ge 0$ by offsetting the system Hamiltonian by a constant operator ω'_1. Let ρ_t denote the system state at time t and let ρ_g be the initial state of the system at $t = 0$. We always assume that ρ_g is the ground state of $\hat{H}_1$, and so we have $\langle \hat{H}_1 \rangle_{\rho_g} = 0$.

The measure of adiabaticity is proposed as follows

Definition 1 The distance between the final state and the ground state of H_2 is measured by

$$\epsilon = \langle \hat{H}_2 \rangle_{\rho_T}. \tag{2}$$

Obviously, if the evolution is adiabatic, i.e., ρ_T is the ground state of H_2, then we have $\epsilon = 0$. In particular, ϵ is closely related to the fidelity of the final state and ground state in the Schrödinger picture (see Appendix C). A small error ϵ implies a large fidelity.

In this paper we also call ϵ the adiabatic approximation error, as ϵ reflects how well we can approximate the evolution as a perfect adiabatic process.

In this paper we only consider λ such that ρ_t, $t \in [0, T]$ can be expanded using Magnus series in the interaction picture. For more details about the expansion in the interaction picture, please refer to Appendix A. If the series expansion is valid in the interaction picture, we can transform back to the Schrödinger picture and write the evolution of the state as (see Appendix A)

$$\rho_t = e^{-\mathrm{i}H_1 t}\left(\rho_g + R(t) + \mathrm{i}\left[\rho_g, \lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \Delta H e^{-\mathrm{i}H_1 t'}\right]\right) e^{\mathrm{i}H_1 t}, \tag{3}$$

where we have $\|R(t)\| = O(\lambda^2)$. A sufficient condition for the Magnus series to converge is given by (see Appendix A)

$$\lambda < \frac{\pi}{\|\Delta H\| \int_0^T f(t)\, dt}. \tag{4}$$

Our aim is to estimate an asymptotic behaviour of ϵ provided $\lambda \to 0$. Furthermore, we will use the obtained estimate to analyze several cases of the adiabatic theorem including those where some difficulties with adiabatic approximation have been encountered.

3 Adiabatic approximation under linear interpolation of the Hamiltonian

The Heisenberg evolution of the expectation of an observable is written as

$$\frac{d}{dt}\langle X(t)\rangle_{\rho_g} = \langle -\mathrm{i}[X(t), H]\rangle_{\rho_g}, \tag{5}$$

where H is the system Hamiltonian. Recall that $\rho_g = |1\rangle\langle 1|$. Since $H_1|1\rangle = \omega_1|1\rangle$, $\langle X(t)\rangle_{\rho_g}$ is a constant of motion under the action of H_1:

$$\frac{d}{dt}\langle X(t)\rangle_{\rho_g} = \langle -\mathrm{i}[X(t), H_1]\rangle_{\rho_g} = 0 = \langle -\mathrm{i}[X(t), \hat{H}_1]\rangle_{\rho_g} \tag{6}$$

for any Hermitian operator $X(t)$.

We will need to study the dynamics of $\langle \hat{H}_2\rangle_{\rho_t} = \langle \hat{H}_2(t)\rangle_{\rho_g}$ in order to solve for ϵ. The time evolution of $\langle \hat{H}_2\rangle_{\rho_t}$ is determined by its generator $\frac{d}{dt}\langle \hat{H}_2\rangle_{\rho_t} = \langle -\mathrm{i}[\hat{H}_2, H(t)]\rangle_{\rho_t}$. For linear interpolating function $f(t) = \frac{t}{T}$, integration of $\frac{d}{dt}\langle \hat{H}_2\rangle_{\rho_t}$ over $[0, T]$ results in the following expression (see details in Appendix B):

