Conditions for the quantum adiabatic approximation

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Abstract

We give a sufficient condition for the quantum adiabatic approximation, which is quantitative and can be used to estimate error caused by this approximation. We also discuss when the traditional condition is sufficient.

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Quantum adiabatic approximation has a long history but recently it is re-examined [1, 2, 3, 4]. Tong et al point out that the traditional used condition is insufficient, which does not guarantee the validity of the adiabatic approximation [4]. In this paper we present a sufficient condition. Our condition is a quantitative one and can be used to estimate error caused by the approximation.

When we make an approximation two things should be specified: (i) A time interval in which we use the approximation and (ii) a parameter that is used to show how good the approximation is. To our knowledge these two things have not been specified for adiabatic approximation. Usually quantum adiabatic approximation is expressed as follows: suppose a quantum system has a finite and discrete spectral decomposition, if at the start time $t = 0$ the system is in the $n$th instantaneous eigenstate, then at a later time the system will remain in the $n$th instantaneous eigenstate up to a phase factor provided the system Hamiltonian varies slowly enough.

Assume the system has finite instantaneous discrete spectrum decomposition

$$H(t) = \sum_m E_m(t) \langle E_m(t) | E_m(t) \rangle.$$ 

And the initial state of the system is

$$|\Psi(0)\rangle = \sum_n c_n(0) |E_n(0)\rangle.$$ 

The adiabatic approximation predicates that at time $t$ the system will be in the state

$$|\Psi_A(t)\rangle = \sum_n c_n(0) e^{-i\alpha_n(t)} e^{-i\beta_n(t)} |E_n(t)\rangle,$$

Where $\alpha_n(t) = \int_0^t E_n(t') dt'$ is the dynamic phase, and $\beta_n(t) = -i \int_0^t (\langle E_n(t') | \frac{d}{dt'} | E_n(t') \rangle) dt'$ is Berry phase [5]. We specify a time interval $[0, T]$ in which we use the adiabatic approximate evolution to simulate the real evolution of the system. Our goal is to find the condition under which the error caused by the approximation is below a value $\epsilon$ we specified.

Suppose the true wave function at time $t$ is

$$|\Psi(t)\rangle = \sum_n c_n(t) e^{-i\alpha_n(t)} e^{-i\beta_n(t)} |E_n(t)\rangle.$$ 

This wave function obeys the Schrödinger equation $i d |\Psi(t)\rangle / dt = H(t) |\Psi(t)\rangle$ (we set
\(h = 1\). From \(i \langle E_m(t) | d | \Psi(t) \rangle / dt = \langle E_m(t) | H(t) | \Psi(t) \rangle\) we obtain

\[
\frac{dc_m(t)}{dt} = - \sum_{n \neq m} c_n(t) \langle E_m | d | E_n \rangle e^{-i(\alpha_n(t) - \alpha_m(t))} e^{-i(\beta_n(t) - \beta_m(t))}.
\]

This differential equation is equivalent to the following integral equation

\[
c_m(t) - c_m(0) = - \sum_{n \neq m} \int_0^t c_n(t') \langle E_m | d | E_n \rangle e^{-i(\alpha_n(t') - \alpha_m(t'))} e^{-i(\beta_n(t') - \beta_m(t'))} dt'.
\]

We assume the adiabatic approximation is very good in the time interval \([0, T]\), which means \(|c_m(t) - c_m(0)| \ll 1\) for arbitrary initial value \(c_m(0)\). Mathematically this assumption requires

\[
\left| \int_0^t \langle E_m | d | E_n \rangle e^{-i(\alpha_n(t') - \alpha_m(t'))} e^{-i(\beta_n(t') - \beta_m(t'))} dt' \right| \ll 1, \ t \in [0, T] \quad (1)
\]

for any \(n \neq m\). Recall a simple physical picture where a two-level atom is presented in a classical field. When the coupling strength between the atom and the field is much smaller than the energy detuning, the population of the atom will not change. Compare the question we are considering with this simple physical picture, intuitively we conjecture that when the adiabatic approximation is a good approximation in the time interval \([0, T]\) we should have

\[
\left| \frac{d}{dt} \left[ \langle E_n | \alpha_n(t') - \alpha_m(t') + \beta_n(t') - \beta_m(t') + \gamma_{mn}(t') \rangle \right] \right| \ll 1, \ t' \in [0, T] \quad (2)
\]

for any \(m \neq n\), where \(\gamma_{mn}(t')\) is the phase of \(\langle E_m | d | E_n \rangle\), i.e., \(\langle E_m | d | E_n \rangle = |A_{mn}(t')| e^{-i\gamma_{mn}(t')}\). We will show that this requirement can be regarded as a qualitative condition for quantum adiabatic approximation.

