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Why the quantitative condition fails to reveal quantum adiabaticity

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Abstract

The quantitative adiabatic condition (QAC), or quantitative condition, is a convenient (*a priori*) tool for estimating the adiabaticity of quantum evolutions. However, the range of the applicability of QAC is not well understood. It has been shown that QAC can become insufficient for guaranteeing the validity of the adiabatic approximation, but under what conditions the QAC would become necessary has become controversial. Furthermore, it is believed that the inability for the QAC to reveal quantum adiabaticity is due to induced resonant transitions. However, it is not clear how to quantify these transitions in general. Here we present a progress to this problem by finding an exact relation that can reveal how transition amplitudes are related to QAC directly. As *a posteriori* condition for quantum adiabaticity, our result is universally applicable to any (non-degenerate) quantum system and gives a clear picture on how QAC could become insufficient or unnecessary for the adiabatic approximation, which is a problem that has gained considerable interest in the literature in recent years.

Keywords: adiabatic computing, quantum adiabatic condition, adiabatic approximation

1. Introduction

The quantum adiabatic theorem (QAT) [1, 2] suggests that a physical system initialized in an eigenstate $\left|E_n\left(t=0\right)\right\rangle$ (commonly the ground state) of a certain gapped time-dependent Hamiltonian $H(t)$, with an eigenvalue E_n, at time t remains in the same instantaneous eigenstate (up to a multiplicative phase factor), provided that the Hamiltonian $H(t)$ varies in a continuous and sufficiently slow way. The adiabatic theorem was first proposed by Born and Fock at the dawn of quantum mechanics [3], who were motivated by the idea of adiabatic invariants of Ehrenfest [4]. Born and Fock's result is restricted to bounded Hamiltonians with discrete energy levels, e.g. 1D harmonic oscillators; their result is not applicable to systems with a continuous spectrum e.g. Hydrogen atom. This restriction was relaxed by Kato in 1950 [5], who found that in the adiabatic limit, the time evolution of a time-dependent Hamiltonian is equivalent to a geometric evolution. Kato's result is applicable to systems including Hydrogen atom, where the ground state is unique and has a gap from the excited states that can have degeneracy. Later, the requirement of the existence of a gap for proving the adiabatic theorem was found to be unnecessary [6].

This intriguing physical property of quantum adiabaticity finds many interesting applications, including but not limited to quantum field theory [7], geometric phase [8], stimulated Raman adiabatic passage [9], energy level crossings in molecules [10, 11], adiabatic quantum computation [12–18], quantum simulation (see e.g. the review [19]), and other applications [20].

1.1. Quantitative adiabatic condition

Despite its long history, the study of the QAT is still a very active field of research. Many works have been performed aiming to achieve a better understanding of the adiabatic theorem. In particular, the problem of quantifying the slowness of adiabatic evolution has not been completely solved. Traditionally [1, 2, 14, 21] the so-called (e.g. see [22]) quantitative adiabatic condition (QAC) or simply quantitative condition (for *all* $m \neq n$):

$$\left|\frac{\left\langle E_m\left(t\right)\middle|\dot{E}_n\left(t\right)\right\rangle}{E_m\left(t\right)-E_n\left(t\right)}\right| \ll 1, \tag{1}$$

was meant to quantify the slowness of $H(t)$ (see appendix A for details on the definitions of the Hamiltonian and eigenvectors). However, QAC was numerically shown to be not a good indicator for revealing the fidelity of the final state [23]. Furthermore, it has been shown that QAC is inconsistent with the QAT [24] and insufficient for maintaining the validity of the adiabatic approximation [22], except for some special cases [25]. The arguments for showing the inconsistency and insufficiency of QAC were constructed [22] from a comparison between two systems, A and B, where A was evolved under a Hamiltonian $H_a\left(t\right)$. The Hamiltonian

$$H_b\left(t\right) = -\,U_a\left(t\right)^{\dagger} H_a\left(t\right) U_a\left(t\right) \tag{2}$$

of system B is related to that of system A through a unitary transformation $U_a\left(t\right) = T\exp\left(-i\int_0^t H_a\left(t'\right)\mathrm{d}t'\right)$ that corresponds to the exact propagator of $H_a\left(t\right)$. It was shown that both systems A and B satisfy the QAC, but at most one of them can fulfill the

adiabatic approximation. This conclusion is consistent with the results performed in an NMR experiment [26].

1.2. Related studies in the literature

Many studies (e.g. [27–33]) have been made trying to understand the inconsistency raised by Marzlin and Sanders [24]. It was argued [29–33] that resonant transitions between energy levels are responsible for the violations of the adiabatic theorem. A refined adiabatic condition has been found [34], which takes into account the effects of resonant energy-level transitions.

On the other hand, the validity of the adiabatic theorem was analyzed from a perturbative-expansion approach [35, 36], which provides a diagrammatic representation for adiabatic dynamics and yields the quantitative condition (in equation (1)) as the first-order approximation. It was argued [37] that the quantitative condition is insufficient for the adiabatic approximation when the Hamiltonian varies rapidly but with a small amplitude. Furthermore, generalizing QAC for open quantum systems [27, 38] and many-body systems [39] have been achieved. Efforts for finding conditions that can replace QAC were made [40–42].

Another line of research related to the adiabatic theorem is to estimate or bound the scaling of the final-state fidelity. Under some general conditions for a gapped Hamiltonian, it was found [43] that the transition probability scales as $O\left(1/T^2\right)$ for a total evolution time T. When the total time is fixed, it was shown [44, 45] that both the minimum eigenvalue gap Δ and the length of the traversed path $L \equiv \int_0^1 \left\| \left| \partial_r \psi\left(r\right) \right\rangle \right\| \mathrm{d}r$, where $r(t)$ is a time-varying parameter in the Hamiltonian, are important.

