A sufficient condition for the validity of quantum adiabatic theorem

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Abstract: In this paper, we attempt to give a sufficient condition of guaranteeing the validity of the proof of quantum adiabatic theorem. The new sufficient condition can clearly remove the inconsistency and counterexample pointed out by K. P. Marzlin and B. C. Sanders [Phys. Rev. Lett. 93, 160408, (2004)].

Keywords: Quantum adiabatic theorem; Integral formalism; Differential formalism; Berry phase. **PACS:** 03.65.-w; 03.65.Ca; 03.65.Vf.

1. Introduction

The quantum adiabatic theorem (QAT) [1-4] is one of the basic results in quantum physics. The role of the QAT in the study of slowly varying quantum mechanical system spans a vast array of fields and applications, such as quantum field [5], Berry phase [6], and adiabatic quantum computation [7]. However, recently, the validity of the application of the QAT had been doubted in reference [8], where Marzlin and Sanders (MS) pointed out an inconsistency. The MS inconsistency led to extensive discussions from physical circles [9-16]. Although there are many different viewpoints as for the inconsistency, there seems to be a general agreement that the origin is due to the insufficient conditions for the QAT.

More recently, we have summarized many different viewpoints of studying the MS inconsistency [17] and we further notice that there, in fact, are two different types of inconsistencies of the QAT in reference [8], that is, MS inconsistency and MS counterexample. Most importantly, these two types are often confused as one! That is the reason why there are many different viewpoints as for the inconsistency of the QAT. Our study shows that [17] resolving the MS counterexample refers to convergence of the Schrödinger integral equation in the adiabatic limit (References [12,14,15,16] refer to this point) and that resolving the MS inconsistency refers to convergence of the Schrödinger differential equation in the adiabatic limit (References [10,13] refer to this point). Nevertheless, a lot of references always pay attention to MS counterexample rather than MS inconsistency. In reference [17] we point out that the MS inconsistency is very important: Recognition of the MS inconsistency would give rise to the necessity of integral formalism. For example, we can only reach a complete QAT through Schrödinger integral equation rather than Schrödinger differential equation. Our main purpose of this paper is to provide a new sufficient condition to rigorously prove the complete QAT through Schrödinger integral equation. Furthermore, the new sufficient condition can clearly remove MS inconsistency and MS counterexample.

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2. The type of proof of quantum adiabatic theorem

In general, there are two types of proofs as for the QAT, differential formalism and integral formalism.

(i) Proof of differential formalism: $\lim_{T \to \infty} \frac{\partial}{\partial s} |\psi(sT)\rangle = \frac{\partial}{\partial s} |\psi(sT)\rangle_A$ (ii) Proof of integral formalism: $\lim_{T \to \infty} |\psi(sT)\rangle = |\psi(sT)\rangle_A$

Here $|\psi(sT)\rangle$ is state vector and $s = \frac{t}{T}$ denotes the scaled dimensionless time variable. The QAT reads

$$\left|\psi(sT)\right\rangle_{A} = \exp\left[-iT\int_{0}^{s} E_{n}\left(sT\right)ds\right] \exp\left[-\int_{0}^{s}\left\langle n\left(sT\right)\right|\frac{\partial}{\partial s}\left|n\left(sT\right)\right\rangle ds\right] \left|n\left(sT\right)\right\rangle$$
(1)

Recently, nevertheless, Wu and Yang [10] have pointed out that the proof of differential formalism (i) is invalid and it may give rise to MS inconsistency. In fact, up to now, many rigorous proofs of QAT are based on the proof of integral formalism (ii) [3,4,18,19], but this point is always neglected by physical circles. That is the reason why there exists MS inconsistency.