$$\begin{aligned}
&\langle \hat{H}_2\rangle_{\rho_T} - \langle \hat{H}_2\rangle_{\rho_g} \\
&\quad = \int_0^T \left(\langle -\mathrm{i}[\hat{H}_2, H(t)]\rangle_{\rho_t}\right) dt \\
&\quad = \int_0^T dt \biggl[-2\bigl(1-f(t)\bigr)\sum_{i\neq 1}(\omega_i - \omega_1)\langle 1|\hat{H}_2|i\rangle\langle i|\hat{H}_2|1\rangle \\
&\qquad \times \int_0^t dt' f(t')\cos\bigl((\omega_i - \omega_1)(t'-t)\bigr)\biggr] \\
&\qquad + \int_0^T dt\, \mathrm{Tr}\bigl\{-\mathrm{i}e^{\mathrm{i}H_1 t}\bigl[\hat{H}_2, \bigl(1-f(t)\bigr)\hat{H}_1\bigr]e^{-\mathrm{i}H_1 t}R(t)\bigr\} && (7) \\
&\quad = \sum_{i\neq 1}\left(-\frac{1}{\lambda_i} + \frac{4\sin^2(\lambda_i T/2)}{T^2\lambda_i^3}\right)\langle 1|\hat{H}_2|i\rangle\langle i|\hat{H}_2|1\rangle \\
&\qquad + \int_0^T dt\, \mathrm{Tr}\left\{-\mathrm{i}e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1-\frac{t}{T}\right)\hat{H}_1\right]e^{-\mathrm{i}H_1 t}R(t)\right\}. && (8)
\end{aligned}$$

As we noted before, $\langle \hat{H}_2\rangle_{\rho_T}$ is exactly zero if ρ_T is the ground state of $\hat{H}_2$. If ρ_T is not the ground state of $\hat{H}_2$, we can determine the bound on $\epsilon = \langle \hat{H}_2\rangle_{\rho_T}$ from the following equality

$$\begin{aligned}
\langle \hat{H}_2\rangle_{\rho_T} - \langle \hat{H}_2\rangle_{\rho_g} &= \int_0^T \langle -\mathrm{i}[\hat{H}_2, H(t)]\rangle_{\rho_t}\, dt \\
&= \int_0^T \langle -\mathrm{i}[H_2, H(t)]\rangle_{\rho_t}\, dt = \langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g}.
\end{aligned} \tag{9}$$

Since

$$\hat{H}_2 = H_2 - \omega_1', \tag{10}$$

the error ϵ can be expressed as

$$\epsilon = \langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g} - \bigl[\omega_1' - \langle H_2\rangle_{\rho_g}\bigr]. \tag{11}$$

With the aid of (8), we can investigate the rate of convergence of ϵ to zero as λ tends to zero in the case where $f(t)$ defines a linear interpolation, as summarized in the following proposition:

Proposition 1 *Assume $\lambda_2 > 0$ (the ground state of H_1 is non-degenerate) and suppose $f(t) = t/T$, which corresponds to the linear interpolation of the Hamiltonian. The estimation of ϵ is given by $\sum_{i\neq 1} \frac{4\lambda^2 \sin^2(\lambda_i T/2)|\langle 1|\Delta H|i\rangle|^2}{T^2\lambda_i^3} + O(\lambda^3)$, which is of the order $O(\frac{\lambda^2}{T^2\lambda_2^3})$ as $\lambda \to 0$.*

Proof Referring to (11) and (9), we need to compute the difference between (8) and $\omega_1' - \langle 1|H_2|1\rangle$. First we write (8) as

$$\begin{aligned}\langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g} &= \sum_{i\neq 1}\left(-\frac{1}{\lambda_i} + \frac{4\sin^2(\lambda_i T/2)}{T^2\lambda_i^3}\right)\langle 1|\hat{H}_2|i\rangle\langle i|\hat{H}_2|1\rangle \\ &\quad + \int_0^T dt\,\mathrm{Tr}\bigl\{-\mathrm{i}e^{\mathrm{i}H_1 t}\bigl[\hat{H}_2, \bigl(1-f(t)\bigr)\hat{H}_1\bigr]e^{-\mathrm{i}H_1 t}R(t)\bigr\} \qquad (12) \\ &= -\sum_{i\neq 1}\frac{\lambda^2|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + \sum_{i\neq 1}\frac{4\lambda^2\sin^2(\lambda_i T/2)|\langle 1|\Delta H|i\rangle|^2}{T^2\lambda_i^3} \\ &\quad + \int_0^T dt\,\mathrm{Tr}\bigl\{-\mathrm{i}e^{\mathrm{i}H_1 t}\bigl[\hat{H}_2, \bigl(1-f(t)\bigr)\hat{H}_1\bigr]e^{-\mathrm{i}H_1 t}R(t)\bigr\}, \qquad (13)\end{aligned}$$