2. Motivation

Instead of questioning the validity of the quantitative condition as an indicator for quantum adiabaticity, we are interested in the question

'*Under what additional conditions would QAC become necessary*?'.

The answer to this question has not been clear [46–48]. Our work is motivated by a recent development achieved in [46], where QAC is argued to be necessary under certain additional assumptions related to the *adiabatic state* $\left|\psi_n^{adi}\left(t\right)\right\rangle$ [8, 46], which is defined by attaching a time-dependent phase factor (essentially the Berry phase [8]) $e^{i\beta_n(t)}$ to the energy eigenstate $\left|E_n\left(t\right)\right\rangle$, i.e.,

$$\left|\psi_n^{adi}\left(t\right)\right\rangle \equiv e^{i\beta_n(t)} \left|E_n\left(t\right)\right\rangle, \tag{3}$$

where

$$\beta_n\left(t\right) \equiv -\int_0^t E_n\left(x\right)\mathrm{d}x + i\int_0^t \left\langle E_n\left(x\right)\middle|\dot{E}_n\left(x\right)\right\rangle \mathrm{d}x. \tag{4}$$

The key result obtained in [46] is that (in our notations) the probability amplitude $c_m\left(t\right) = \left\langle E_m\left(t\right)\middle|\psi\left(t\right)\right\rangle$ for the eigenstate $\left|E_m\left(t\right)\right\rangle$ at time t is given by the following expression:

Table 1. Summary of various terms and symbols.

Terms	Meaning
Quantum adiabatic theorem	This theorem states that for general physical systems initialized in an eigenstate (e.g. ground state) with respect to a time-dependent Hamiltonian, the transition to other (instantaneous) eigenstate is small provided that the variation of the Hamiltonian is sufficiently slow.
Quantitative adiabatic condition (QAC) (or quantitative condition)	A condition traditionally considered as a necessary and sufficient condition for the validity of the adiabatic approximation (see equation (1)), i.e., $\left\vert \frac{\langle E_m(t) \vert \dot{E}_n(t)\rangle}{E_m(t)-E_n(t)} \right\vert \ll 1$.
Adiabatic approximation	An approximation that replaces the exact state $\vert\psi(t)\rangle$ with the adiabatic state $\vert\psi_n^{adi}(t)\rangle$, which leads to $\vert c_m(t)\vert \ll 1$ for all $m \neq n$.
Adiabatic state $\vert\psi_n^{adi}(t)\rangle$	Defined by $\vert\psi_n^{adi}(t)\rangle \equiv e^{i\beta_n(t)}\vert E_n(t)\rangle$, where $\vert E_n(t)\rangle$ is the instantaneous eigenstate (with eigenvalue $E_n(t)$) of the Hamiltonian $H(t)$, and $\beta_n(t) \equiv -\int_0^t E_n(x)\,\mathrm{d}x + i\int_0^t \langle E_n(x)\vert\dot{E}_n(x)\rangle\,\mathrm{d}x$ (see equation (3)).
Difference vector $\vert D(t)\rangle$	Defined by $\vert D(t)\rangle \equiv \vert\psi(t)\rangle - \vert\psi_n^{adi}(t)\rangle$, the difference between the exact time-evolved state $\vert\psi(t)\rangle$ and the adiabatic state $\vert\psi_n^{adi}(t)\rangle$ (see equation (8))

$$c_m(t) \approx i e^{i\beta_n(t)} \frac{\langle E_m(t)\vert\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}, \tag{5}$$

which leads to the conclusion that if the adiabatic approximation is valid, i.e., the probability amplitude c_m for all eigenstates $m \neq n$ are small, $\vert c_m(t)\vert \ll 1$, then the QAC (cf equation (1)) necessarily holds (for a summary of the definitions of various terms, see table (1)).

For comparison, a similar expression (in our notation) was given by Schiff [1] as

$$c_m(t) \approx \frac{\langle E_m(t)\vert\dot{H}\vert E_n(t)\rangle}{i\big(E_m(t)-E_n(t)\big)^2}\Big(e^{i(E_m-E_n)t}-1\Big), \tag{6}$$

$$= i\frac{\langle E_m(t)\vert\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}\Big(e^{i(E_m-E_n)t}-1\Big). \tag{7}$$

The derivation from the first line to the second line is provided in appendix B. These two expressions (in equations (5) and (7)) predict the validity of the adiabatic approximation when the quantitative condition (cf equation (1)) is satisfied.

However, the result in [46] was not uncontroversial [47, 48]. Zhao and Wu [47] argued that the contribution of the missing term in the result in [46] is underestimated. Comparat [48] pointed out that the non-rigorous use of the approximation sign '≈' in [46] leads to an obscure meaning for quantum adiabaticity. This problem is avoided in our derivation. Tong's reply [49] emphasized the connection with the adiabatic state in his result, but did not resolve the oppositions completely.

3. Summary of results

We present new results that aim to

1. Settle the existing controversy in the literature [46–49] by deriving an exact expression (cf equation (9)) for the transition amplitude $c_m(t)$, which contains correction terms missing in the previous result (shown in equation (5)), and
2. explore the properties of the correction term (cf equation (22)) for equation (5), which helps us understand better the connection between QAC and the adiabatic approximation.