On the other hand, to guarantee the validity of the proof of integral formalism (ii), there needs a sufficient condition. Unfortunately, the traditional adiabatic condition [20], $\langle n(t) | \frac{\partial}{\partial t} | m(t) \rangle = 0$

 $(n \neq m)$, is insufficient and hence can not guarantee the validity of the proof of integral formalism (ii). That is the reason why there exists MS counterexample. In fact, the traditional adiabatic condition, $\langle n(t) | \frac{\partial}{\partial t} | m(t) \rangle = 0$ $(n \neq m)$, is just based on the proof of differential formalism (i) [20] and hence is invalid [10].

In the next section, we attempt to give a sufficient condition of guaranteeing the validity of the proof of integral formalism (ii).

3. The validity of quantum adiabatic theorem

First, we attempt to give an exact expression of Berry phase. In fact, there may be, in the adiabatic limit $T \to \infty$, that $\lim_{T \to \infty} |n(sT)\rangle$ does not exist and that

$$\lim_{T\to\infty}\frac{\partial}{\partial s}|n(sT)\rangle\neq\frac{\partial}{\partial s}\lim_{T\to\infty}|n(sT)\rangle.$$

That means, in the adiabatic limit, the Berry phase, which reads $i\oint \lim_{T\to\infty} \langle n(sT)|d|n(sT)\rangle$

[21], has no meaning. Therefore, if we require that the Berry phase makes good sense, then the theorem 3.1 given as follow must hold.

Theorem 3.1. If
$$\lim_{T \to \infty} |n(sT)\rangle = |n(s)\rangle$$
 and if $\lim_{T \to \infty} \frac{\partial}{\partial s} |n(sT)\rangle = \frac{\partial}{\partial s} \lim_{T \to \infty} |n(sT)\rangle$ [22], then

Berry phase is given by

$$\gamma(C) = \lim_{T \to \infty} i \oint \langle n(sT) | d | n(sT) \rangle = i \oint \lim_{T \to \infty} \langle n(sT) | d | n(sT) \rangle = i \oint \langle n(s) | d | n(s) \rangle$$

Proof. Using the bounded convergence theorem of Lebesgue [23], the proof is complete.

In this paper, we always suppose the theorem 3.1 holds. That is to say, the theorem 3.1 is an important postulate of guaranteeing the validity of QAT.

In reference [17] we have noted that if we want to prove the QAT, we only need to prove that

$$\lim_{T \to \infty} |\phi(sT)\rangle = \lim_{T \to \infty} \exp\left[-\int_0^s \langle m(sT) | \frac{\partial}{\partial s} | m(sT)\rangle\right] |m(0)\rangle$$

$$= \exp\left[-\int_0^s \langle m(sT) | \frac{\partial}{\partial s} | m(sT)\rangle\right] |m(0)\rangle$$
(2)

Here $|\phi(sT)\rangle$ satisfies the Schrödinger integral equation,

$$\left|\phi(sT)\right\rangle = \left|\phi(0)\right\rangle - \int_{0}^{s} K_{T}\left(s^{\dagger}\right) \phi\left(s^{\dagger}T\right) ds^{\dagger}, \qquad (3)$$

where

$$K_{T}(s) = \sum_{j} \sum_{k} \exp\left[iT \int_{0}^{s} E_{j}(s'T) - E_{k}(s'T) ds'\right] \langle j(sT)|\frac{\partial}{\partial s}|k(sT)\rangle |j(0)\rangle \langle k(0)|.$$
(4)

Second, if we take $|\phi(sT)\rangle = W_T(s)|\phi(0)\rangle$, then our main result is as follow:

Theorem 3.2. If $W_T(s)$ fulfills four conditions as follows:

(a) The Schrödinger integral equation reads

$$W_T(s) = I - \int_0^s K_T(s') W_T(s') ds', \qquad (5)$$

where $K_T(s)$ is defined by equation (4);

(b) For an arbitrary eigenstate $|n(sT)\rangle$, there have

$$\lim_{T \to \infty} |n(sT)\rangle = |n(s)\rangle \text{ and } \lim_{T \to \infty} \frac{\partial}{\partial s} |n(sT)\rangle = \frac{\partial}{\partial s} \lim_{T \to \infty} |n(sT)\rangle;$$