by noting that

$$\sum_{i\neq 1}\frac{|\langle 1|\hat{H}_2|i\rangle|^2}{\lambda_i} = \sum_{i\neq 1}\frac{|\langle 1|H_1 + \lambda\Delta H - \omega_1'|i\rangle|^2}{\lambda_i} = \sum_{i\neq 1}\frac{\lambda^2|\langle 1|\Delta H|i\rangle|^2}{\lambda_i}. \qquad (14)$$

Moreover, by the definition of the notation $O(\cdot)$ in Section 2 we can write $\sum_{i\neq 1}\frac{4\lambda^2\sin^2(\lambda_i T/2)|\langle 1|\Delta H|i\rangle|^2}{T^2\lambda_i^3} = O(\frac{\lambda^2}{T^2\lambda_2^3})$.

Denote $\bar{H} = \max_{f(t)\in(0,1)}\|H(t)\|$. Since

$$\left\|\int_0^T dt\,\mathrm{Tr}\bigl\{-\mathrm{i}e^{\mathrm{i}H_1 t}\bigl[\hat{H}_2, \bigl(1-f(t)\bigr)\hat{H}_1\bigr]e^{-\mathrm{i}H_1 t}R(t)\bigr\}\right\| \le \frac{T\lambda}{2}\bar{H}^2\|R(t)\| \qquad (15)$$

is $O(\lambda^3)$, we can further write (13) as

$$\langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g} = -\sum_{i\neq 1}\frac{\lambda^2|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + \sum_{i\neq 1}\frac{4\lambda^2\sin^2(\lambda_i T/2)|\langle 1|\Delta H|i\rangle|^2}{T^2\lambda_i^3} + O\bigl(\lambda^3\bigr). \qquad (16)$$

Next we will calculate $\omega_1' - \langle 1|H_2|1\rangle$. We have

$$\langle 1|H_2|1\rangle = \langle 1|H_1 + \lambda\Delta H|1\rangle = \omega_1 + \lambda\langle 1|\Delta H|1\rangle. \qquad (17)$$

The smallest eigenvalue ω_1' of H_2 can be calculated using the first-order time-independent perturbation theory for non-degenerate system. Assume H_1 is the unperturbed Hamiltonian and the perturbation is $\lambda\Delta H$, then the lowest eigenvalue of the perturbed Hamiltonian $H_1 + \lambda\Delta H$ can be written as series in terms of λ and ω_1 [28]:

$$\omega_1' = \omega_1 + \lambda\langle 1|\Delta H|1\rangle - \lambda^2\sum_{i\neq 1}\frac{|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + O\bigl(\lambda^3\bigr). \qquad (18)$$

Thus we conclude

$$\omega_1' - \langle H_2\rangle_{\rho_g} = \omega_1' - \langle 1|H_2|1\rangle = -\lambda^2 \sum_{i\neq 1} \frac{|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + O(\lambda^3). \tag{19}$$

Comparing (16) and (19), the terms $-\lambda^2 \sum_{i\neq 1} \frac{|\langle 1|\Delta H|i\rangle|^2}{\lambda_i}$ cancel and so the error ϵ is estimated by

$$\begin{aligned}\epsilon &= \sum_{i\neq 1} \frac{4\lambda^2 \sin^2(\lambda_i T/2)|\langle 1|\Delta H|i\rangle|^2}{T^2\lambda_i^3} + O(\lambda^3) \\ &= O\left(\frac{\lambda^2}{T^2\lambda_2^3}\right), \quad \lambda \to 0. \end{aligned}\tag{20}$$