Our approach can be formulated conveniently with the use of the difference vector $\left|D(t)\right\rangle$, which is defined by the difference between the exact state $\left|\psi(t)\right\rangle$ and the adiabatic states $\left|\psi_n^{adi}(t)\right\rangle$ (cf equation (3)):

$$\left|D(t)\right\rangle \equiv \left|\psi(t)\right\rangle - \left|\psi_n^{adi}(t)\right\rangle. \tag{8}$$

3.1. Our main result and its consequences

Our main result contains an *exact* expression for $c_m(t)$, namely (compare with equation (5))

$$c_m(t) = \underbrace{ie^{i\beta_n(t)}\frac{\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}{E_m(t)-E_n(t)}}_{\equiv Q_m(t)\ \text{Result in [46]}} \underbrace{-E_n(t)\frac{\left\langle E_m(t)\middle|D(t)\right\rangle}{E_m(t)-E_n(t)} + i\frac{\left\langle E_m(t)\middle|\dot{D}(t)\right\rangle}{E_m(t)-E_n(t)}}_{\equiv R_m(t)\quad \text{Correction terms}}, \tag{9}$$

which reduces to the result in [46] (cf equation (5)) when the magnitude $\left|R_m(t)\right|$ of the correction term is small; for example when both $\left|D(t)\right\rangle = 0$ and $\left|\dot{D}(t)\right\rangle = 0$. These two conditions correspond to the key assumptions made in [46]. Furthermore, our result in equation (9) also indicates a condition (cf equation (25)) more general than the result in [46].

The exact expression in equation (9) implies many new results, which are listed as follows:

- The result of [46] was obtained by assuming that both $\left|D(t)\right\rangle$ and $\left|\dot{D}(t)\right\rangle$ can be ignored, i.e., $\left|D(t)\right\rangle \approx 0$ and $\left|\dot{D}(t)\right\rangle \approx 0$. However [46] did not tell us how small these terms should be. Our expression gives the quantitative criteria, namely:

$$\left\| \left| D\left(t\right)\right\rangle \right\| \ll \left| \frac{E_m\left(t\right) - E_n\left(t\right)}{E_n\left(t\right)} \right| \quad \text{and} \quad \left\| \left| \dot{D}\left(t\right)\right\rangle \right\| \ll \left| E_m\left(t\right) - E_n\left(t\right) \right|. \tag{10}$$

- Furthermore, from our expression, we can obtain the same conclusion as in [46] by requiring a more general condition

$$\left\| i\left| \dot{D}\left(t\right)\right\rangle - E_n\left(t\right) \left| D\left(t\right)\right\rangle \right\| \ll \left| E_m\left(t\right) - E_n\left(t\right) \right|. \tag{11}$$

- One of the criticisms on the result of [46] was that one can find a counter example that violates the quantitative condition but fulfills the adiabatic condition [48]. Our expression indicates that this situation is possible when our correction term cancels with the first term in equation (9).
- In the limiting case where the transition amplitude equals exactly the right hand side of equation (5), i.e.,

$$c_m\left(t\right) = ie^{i\beta_n\left(t\right)} \frac{\left\langle E_m\left(t\right) \left| \dot{E}_n\left(t\right)\right\rangle \right.}{E_m\left(t\right) - E_n\left(t\right)}, \tag{12}$$

  we found that this condition is equivalent to

$$i\left| \dot{D}\left(t\right)\right\rangle = E_n\left(t\right) \left| D\left(t\right)\right\rangle. \tag{13}$$

- We also found that the condition of $\left| \dot{D}\left(t\right)\right\rangle = 0$ implies that both $c_m\left(t\right) = 0$ and $\left| D\left(t\right)\right\rangle = 0$. In other words, for any time-evolving quantum state $\left| \psi\left(t\right)\right\rangle$, if $\left| \dot{\psi}\left(t\right)\right\rangle = \left| \dot{\psi}_n^{adi}\left(t\right)\right\rangle$, then this quantum state must equal $\left| \psi_n^{adi}\left(t\right)\right\rangle$ as well, i.e., $\left| \psi\left(t\right)\right\rangle = \left| \psi_n^{adi}\left(t\right)\right\rangle$.

Finally, we note that the fact that our main expression is an exact result eliminates unnecessary debate over the correctness of applying approximation, as happened [47, 50] for the results of [24] and [46].

3.2. Organization of the report

Before we go into the details, we emphasize that the goal of this work is not to look for a new condition that can take the role of QAC for adiabatic approximation. Indeed, the QAC is a convenient a *priori* condition for estimating the validity of the adiabatic approximation, although the range of the applicability is not clear. Instead, as a *posteriori* condition, we aim to offer a better picture that helps understand *why the QAC fails to reveal the adiabatic approximation*—a problem that has gained considerable interest in the literature in recent years. Although some mathematical steps in our derivation may look tricky, only materials in elementary quantum mechanics are involved.

The rest of this report is organized as follows:

In section 'Derivation of the main result': we provide a detailed step-by-step guide for the derivation of our main result in equation (9).

In section 'Discussion on the main result': we focus on the properties of the first term and the corrections terms in equation (9). The necessity of the quantitative condition is discussed. The implications of our expression are also explored.

In section 'Illustrative example': here we consider our results based on the Schwinger's spin-1/2 Hamiltonian. This model is well-studied, and is one of the few time-dependent models that are exactly solvable, providing us a good testing ground for illustrating our findings. Furthermore, numerical simulations are performed for this model. The most interesting case here is probably the result in figure 1(d), where the quantitative condition is violated but the adiabatic approximation is still valid. This case shows that the adiabatic condition is not necessary for the adiabatic approximation in general.