In the above we have specified the time interval \([0, T]\) we use the adiabatic approximation. Now we specify a small number \(\epsilon\) to show how good the approximation will be in this time interval. We require

\[
\left| \int_0^t \langle E_m | d | E_n \rangle e^{-i(\alpha_n(t') - \alpha_m(t'))} e^{-i(\beta_n(t') - \beta_m(t'))} dt' \right| \leq \epsilon, \ t \in [0, T] \quad (3)
\]

for any \(n \neq m\). Obviously the smaller \(\epsilon\) is, the better the adiabatic approximation will be. So the parameter \(\epsilon\) can be used to tell how good the adiabatic approximation is in the time interval \([0, T]\). We think this inequality is the sufficient and necessary condition for quantum adiabatic approximation. When we want to know whether quantum adiabatic approximation is a good approximation (specified by \(\epsilon\)) for a system evolution in the time interval \([0, T]\), we can check whether the system Hamiltonian satisfies the above inequality.
or not. When this check is not easy to accomplish, some sufficient conditions that are easy
to check can be used.

We define

$$G_{mn} = \left| \int_0^t \langle E_m \frac{d}{dt'} | E_n \rangle e^{-i(\alpha_n(t')-\alpha_m(t'))} e^{-i(\beta_n(t')-\beta_m(t'))} dt' \right|$$

$$= \left| \int_0^t \langle E_m \frac{d}{dt'} | E_n \rangle e^{-i\theta_{mn}(t')} dt' \right|,$$

where $\theta_{mn}(t') = \alpha_n(t') - \alpha_m(t') + \beta_n(t') - \beta_m(t') + \gamma_{mn}(t')$. Notice that

$$G_{mn} \leq \int_0^t \langle E_m \frac{d}{dt'} | E_n \rangle dt' \leq T \max_{t' \in [0,T]} \left| \langle E_m \frac{d}{dt'} | E_n \rangle \right|.$$

So when

$$T \max_{t' \in [0,T]} \left| \langle E_m \frac{d}{dt'} | E_n \rangle \right| \leq \epsilon \quad (4)$$

for any $m \neq n$ we can say in the time interval $[0, T]$ the adiabatic approximation is a good
approximation under the error rate we specify by $\epsilon$. Physically this situation means the
eigenstates change little in the time interval $[0, T]$. In the limit case, i.e., $\langle E_m \frac{d}{dt} | E_n \rangle = 0$
for any $m \neq n$, $\frac{d}{dt} | E_n \rangle$ is always proportional to $| E_n \rangle$ or $| E_n \rangle$ is a constant vector, which means
$| E_n(t') \rangle$ is equivalent to $| E_n(0) \rangle$ up to a phase factor. When $T \max_{t' \in [0,T]} \left| \langle E_m \frac{d}{dt'} | E_n \rangle \right| \leq \epsilon$
is not satisfied, we make some assumptions for further discussion. (i) We assume $\theta_{mn}(t')$
is an increasing (or decreasing) function in the interval $t' \in [0, T]$, so we can write

$$G_{mn} = \left| \int_0^t |A_{mn}(t')| e^{-i\theta_{mn}(t')} dt' \right|$$

$$= \left| \int_{\theta_{mn}(0)}^{\theta_{mn}(t)} A_{mn}(t' \theta_{mn}) \frac{dt'(\theta_{mn})}{d\theta_{mn}} e^{-i\theta_{mn}} d\theta_{mn} \right|$$

$$\leq \left| \int_{\theta_{mn}(0)}^{\theta_{mn}(t)} A_{mn}(t' \theta_{mn}) \frac{dt'(\theta_{mn})}{d\theta_{mn}} \cos \theta_{mn} d\theta_{mn} \right| + \left| \int_{\theta_{mn}(0)}^{\theta_{mn}(t)} A_{mn}(t' \theta_{mn}) \frac{dt'(\theta_{mn})}{d\theta_{mn}} \sin \theta_{mn} d\theta_{mn} \right|.$$