□

4 Error estimation for arbitrary interpolations

The approach derived in the previous section can be easily generalized for arbitrary given continuous interpolating functions. The generalization can simply be done by replacing the linear interpolation function with the given continuous function $f(t)$ and then recalculating the double integration

$$A_i(T) = -2\int_0^T dt \int_0^t dt' \left(1 - \frac{t}{T}\right)\lambda_i f(t') \cos\bigl(\lambda_i(t'-t)\bigr) \tag{21}$$

in (7). The error estimation can easily be obtained from the proof of Proposition 1:

Proposition 2 *For an arbitrarily given $f(t)$, the error estimation is given by*

$$\epsilon = \lambda^2 \sum_{i\neq 1} A_i(T)\bigl|\langle 1|\Delta H|i\rangle\bigr|^2 + \lambda^2 \sum_{i\neq 1} \frac{|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + O(\lambda^3) \tag{22}$$

as $\lambda \to 0$.

Proof ϵ is still calculated by (11), using $\langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g}$ and $\omega_1' - \langle H_2\rangle_{\rho_g}$. We have

$$\langle H_2\rangle_{\rho_T} - \langle H_2\rangle_{\rho_g} = \sum_{i\neq 1} A_i(T)\lambda^2\bigl|\langle 1|\Delta H|i\rangle\bigr|^2 + O(\lambda^3) \tag{23}$$

and

$$\omega_1' - \langle H_2\rangle_{\rho_g} = -\lambda^2 \sum_{i\neq 1} \frac{|\langle 1|\Delta H|i\rangle|^2}{\lambda_i} + O(\lambda^3). \tag{24}$$

□

It must be pointed out that $A(T)$ is very easy to calculate with the aid of any softwares that can perform symbolic integration, and therefore it is straightforward to apply Proposition 2 to find the error estimation for a given interpolating function, as we are going to do in the next section.

5 Examples

5.1 Linear interpolation: $f(t) = t/T$

By Proposition 1, the error estimation is $\epsilon = \sum_{i\neq 1} \frac{4\sin^2(\lambda_i T/2)}{T^2\lambda_i^3} |\langle 1|\Delta H|i\rangle|^2\lambda^2 + O(\lambda^3)$ as $\lambda \to 0$. Since $\sin^2(\lambda_i T/2)$ and ΔH are bounded, this error term is primarily determined by $\frac{\lambda}{T}$ which is the average speed of the variation of the system Hamiltonian, and $\frac{1}{\lambda_i}$ which is the inverse of the energy gap between the ground and ith eigenstates of H_1, as $\lambda \to 0$. In particular, we have

$$\lim_{\lambda\to 0} \frac{\epsilon}{(\frac{\lambda}{T})^2} = \sum_{i\neq 1} \frac{4\sin^2(\lambda_i T/2)}{\lambda_i^3} \bigl|\langle 1|\Delta H|i\rangle\bigr|^2. \tag{25}$$

Therefore, when the inverse of the energy gaps $\frac{1}{\lambda_i}$ are fixed values, the approximation error ϵ is estimated to be proportional to the square of the average speed of the variation of the Hamiltonian, which is $(\frac{\lambda}{T})^2$, as $\lambda \to 0$.

5.2 Quadratic interpolation: $f(t) = t^2/T^2$

Replace $f(t)$ with a nonlinear function $f(t) = \frac{t^2}{T^2}$ in (7) and we recalculate the integral to be

$$\sum_{i\neq 1} A_i(T) = \sum_{i\neq 1}\left(-\frac{1}{\lambda_i} + \frac{16\sin^2(\frac{T\lambda_i}{2}) + 4T^2\lambda_i^2 - 8T\lambda_i\sin(T\lambda_i)}{T^4\lambda_i^5}\right)\bigl|\langle 1|\Delta H|i\rangle\bigr|^2. \tag{26}$$