4. Derivation of the main result

We are now ready to derive the exact expression in equation (9). To this end, consider for some $m \neq n$ the following expression:

$$\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|D(t)\right\rangle, \tag{14}$$

which can be separated into two different terms, i.e.,

$$\underbrace{\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|\psi(t)\right\rangle}_{=\left(E_m(t)-E_n(t)\right)c_m(t)} - \underbrace{\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|\psi_n^{adi}(t)\right\rangle}_{=ie^{i\beta_n(t)}\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}, \tag{15}$$

from the definition (cf equation (8)) of the difference vector $\left|D(t)\right\rangle$. These two terms can be simplified as follows:

First term the first term is equal to

$$\left(E_m(t) - E_n(t)\right)c_m(t), \tag{16}$$

which comes from the Schrödinger equation that makes

$$i\left\langle E_m(t)\middle|\dot{\psi}(t)\right\rangle = \left\langle E_m(t)\right| H(t) \left|\psi(t)\right\rangle, \tag{17}$$

followed by the Hermitian property, $H^{\dagger}(t) = H(t)$, of $H(t)$ that gives

$$\left\langle E_m(t)\middle|H(t) = E_m(t)\left\langle E_m(t)\right|, \right. \tag{18}$$

and the definition of the transition amplitude $c_m(t) = \left\langle E_m(t)\middle|\psi(t)\right\rangle$.

Second term note that we have the orthogonal condition where

$$\left\langle E_m(t)\middle|\psi_n^{adi}(t)\right\rangle = \left\langle E_m(t)\middle|E_n(t)\right\rangle = 0 \tag{19}$$

for all eigenstates $m \neq n$. The second term therefore contains only the first part $i\left\langle E_m(t)\right|\left|\frac{\mathrm{d}}{\mathrm{d}t}\right|\psi_n^{adi}(t)\rangle$, which is equal to $ie^{i\beta_n(t)}\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle$ from the definition (cf equation (3)) of the adiabatic state $\left|\psi_n^{adi}(t)\right\rangle$.

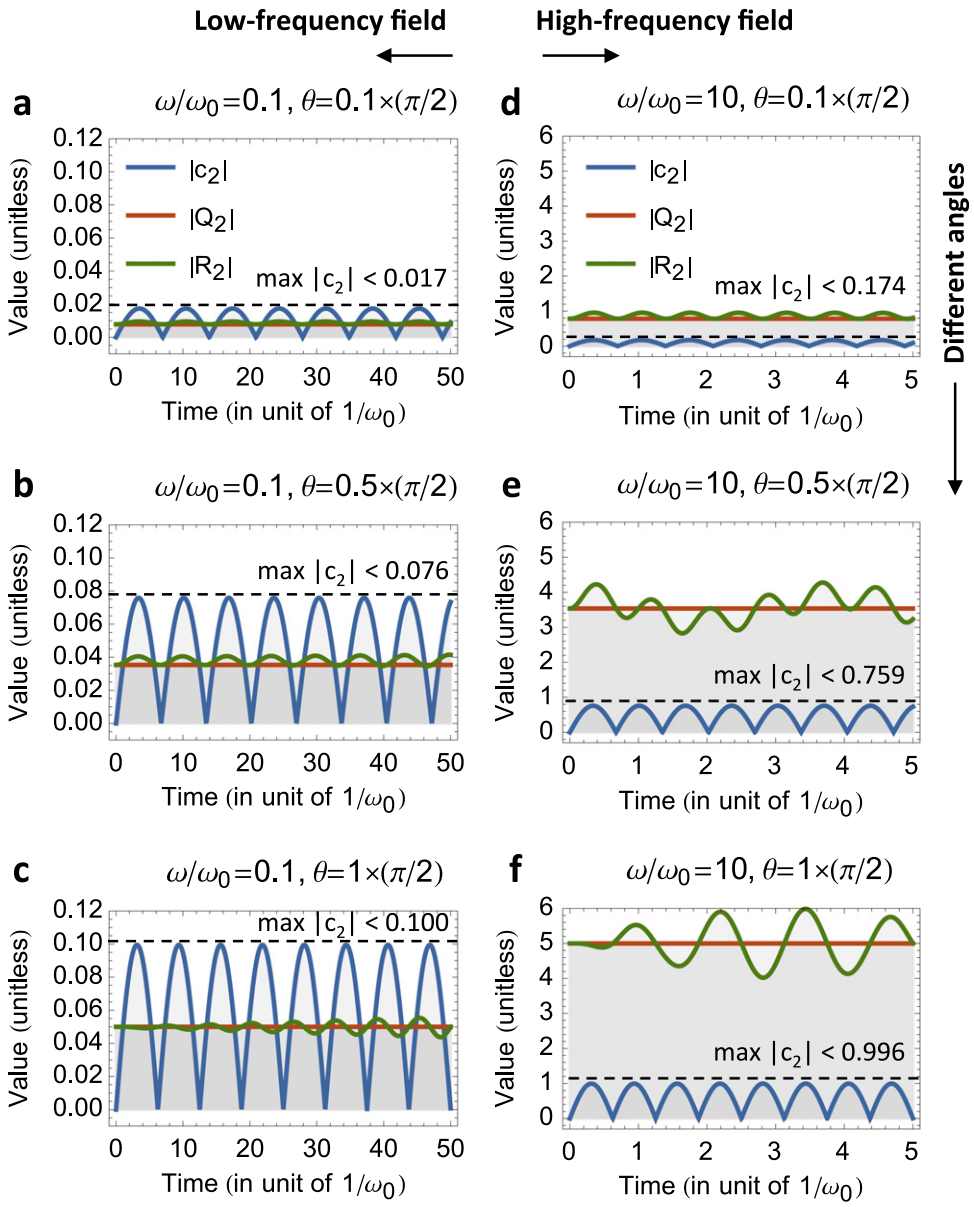

Figure 1. Time variations of the amplitude $|c_2(t)|$, $|Q_2(t)|$, and $|R_2(t)|$ of the terms in equation (9). (a)–(c) correspond to the cases with slow ($\omega/\omega_0 = 0.1$) driving fields. (d)–(f) are showing the cases with fast ($\omega/\omega_0 = 10$) driving fields.