(ii) We assume $\left| A_{mn}(t' \theta_{mn}) \frac{dt' \theta_{mn}}{d\theta_{mn}} \right|$ is an not-decreasing (or not-increasing) function in
the interval $\theta_{mn} \in [\theta_{mn}(0), \theta_{mn}(T)]$, i.e., $\left| A_{mn}(t') \frac{dt'}{d\theta_{mn}(t')} \right|$ is an not-decreasing (or not-increasing) function in the interval $t' \in [0, T]$. According to integral mean value theorems
we have

\[ G_{mn} \leq 4 \max_{\theta_{mn} \in [\theta_{mn}(0), \theta_{mn}(T)]} \left| \frac{A_{mn}(t') \, dt'}{d\theta_{mn}(t') / dt'} \right| \]

\[ = 4 \max_{t' \in [0,T]} \left| \frac{A_{mn}(t')}{d\theta_{mn}(t') / dt'} \right|. \]

In deriving this inequality we use the following real function integral mean value theorems:

1. In the interval \( x \in [a, b] \), \( f(x) \) is a not-increasing and not-negative function and \( g(x) \) is integrable, then we have \( \int_a^b f(x)g(x)dx = f(a) \int_a^c g(x)dx, a < c < b \).
2. In the interval \( x \in [a, b] \), \( f(x) \) is a not-decreasing and not-negative function and \( g(x) \) is integrable, then we have \( \int_a^b f(x)g(x)dx = f(b) \int_a^b g(x)dx, a < c < b \).

Generally, the above two assumptions are incorrect, but we can always divide the interval \([0, T]\) into \( N_{mn}(T) \) small intervals and in each one the above two assumptions are correct \(6\). Now we have

\[
G_{mn} \leq 4N_{mn}(T) \max_{t' \in [0,T]} \left| \frac{A_{mn}(t')}{d\theta_{mn}(t') / dt'} \right|
\]

\[
= 4N_{mn}(T) \max_{t' \in [0,T]} \left| \frac{\langle E_m | \frac{d}{dt} | E_n \rangle}{\frac{d}{dt}[\alpha_n(t') - \alpha_m(t') + \beta_n(t') - \beta_m(t') + \gamma_{mn}(t')]} \right| \leq \epsilon \tag{5}
\]

for any \( m \neq n \) we can claim that in the time interval \([0, T]\) the adiabatic approximation is a good approximation. But when this inequality is not satisfied we can not certainly claim the adiabatic approximation is not a good approximation \( \text{specified by } \epsilon \) in the time interval \([0, T]\). Inequalities (4) and (5) are sufficient conditions for the adiabatic approximation, they are not necessary. Qualitatively inequality (5) implies

\[
\left| \frac{\langle E_m | \frac{d}{dt} | E_n \rangle}{\frac{d}{dt}[\alpha_n(t') - \alpha_m(t') + \beta_n(t') - \beta_m(t') + \gamma_{mn}(t')]} \right| \ll 1. \tag{6}
\]

This is just our previous conjecture came from analog with a simple physical picture.

When there exists a special basis and the instantaneous eigenstate vectors \( |E_n \rangle \) expressed in this basis are always real, \( i.e. \), the system Hamiltonian in this basis is real, we can find that \( \langle E_m | \frac{d}{dt} | E_n \rangle \) is real and Berry phase \( \beta_m(t') \) is zero. In this situation we have

\[
d\theta_{mn}(t') / dt' = \frac{d}{dt'} [\alpha_n(t') - \alpha_m(t')]
= E_n(t') - E_m(t').
\]
Inequalities (5) and (6) can be written as

\[ 4N_{mn}(T) \max_{t' \in [0,T]} \left| \frac{\langle E_m | \frac{d}{dt} | E_n \rangle}{E_n (t') - E_m (t')} \right| \leq \epsilon, \]

and

\[ \left| \frac{\langle E_m | \frac{d}{dt} | E_n \rangle}{E_n (t') - E_m (t')} \right| \ll 1. \]

This inequality is the traditional sufficient condition for quantum adiabatic approximation, they are correct when Hamiltonian is a real matrix in a certain basis.

The quantum adiabatic approximation is not perfect except for the trivial case where \( \langle E_m | \frac{d}{dt} | E_n \rangle = 0 \) for any \( m \neq n \), so applying a parameter to estimate error is necessary when we use this approximation in a certain time interval. First we can check the inequality (3). When inequality (3) is not easy to check, we can check inequalities (4) and (5), they are sufficient conditions for adiabatic approximation. Qualitatively we can check inequality (6).

In conclusion we give a sufficient condition for quantum adiabatic approximation, which is quantitative and can be used to analyze error caused by adiabatic approximation. We point out that the widely used traditional sufficient condition are correct only when the system Hamiltonian can be presented by a real matrix, Berry phase is always zero in this situation.

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[6] Here we assume \( \theta_{mn} (t') \) is not a constant.