By Proposition 2, for sufficiently small λ, the error is estimated to be of order of λ^2:

$$\begin{aligned}\epsilon_{\text{quad}} &= \lambda^2 \sum_{i\neq 1} \frac{16\sin^2(\frac{T\lambda_i}{2}) + 4T^2\lambda_i^2 - 8T\lambda_i\sin(T\lambda_i)}{T^4\lambda_i^5}\bigl|\langle 1|\Delta H|i\rangle\bigr|^2 + O\bigl(\lambda^3\bigr) \\ &= \left(\frac{\lambda}{T}\right)^2 \sum_{i\neq 1}\left[\frac{16\sin^2(\frac{T\lambda_i}{2})}{T^2\lambda_i^5} + \frac{4}{\lambda_i^3} - \frac{8\sin(T\lambda_i)}{T\lambda_i^4}\right]\bigl|\langle 1|\Delta H|i\rangle\bigr|^2 + O\bigl(\lambda^3\bigr).\end{aligned} \tag{27}$$

That is, in contrast to the linear interpolation case, we have

$$\lim_{\lambda\to 0} \frac{\epsilon_{\text{quad}}}{(\frac{\lambda}{T})^2} = \sum_{i\neq 1}\left[\frac{16\sin^2(\frac{T\lambda_i}{2})}{T^2\lambda_i^5} + \frac{4}{\lambda_i^3} - \frac{8\sin(T\lambda_i)}{T\lambda_i^4}\right]\bigl|\langle 1|\Delta H|i\rangle\bigr|^2. \tag{28}$$

This calculation shows that if the evolution speed is infinitely slow, then the system dynamics is adiabatic during $t \in [0, T]$. However, the scaling of ϵ_{quad} with respect of the square of the average evolution speed $\frac{\lambda}{T}$ is not as simple as in the linear case, where the scaling of ϵ with respect of $(\frac{\lambda}{T})^2$ is primarily determined by the inverse of the energy gaps as $\lambda \to 0$. In the quadratic case, this scaling is primarily determined by a complex factor $[\frac{16\sin^2(\frac{T\lambda_i}{2})}{T^2\lambda_i^5} + \frac{4}{\lambda_i^3} - \frac{8\sin(T\lambda_i)}{T\lambda_i^4}]$ which depends mainly on the inverse of the energy gaps $\{\lambda_i\}$ and the inverse of the evolution time T.

5.3 Interpolation with decaying resonant terms

Here we assume a linear interpolating function with an additional oscillating term that gradually decays to zero. That is,

$$f(t) = \frac{t}{T} + g\left(1 - \frac{t}{T}\right)\sin(\lambda_c t),$$

where λ_c is the oscillating frequency of the perturbation. Ortigoso observed in [25] the inconsistency in the applicability of the adiabatic theorem when the Hamiltonian contains resonant terms whose amplitudes go asymptotically to zero.

Replace $f(t)$ with $f(t) = \frac{t}{T} + g(1 - \frac{t}{T})\sin(\lambda_c t)$ in (7) and we recalculate the integral to be

$$\sum_{i\neq 1} A_i(T) = \sum_{i\neq 1} \frac{Q_1(g, T, \lambda_i, \lambda_c)}{T^2(2\lambda_i^{11} - 8\lambda_i^9\lambda_c^2 + 12\lambda_i^7\lambda_c^4 - 8\lambda_i^5\lambda_c^6 + 2\lambda_i^3\lambda_c^8)}. \tag{29}$$

Q_1 is a function of four parameters. In particular, we note that each term in (29) is well defined for all λ_c, including $\lambda_c = \lambda_i$, since as $\lambda_c \to \lambda_i$, the ith term in (29) approaches

$$\begin{aligned}
&\biggl[-128\sin^2\left(\frac{T\lambda_i}{2}\right) - 16g\sin(T\lambda_i) + 8g\sin(2T\lambda_i) + g^2 \\
&\quad + g^2\bigl(2\sin^2(T\lambda_i) - 1\bigr) - 32T^2\lambda^2 - 16gT\lambda_i + 2g^2T^4\lambda_i^4 \\
&\quad + 16gT^2\lambda_i^2\sin(T\lambda_i) - 16gT\lambda_i\left(2\sin^2\left(\frac{T\lambda_i}{2}\right) - 1\right) \\
&\quad - 2g^2T^2\lambda_i^2\bigl(2\sin^2(T\lambda_i) - 1\bigr) - 2g^2T\lambda_i\sin(2T\lambda_i)\biggr]\Big/ 32T^2\lambda_i^3 \\
&= -\frac{1}{\lambda_i} + \frac{g^2}{16}T^2\lambda_i + \frac{g}{2\lambda_i}\sin(T\lambda_i) - \frac{g^2}{16\lambda_i}\bigl(2\sin^2(T\lambda_i) - 1\bigr) + Q(T),
\end{aligned} \tag{30}$$