In summary, we now have the following relation:

$$\langle E_m|\left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n\right)|D\rangle = (E_m - E_n)c_m - ie^{i\beta_n}\langle E_m|\dot{E}_n\rangle. \tag{20}$$

Next, through a simple rearrangement of the terms in this relation, we obtained the exact expression of $c_m(t)$ advertised earlier in equation (9).

5. Discussion on the main result

The first term,

$$Q_m(t) \equiv ie^{i\beta_n(t)} \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)}, \tag{21}$$

on the right hand side of equation (9) is closely related to the QAC (cf equation (1)) and was obtained in [46], which asserted that the QAC (cf equation (1)) is necessary subject to the condition that both '$|D(t)\rangle \approx 0$' and '$|\dot{D}(t)\rangle \approx 0$'. However, our result in equation (9) not only quantifies (cf equation (23)) the size of $|D(t)\rangle$ and $|\dot{D}\rangle$ for the validity of QAC (which is needed to justify the result in [46]), but also reveals a more general condition (cf equation (25)) that can lead to the same conclusion for the validity of the QAC.

The second term,

$$R_m(t) \equiv -E_n(t)\frac{\langle E_m(t)|D(t)\rangle}{E_m(t) - E_n(t)} + i\frac{\langle E_m(t)|\dot{D}(t)\rangle}{E_m(t) - E_n(t)}, \tag{22}$$

represents the correction to the result obtained in [46]. Remarkably, provided that the absolute value of $R_m(t)$ is small compared with unity, i.e., $|R_m(t)| \ll 1$, the QAC in equation (1) is necessary for the validity of the adiabatic approximation.

5.1. On the necessity of QAC

Having derived our main expression shown in equation (9), we are now ready to explore further the consequences of this expression. Here we consider the conditions that make the QAC (cf equation (1)) become necessary when the adiabatic approximation is valid, i.e., $|c_m| \ll 1$ for all $m \neq n$. We shall answer the following question: 'under what conditions does the correction term $R_m(t)$ in equation (9) vanish?'

First of all, the correction term contains both $|D(t)\rangle$ and $|\dot{D}(t)\rangle$. Clearly, the QAC is necessary for the adiabatic approximation, provided that the vector norms (or the projection to $|E_m(t)\rangle$) of both $|D(t)\rangle$ and $|\dot{D}(t)\rangle$ are small, compared with $|(E_m(t) - E_n(t))/E_n(t)|$ and $|E_m(t) - E_n(t)|$ respectively, i.e.,

$$\||D\rangle\| \ll \left|\frac{E_m - E_n}{E_n}\right| \quad \& \quad \||\dot{D}\rangle\| \ll |E_m - E_n|. \tag{23}$$

In fact, in [46] it was explicitly assumed that both '$|D(t)\rangle \approx 0$' and '$|\dot{D}(t)\rangle \approx 0$' in order to obtain the result in equation (5) (see equations (7) and (9) of [46]). Here the conditions in equation (23) provide a quantitative meaning about the approximations '$|D(t)\rangle \approx 0$' and '$|\dot{D}(t)\rangle \approx 0$' employed in [46], and help clarify the ambiguity that caused the controversy [47, 48].

5.2. Generalization

Of course, the necessity of QAC (cf equation (5)) is valid as long as the correction term $R_m(t)$ becomes sufficiently small. Requiring both '$\left|D(t)\right\rangle \approx 0$' and '$\left|\dot{D}(t)\right\rangle \approx 0$' as in [46] is just one possibility. Generally, from equation (22), it is sufficient to require the vector norm of the linear combination

$$i\left|\dot{D}(t)\right\rangle - E_n(t)\left|D(t)\right\rangle, \tag{24}$$

to be small compared with the absolute value of the energy gap $E_m(t) - E_n(t)$, i.e.,

$$\left\| i\left|\dot{D}(t)\right\rangle - E_n(t)\left|D(t)\right\rangle \right\| \ll \left|E_m(t) - E_n(t)\right|, \tag{25}$$

which covers more possibilities other than just requiring '$\left|D(t)\right\rangle \approx 0$' and '$\left|\dot{D}(t)\right\rangle \approx 0$'. In other words, as long as the condition in equation (25) holds, the QAC (cf equation (1)) implies the adiabatic approximation where $\left|c_m(t)\right| \ll 1$ for all $m \neq n$, and vice versa.

5.3. Properties of the correction term

In the following, we shall show that the condition requiring the correction term to vanish, i.e., $R_m(t) = 0$, implies the following result: for each $m \neq n$, the probability amplitude $c_m(t) = \left\langle E_m(t)\middle|\psi(t)\right\rangle$ is given by the following expression (cf equation (5)):

$$c_m(t) = ie^{i\beta_n(t)}\frac{\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}{E_m(t) - E_n(t)}, \tag{26}$$

if and only if

$$\left|\dot{D}(t)\right\rangle = -iE_n\left|D(t)\right\rangle. \tag{27}$$

In other words, the probability amplitude $c_m(t)$ is given exactly by the expression in equation (5), with the approximation sign changed to the equal sign in equation (26)). Furthermore, from equation (9), it is equivalent to show the following relationship:

$$R_m(t) = 0 \quad \Leftrightarrow \quad i\left|\dot{D}(t)\right\rangle = E_n(t)\left|D(t)\right\rangle. \tag{28}$$

Proof. The proof for the backward direction, i.e.,

$$i\left|\dot{D}(t)\right\rangle = E_n(t)\left|D(t)\right\rangle \Rightarrow R_m(t) = 0, \tag{29}$$

is trivial from the definition of $R_m(t)$ (cf equation (22)). Therefore, we shall focus on the forward direction, i.e.,

$$R_m(t) = 0 \;\Rightarrow\; i\left|\dot{D}(t)\right\rangle = E_n(t)\left|D(t)\right\rangle, \tag{30}$$

of the proof.

Step 1 : From the definition of $R_m(t)$ (cf equation (22)), for each $m \neq n$, we have

$$\left\langle E_m(t) \right| \left(E_n(t) \left| D(t) \right\rangle - i \left| \dot{D}(t) \right\rangle \right) = 0, \tag{31}$$

which implies that the vector $E_n(t)\left|D(t)\right\rangle - i\left|\dot{D}(t)\right\rangle$ is orthogonal to all the basis vectors $\left|E_m(t)\right\rangle$. In other words, this vector belongs to the subspace spanned by the vector $\left|E_n(t)\right\rangle$ only.

Step 2 : Consequently, we can write

$$E_n(t)\left|D(t)\right\rangle - i\left|\dot{D}(t)\right\rangle = \lambda \left|E_n(t)\right\rangle, \tag{32}$$

for some complex number λ. Since the eigenstate is assumed to be normalized $\left\langle E_n(t) \middle| E_n(t) \right\rangle = 1$, we can also write

$$E_n(t)\left\langle E_n(t)\middle|D(t)\right\rangle - i\left\langle E_n(t)\middle|\dot{D}(t)\right\rangle = \lambda. \tag{33}$$

Next, we shall show that λ can only be zero, i.e., $\lambda = 0$.

Step 3 : Let us consider from the definition of the difference vector $\left|D(t)\right\rangle$ (cf equation (8)), which gives

$$\left\langle E_n(t)\middle|\dot{D}(t)\right\rangle = \underbrace{\underbrace{\left\langle E_n(t)\middle|\dot{\psi}(t)\right\rangle}_{=-iE_n(t)\left\langle E_n(t)\middle|\psi(t)\right\rangle} - \underbrace{\left\langle E_n(t)\middle|\dot{\psi}_n^{adi}(t)\right\rangle}_{=-ie^{i\beta_n(t)}E_n(t)}}_{=-iE_n(t)\left\langle E_n(t)\middle|D(t)\right\rangle}. \tag{34}$$

From the Schrödinger equation,

$$\left\langle E_n(t)\middle|\dot{\psi}(t)\right\rangle = -i\left\langle E_n(t)\middle|H(t)\middle|\psi(t)\right\rangle, \tag{35}$$

and from the Hermitian property of $H(t)$, the first term on the right of equation (34) becomes

$$\left\langle E_n(t)\middle|\dot{\psi}(t)\right\rangle = -iE_n(t)\left\langle E_n(t)\middle|\psi(t)\right\rangle. \tag{36}$$

On the other hand, from the definition of the adiabatic state $\left|\psi_n^{adi}(t)\right\rangle$ in equation (3), we have

$$\left|\dot{\psi}_n^{adi}(t)\right\rangle = e^{i\beta_n(t)}\left|\dot{E}_n(t)\right\rangle - e^{i\beta_n(t)}\left(iE_n(t) + \left\langle E_n(t)\middle|\dot{E}_n(t)\right\rangle\right)\left|E_n(t)\right\rangle, \tag{37}$$

which implies that the second term on the right of equation (34) becomes

$$\left\langle E_n(t)\middle|\dot{\psi}_n^{adi}(t)\right\rangle = -ie^{i\beta_n(t)}E_n(t). \tag{38}$$

Combing these results, we finally have

$$\left\langle E_n(t)\middle|\dot{D}(t)\right\rangle = -iE_n(t)\left\langle E_n(t)\middle|D(t)\right\rangle \tag{39}$$

(note that $\left\langle E_n(t)\middle|D(t)\right\rangle = \left\langle E_n(t)\middle|\psi(t)\right\rangle - e^{i\beta_n(t)}$ from the definition of $\left|D(t)\right\rangle$). This means that λ is exactly equal to zero, $\lambda = 0$, which further implies that

$$i\left|\dot{D}(t)\right\rangle = E_n(t)\left|D(t)\right\rangle, \tag{40}$$

and completes the proof. □

5.4. Consequences of $\left|\dot{D}(t)\right\rangle = 0$

We have shown that whenever we set both $\left|D\left(t\right)\right\rangle = 0$ and $\left|\dot{D}\left(t\right)\right\rangle = 0$ (which are also a solution to equation (27)), then we can recover the result in [46] (cf equation (5) and equation (26)). Here we show a stronger result, namely the condition of $\left|\dot{D}\left(t\right)\right\rangle = 0$ implies that the system can only be in the eigenstate (ground state) $\left|E_n\left(t\right)\right\rangle$ i.e., all $c_m = 0$ for $m \neq n$.

More precisely, for all $m \neq n$ and $E_i\left(t\right) \neq 0$,

$$\left|\dot{D}\left(t\right)\right\rangle = 0 \quad \Rightarrow \quad \left|D\left(t\right)\right\rangle = 0 \ \ \& \ \ c_m\left(t\right) = 0. \tag{41}$$

Proof. First of all, from equation (8), we can write

$$c_n\left(t\right) = e^{i\beta_n\left(t\right)} + \frac{i\left\langle E_n\left(t\right)\middle|\dot{D}\left(t\right)\right\rangle}{E_n\left(t\right)}. \tag{42}$$

Now setting $\left|\dot{D}\left(t\right)\right\rangle = 0$ implies

$$c_n\left(t\right) = \left\langle E_n\left(t\right)\middle|\psi\left(t\right)\right\rangle = e^{i\beta_n\left(t\right)}. \tag{43}$$

Since the time-evolving state is normalized, i.e., $\left|\left|\left|\psi\left(t\right)\right\rangle\right|\right| = 1$, it means that all $c_m = 0$ for $m \neq n$, and

$$\left|\psi\left(t\right)\right\rangle = e^{i\beta_n\left(t\right)}\left|E_n\left(t\right)\right\rangle \equiv \left|\psi_n^{adi}\left(t\right)\right\rangle \tag{44}$$

(i.e., $\left|D\left(t\right)\right\rangle = 0$). □

From equation (9), these results also imply that $\left\langle E_m\left(t\right)\middle|\dot{E}_n\left(t\right)\right\rangle = 0$ for $m \neq n$ whenever $\left|\dot{D}\left(t\right)\right\rangle = 0$.