where $Q(T)$ is a complicated fraction with T being in its denominator. The error resulting from the ith term is given by

$$\begin{aligned}
\epsilon_i &= \bigl|\langle 1|\Delta H|i\rangle\bigr|^2\left[\frac{g^2T^4\lambda_i}{16} + \frac{gT^2\sin(T\lambda_i)}{2\lambda_i} - \frac{g^2T^2(2\sin^2(T\lambda_i) - 1)}{16\lambda_i} + T^2Q(T)\right]\left(\frac{\lambda}{T}\right)^2 \\
&\quad + O\bigl(\lambda^3\bigr)
\end{aligned} \tag{31}$$

as $\lambda \to 0$. We have

$$\begin{aligned}
&\lim_{\lambda\to 0}\frac{\epsilon_i}{(\frac{\lambda}{T})^2} \\
&\quad = \bigl|\langle 1|\Delta H|i\rangle\bigr|^2\left[\frac{g^2T^4\lambda_i}{16} + \frac{gT^2\sin(T\lambda_i)}{2\lambda_i} - \frac{g^2T^2(2\sin^2(T\lambda_i) - 1)}{16\lambda_i} + T^2Q(T)\right].
\end{aligned} \tag{32}$$

The scaling of ϵ_i with respect of $(\frac{\lambda}{T})^2$ is additionally determined by T^2 and T^4, as compared to the quadratic case. This is where adiabatic approximation error may not be small if the average evolution speed is slow. In particular by (32), if one chooses a comparably large value for T in an adiabatic evolution experiment, the adiabatic approximation error may not decrease as expected when one applies a slow evolution speed $\frac{\lambda}{T}$.

In order to further illustrate this point, we can heuristically compare the speed of convergence of ϵ to zero observed in this case and the quadratic case, as the speed of the adiabatic process (λ/T) reduces and the evolution horizon T increases. The difference in the speed of convergence can be clearly seen using the ratio

$$\lim_{T\to\infty}\left(\lim_{(\lambda/T)\to 0}\frac{\epsilon_i}{\epsilon_{\text{quad}}}\right) = \infty. \tag{33}$$

Therefore, the rate of convergence considered in this subsection is slower than that in the quadratic or linear case. That is, ϵ goes to zero as $\lambda \to 0$ at a much slower rate than in the linear interpolation case or the quadratic interpolation case if T is large. Furthermore, the larger T is, the slower the convergence.

6 Conclusion

In this paper we provide a rigorous analysis of the time-dependent evolution of Hamiltonian-varying quantum systems. As we calculated, the adiabatic approximation error is not proportional to the average speed of the variation of the system Hamiltonian and the inverse of the energy gaps in many cases. The results in this paper may provide guidelines when applying complicated interpolation for adiabatic evolution.

Appendix A

The Magnus expansion is proposed to solve the following time-dependent equation [29]

$$\frac{dY(t)}{dt} = A(t)Y(t). \tag{34}$$

The solution of the above equation can be written as

$$Y(t) = \exp\left(\sum_{k=1}^{\infty} \Omega_k(t)\right) Y(0), \tag{35}$$

where the first three terms in the Magnus series $\{\Omega_k, k = 1, 2, \ldots, \infty\}$ are calculated by

$$\begin{aligned}
\Omega_1(t) &= \int_0^t A(t_1)\, dt_1, \\
\Omega_2(t) &= \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 \big[A(t_1), A(t_2)\big], \\
\Omega_3(t) &= \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \big(\big[A(t_1), \big[A(t_2), A(t_3)\big]\big] + \big[A(t_3), \big[A(t_2), A(t_1)\big]\big]\big).
\end{aligned} \tag{36}$$

The rest terms in the Magnus series can also be written as the integrals of nested commutators.