6. Illustrative example

Here we explore the behavior of various terms in our main result (cf equation (9)), with a simple but illustrative example, namely Schwinger's spin-half Hamiltonian [51],

$$H\left(t\right) = \vec{\sigma}\cdot\vec{B}\left(t\right) \equiv \frac{\hbar\omega_0}{2}\left(\sigma_x \sin\theta\cos\omega t + \sigma_y \sin\theta\sin\omega t + \sigma_z\cos\theta\right), \tag{45}$$

or in the matrix form:

$$H_S\left(t\right) = \frac{\hbar\omega_0}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\omega t}\\ \sin\theta e^{i\omega t} & -\cos\theta\end{pmatrix}. \tag{46}$$

This Hamiltonian describes a time-dependent field (with a frequency ω) rotating around the z-axis (at an angle θ), where the field strength is characterized by ω_0. The exact solution can be found analytically (e.g. see [32, 46, 51]), which is also summarized in table 2.

Table 2. Schwinger's spin-half Hamiltonian.

Terms	Expression
Hamiltonian:	$H_S(t) = \frac{\omega_0}{2}\left(\left(\sigma_x \cos\omega t + \sigma_y \sin\omega t\right)\sin\theta + \sigma_z \cos\theta\right)$
Eigenvalues:	$E_1(t) = -\omega_0/2$ and $E_2(t) = \omega_0/2$
Eigenvectors:	$\left\|E_1(t)\right\rangle = \left(e^{-i\omega t/2}\sin(\theta/2), -e^{i\omega t/2}\cos(\theta/2)\right)^T$,
	$\left\|E_2(t)\right\rangle = \left(e^{-i\omega t/2}\cos(\theta/2), e^{i\omega t/2}\sin(\theta/2)\right)^T$.
Initial state:	$\left\|\psi(t=0)\right\rangle = \left\|E_1(t=0)\right\rangle$
Time evolution:	$\left\|\psi(t)\right\rangle = c_1(t)\left\|E_1(t)\right\rangle + c_2\left\|E_2(t)\right\rangle$, where
	$c_1(t) = \cos(\tilde{\omega}t/2) + i\sin(\tilde{\omega}t/2)(\omega_0 - \omega\cos\theta)/\tilde{\omega}$,
	$c_2(t) = i(\omega/\tilde{\omega})\sin\theta\sin(\tilde{\omega}t/2)$,
	$\tilde{\omega} = \sqrt{\omega_0^2 + \omega^2 - 2\omega_0\omega\cos\theta}$.

6.1. Calculations of $Q_2(t)$ and $R_2(t)$

The quantity $Q_2(t)$,

$$Q_2(t) \equiv ie^{i\beta_1(t)}\frac{\left\langle E_2(t)\middle|\dot{E}_1(t)\right\rangle}{E_2(t) - E_1(t)}, \tag{47}$$

is the two-level case (cf equation (21)) of the first term on the right hand side of equation (9). First of all, using the results listed in table 2, we have

$$\left\langle E_1(t)\middle|\dot{E}_1(t)\right\rangle = i\frac{\omega}{2}\cos\theta. \tag{48}$$

This gives the expression for $\beta_1(t)$:

$$\beta_1(t) = \frac{\omega_0 t}{2} - \frac{\omega t}{2}\cos\theta. \tag{49}$$

Similarly, the cross-term is

$$\left\langle E_2(t)\middle|\dot{E}_1(t)\right\rangle = \frac{-i\omega}{2}\sin\theta. \tag{50}$$

Therefore, we have an exact expression for $Q_2(t)$:

$$Q_2(t) = e^{i\beta_1(t)}(\omega/2\omega_0)\sin\theta. \tag{51}$$

On the other hand, the quantity $R_2(t)$ is the two-level case of the correction to the result obtained in [46]. It can be calculated with the knowledge of $c_2(t)$ and $Q_2(t)$, i.e., $R_2(t) = c_2(t) - Q_2(t)$, which is

$$R_2(t) = \omega\sin\theta\left[i\sin\left(\frac{\tilde{\omega}t}{2}\right)\Big/\tilde{\omega} - e^{i\beta_1(t)}\Big/2\omega_0\right]. \tag{52}$$

6.2. Numerical results

The time variations of the amplitude $\left|c_2\left(t\right)\right|$, $\left|Q_2\left(t\right)\right|$, and $\left|R_2\left(t\right)\right|$ are shown in figure 1 for cases subject to slow ($\omega/\omega_0 = 0.1$) and fast ($\omega/\omega_0 = 10$) driving fields. With slow driving fields (figures 1(a)–(c)), the system stays close ($\left|c_2\right| \ll 1$) to the instantaneous ground state $\left|E_1\left(t\right)\right\rangle$ of the total Hamiltonian $H_S\left(t\right)$ as expected, independent of the value of θ. For fast driving fields (figures 1(d)–(f)), the system can stay close to the instantaneous ground state only when θ is small. Particularly, the case in figure 1(d) is related to the debate [47–49] on the result of [46], where it was suggested [48] that one can have the adiabatic approximation ($\left|c_2\right| \ll 1$ for all times) without QAC (i.e., $\left|Q_2\left(t\right)\right|$ is not small). Our result clearly indicates that in this case, the $R_2\left(t\right)$ term cancels the $Q_2\left(t\right)$ term to make the $\left|c_2\left(t\right)\right|$ term small, as expected from equation (9). In other words, we have identified a case where the adiabatic approximation holds, but $Q_2\left(t\right)$ is not small, which means that QAC is not necessary.