The dynamical equation of the quantum state in interaction picture is given by

$$\mathrm{i}\frac{\partial|\psi_I(t)\rangle}{\partial t} = e^{\mathrm{i}H_1 t}\lambda f(t)\Delta H e^{-\mathrm{i}H_1 t}\big|\psi_I(t)\big\rangle, \tag{37}$$

where $|\psi(t)\rangle = e^{-\mathrm{i}H_1 t}|\psi_I(t)\rangle$. Applying the Magnus expansion to (37) yields

$$\big|\psi_I(t)\big\rangle = \left(1 - \mathrm{i}\lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f\big(t'\big)\Delta H e^{-\mathrm{i}H_1 t'} + R_0(t)\right)\big|\psi(0)\big\rangle, \tag{38}$$

where $R_0(t)$ includes all the higher-order terms as determined by $\{\Omega_k\}$. Obviously, $\|R_0(t)\|$ is of the order $O(\lambda^2)$. Transforming back to Schrödinger picture we obtain the expression for the density operator as

$$\begin{aligned}\rho_t &= e^{-\mathrm{i}H_1 t}\left(1 - \mathrm{i}\lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \Delta H e^{-\mathrm{i}H_1 t'} + R_0(t)\right) \\ &\quad \times \rho_g \left(1 + \mathrm{i}\lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \Delta H e^{-\mathrm{i}H_1 t'} + R_0^\dagger(t)\right) e^{\mathrm{i}H_1 t} \\ &= e^{-\mathrm{i}H_1 t}\left(\rho_g + R(t) + \mathrm{i}\left[\rho_g, \lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \Delta H e^{-\mathrm{i}H_1 t'}\right]\right) e^{\mathrm{i}H_1 t}.\end{aligned} \tag{39}$$

Obviously, $\|R(t)\|$ is also of the order $O(\lambda^2)$.

An explicit condition for the Magnus series to converge is given by [29]

$$\|\Delta H\| \int_0^T \lambda f(t)\, dt < \pi. \tag{40}$$

Appendix B

The derivative of $\langle \hat{H}_2 \rangle_{\rho_t}$ is calculated as

$$\begin{aligned}&\frac{d}{dt}\langle \hat{H}_2 \rangle_{\rho_t} \\ &\quad = \left\langle -\mathrm{i}\left[\hat{H}_2, H_1 + f(t)(H_2 - H_1)\right]\right\rangle_{\rho_t} \\ &\quad = \left\langle -\mathrm{i}\left[\hat{H}_2, \hat{H}_1 + f(t)(\hat{H}_2 - \hat{H}_1)\right]\right\rangle_{\rho_t} \\ &\quad = \left\langle -\mathrm{i}e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t}\right\rangle_{\rho_g + \mathrm{i}[\rho_g, \lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t')(\Delta H) e^{-\mathrm{i}H_1 t'}] + R(t)} \\ &\quad = -\left\langle \left[e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t}, \lambda \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \Delta H e^{-\mathrm{i}H_1 t'}\right]\right\rangle_{\rho_g} \\ &\qquad + \mathrm{Tr}\left\{-\mathrm{i}e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t} R(t)\right\} \\ &\quad = -\left\langle \left[e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t}, \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \hat{H}_2 e^{-\mathrm{i}H_1 t'}\right]\right\rangle_{\rho_g} \\ &\qquad + \mathrm{Tr}\left\{-\mathrm{i}e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t} R(t)\right\},\end{aligned} \tag{41}$$

where we made use of the relation (6) and $\lambda \Delta H = \hat{H}_2 - \hat{H}_1 + \omega_1' - \omega_1$. Calculating (41) further leads to