7. Conclusion

In summary, we have presented an exact expression for the probability amplitude (cf equation (9)) that identifies the missing corrections of the previous result in the literature [46]. From this expression, we are able to quantify the condition (cf equation (27)) for the traditional QAC to become a valid necessary condition for the adiabatic approximation. As an illustrating example, a numerical analysis on Schwinger's Hamiltonian is performed to demonstrate the role of the correction term for maintaining quantum adiabaticity. These results provide a complementary understanding of the reasons for the breakdown of QAC in various scenarios.

In particular, the fact that we did not apply any approximation to our main result gives us a transparent picture for settling a debate [46–49], which involves the question 'under what additional conditions would QAC become necessary?'. Our result provides a quantitative answer to this question, namely, as long as the vector norms of both $|D\rangle$ and $|\dot{D}\rangle$ are also sufficiently small (cf equation (10)), which were approximated to be zero in Tong's paper [46].

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Appendix A. Hamiltonian and eigenvectors

We consider a time-dependent Hamiltonian $H(t)$ which drives the evolution of an N-dimensional quantum system. For an integer $i \in \{1, 2, 3, \ldots, N\}$, let the real number $E_i\left(t\right)$ and

the vector $\left|E_i\left(t\right)\right\rangle$ represent the instantaneous eigenvalues and orthonormal eigenstates of the Hamiltonian $H(t)$ respectively, i.e.,

$$H\left(t\right)\left|E_i\left(t\right)\right\rangle = E_i\left(t\right)\left|E_i\left(t\right)\right\rangle. \tag{A.1}$$

As usual, the evolution of the quantum state $\left|\psi\left(t\right)\right\rangle$ at any time t is governed by the Schrödinger equation,

$$i\left|\dot{\psi}\left(t\right)\right\rangle = H\left(t\right)\left|\psi\left(t\right)\right\rangle. \tag{A.2}$$

Here we assume that the system is initialized at $t = 0$ in one of the eigenstates, i.e.,

$$\left|\psi\left(0\right)\right\rangle = \left|E_n\left(0\right)\right\rangle, \tag{A.3}$$

including the ground state. Furthermore, the time-dependent state $\left|\psi\left(t\right)\right\rangle$ can be expanded by the completely orthogonal set $\left\{\left|E_i\left(t\right)\right\rangle\right\}$ of the energy eigenbasis as

$$\left|\psi\left(t\right)\right\rangle = \sum_i c_i\left(t\right)\left|E_i\left(t\right)\right\rangle, \tag{A.4}$$

where $c_i\left(t\right) = \left\langle E_i\left(t\right)\middle|\psi\left(t\right)\right\rangle$ is the expansion coefficient with norm less than one, i.e., $\left|c_i\left(t\right)\right| \leqslant 1$, since the whole quantum state is assumed to be normalized, i.e., $\left|\left|\left|\psi\left(t\right)\right\rangle\right|\right| = 1$.

Appendix B. Transformation of Schiff's expression

In the book of Schiff [1], the following expression (in our notation) was given:

$$c_m\left(t\right) \approx \frac{\left\langle E_m\left(t\right)\middle|\dot{H}\middle|E_n\left(t\right)\right\rangle}{i\left(E_m\left(t\right) - E_n\left(t\right)\right)^2}\left(e^{i\left(E_m - E_n\right)t} - 1\right). \tag{B.1}$$

We are going to transform it to another form.

First, note that

$$\left\langle E_m\left(t\right)\middle|E_n\left(t\right)\right\rangle = 0 \tag{B.2}$$

for all $m \neq n$. Therefore, the result

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle E_m\left(t\right)\middle|E_n\left(t\right)\right\rangle = 0 \tag{B.3}$$

implies that

$$\left\langle \dot{E}_m\left(t\right)\middle|E_n\left(t\right)\right\rangle = -\left\langle E_m\left(t\right)\middle|\dot{E}_n\left(t\right)\right\rangle. \tag{B.4}$$

Second, since it is also true that

$$\left\langle E_m\left(t\right)\middle|H\middle|E_n\left(t\right)\right\rangle = 0 \tag{B.5}$$

for all $m \neq n$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle E_m(t)\middle|H(t)\middle|E_n(t)\right\rangle = 0, \tag{B.6}$$

which implies that

$$\left\langle \dot{E}_m(t)\middle|H(t)\middle|E_n(t)\right\rangle + \left\langle E_m(t)\middle|H\middle|\dot{E}_n(t)\right\rangle + \left\langle E_m(t)\middle|\dot{H}(t)\middle|E_n(t)\right\rangle = 0, \tag{B.7}$$

and hence

$$E_n(t)\left\langle \dot{E}_m(t)\middle|E_n(t)\right\rangle + \left\langle E_m(t)\middle|\dot{H}\middle|E_n(t)\right\rangle + E_m(t)\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle = 0. \tag{B.8}$$

Combining these results, we have

$$\frac{\left\langle E_m(t)\middle|\dot{H}\middle|E_n(t)\right\rangle}{E_m(t) - E_n(t)} = -\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle, \tag{B.9}$$

which changes Schiff's expression as

$$c_m(t) \approx i\frac{\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}{E_m(t) - E_n(t)}\left(e^{i(E_m - E_n)t} - 1\right). \tag{B.10}$$

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