$$\begin{aligned}&\frac{d}{dt}\langle \hat{H}_2 \rangle_{\rho_t} \\ &\quad = -\left(1 - f(t)\right)\left\langle e^{\mathrm{i}\omega_1 t}\hat{H}_2 \hat{H}_1 e^{-\mathrm{i}H_1 t} \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \hat{H}_2 e^{-\mathrm{i}\omega_1 t'} \right. \\ &\qquad \left. + \int_0^t dt' e^{\mathrm{i}\omega_1 t'} f(t') \hat{H}_2 e^{-\mathrm{i}H_1 t'} e^{\mathrm{i}H_1 t}\hat{H}_1 \hat{H}_2 e^{-\mathrm{i}\omega_1 t}\right\rangle_{\rho_g} \\ &\qquad + \mathrm{Tr}\left\{-\mathrm{i}e^{\mathrm{i}H_1 t}\left[\hat{H}_2, \left(1 - f(t)\right)\hat{H}_1\right] e^{-\mathrm{i}H_1 t} R(t)\right\} \\ &\quad = -\left(1 - f(t)\right)\left\langle e^{\mathrm{i}\omega_1 t}\hat{H}_2 \hat{H}_1 \sum |i\rangle\langle i| e^{-\mathrm{i}H_1 t} \int_0^t dt' e^{\mathrm{i}H_1 t'} f(t') \hat{H}_2 e^{-\mathrm{i}\omega_1 t'}\right.\end{aligned}$$

$$
\begin{aligned}
&+\int_0^t dt' e^{\mathrm{i}\omega_1 t'} f(t')\hat{H}_2 e^{-\mathrm{i}H_1 t'} e^{\mathrm{i}H_1 t} \sum |i\rangle\langle i|\hat{H}_1\hat{H}_2 e^{-\mathrm{i}\omega_1 t}\Big\rangle_{\rho_g} \\
&+\mathrm{Tr}\big\{-ie^{\mathrm{i}H_1 t}\big[\hat{H}_2, \big(1-f(t)\big)\hat{H}_1\big]e^{-\mathrm{i}H_1 t}R(t)\big\} \\
=&-\big(1-f(t)\big)\sum_{i\neq 1}(\omega_i-\omega_1)\big\langle\hat{H}_2|i\rangle\langle i|\hat{H}_2\big\rangle_{\rho_g}\int_0^t dt' f(t')\big(e^{\mathrm{i}(\omega_i-\omega_1)(t'-t)}+e^{\mathrm{i}(\omega_i-\omega_1)(t-t')}\big) \\
&+\mathrm{Tr}\big\{-\mathrm{i}e^{\mathrm{i}H_1 t}\big[\hat{H}_2, \big(1-f(t)\big)\hat{H}_1\big]e^{-\mathrm{i}H_1 t}R(t)\big\} \\
=&-2\big(1-f(t)\big)\sum_{i\neq 1}(\omega_i-\omega_1)\langle 1|\hat{H}_2|i\rangle\langle i|\hat{H}_2|1\rangle\int_0^t dt' f(t')\cos\big((\omega_i-\omega_1)(t'-t)\big) \\
&+\mathrm{Tr}\big\{-\mathrm{i}e^{\mathrm{i}H_1 t}\big[\hat{H}_2, \big(1-f(t)\big)\hat{H}_1\big]e^{-\mathrm{i}H_1 t}R(t)\big\}.
\end{aligned} \tag{42}
$$

With the linear interpolating function $f(t) = \frac{t}{T}$, the direct integration of (42) over $[0, T]$ gives (8).

Appendix C

The state of the system will remain a pure state during the evolution. Therefore, we can express the final state as $\rho_T = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \sum_{i=1}^N c_i|i'\rangle$. Using this expression, the error measure ϵ defined by (2) can be written as

$$\epsilon = \langle\hat{H}_2\rangle_{\rho_T} = \langle\psi|\hat{H}_2|\psi\rangle = \sum_{i=2}^N |c_i|^2\lambda'_i \geq \sum_{i=2}^N |c_i|^2\lambda'_2. \tag{43}$$

The fidelity of the final state and the ground state $|1'\rangle$ is calculated by

$$F\big(|\psi\rangle, |1'\rangle\big) = \sqrt{\big|\langle\psi|1'\rangle\big|^2} = \sqrt{|c_1|^2} = \sqrt{1-\sum_{i=2}^N |c_i|^2} \geq \sqrt{1-\frac{\epsilon}{\lambda'_2}}. \tag{44}$$

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
YP conceived the idea, formulated the theory, carried out the calculations. YP wrote the paper with the contribution from VU. All authors commented on the manuscript. All authors read and approved the final manuscript.

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