(c) $\langle j(sT) | \frac{\partial}{\partial s} | k(sT) \rangle \neq 0$ $(j \neq k);$

(d) $\lim_{T \to \infty} \int_0^s \exp\left[iT \int_0^s E_j(\sigma T) - E_k(\sigma T) d\sigma\right] ds = 0 \quad (j \neq k) \text{ as for any } s \in [0,1];$

then there holds $\lim_{T \to \infty} W_T(s) = \sum_{k} \exp\left[-\int_0^s \left\langle k(s') \right| \frac{\partial}{\partial s'} \left| k(s') \right\rangle ds' \right] \left| k(0) \right\rangle \left\langle k(0) \right|.$

Before proving this theorem, we need to prepare two lemmas.

Lemma 3.3. If
$$\lim_{T \to \infty} \int_0^s \exp\left[iT \int_0^s E_j(\sigma T) - E_k(\sigma T) d\sigma\right] ds = 0 \quad (j \neq k)$$
 as for any

 $s \in [0,1]$, then there holds

$$\lim_{T\to\infty}\int_0^s \exp\left[iT\int_0^s E_j(\sigma T) - E_k(\sigma T)d\sigma\right]f(s)ds = 0 \quad (j \neq k),$$

where f(s) is any integrable function on the interval [0,1].

Proof. Using the general Riemann-Lebesgue lemma [24], we note that the lemma 3.3 holds.

Lemma 3.4. If the lemma 3.3 holds, then, for any integrable function $f_T(s)$ which is uniform convergence to f(s), i.e., $\lim_{T \to \infty} \sup_{s \in [0,1]} |f_T(s) - f(s)| = 0$, there holds,

$$\lim_{T \to \infty} \int_0^s \exp\left[iT \int_0^s E_j(\sigma T) - E_k(\sigma T) d\sigma\right] f_T(s) ds$$

=
$$\lim_{T \to \infty} \int_0^s \exp\left[iT \int_0^s E_j(\sigma T) - E_k(\sigma T) d\sigma\right] f(s) ds = 0$$
 ($j \neq k$)

Proof. Let
$$g_T(s) = \exp\left[iT\int_0^s E_j(\sigma T) - E_k(\sigma T)d\sigma\right] \quad (j \neq k)$$
, then there holds,
 $\left|\int_0^s g_T(s')f_T(s')ds' - \int_0^s g_T(s')f(s')ds'\right| \le \int_0^s \left|f_T(s') - f(s')ds'\right| \le \sup_{s' \in [0,s]} \left|f_T(s') - f(s')s'\right| \le \int_0^s \left|f_T(s') - f(s')ds'\right| \le \int_0^s$

If we note that $\lim_{T \to \infty} \sup_{s \in [0,1]} |f_T(s) - f(s)| = 0$, then we have proved the lemma 3.4. \Box

Now, we start to prove the theorem 3.2.

Proof. Clearly, the equation (5) can be written as, $W_T(s) = \exp\left[-\int_0^s K_T(s')ds'\right]$ Furthermore, $K_T(s)$ can be separated into two parts, that is, $K_T(s) = K_T^{(1)}(s) + K_T^{(2)}(s)$ where $K_T^{(1)}(s) = \sum_k \langle k(sT) | \frac{\partial}{\partial s} | k(sT) \rangle | k(0) \rangle \langle k(0) |$,

and
$$K_T^{(2)}(s) = \sum_{j \neq k} \exp\left[iT \int_0^s E_j(sT) - E_k(sT) ds\right] \langle j(sT) | \frac{\partial}{\partial s} | k(sT) \rangle | j(0) \rangle \langle k(0) | s$$

On the one hand, conditions (b), (d) and lemma 3.4 will guarantee that

$$\lim_{T \to \infty} \int_0^s K_T^{(2)}(s') ds' = 0.$$
 (6)

On the other hand, the bounded convergence theorem of Lebesgue [23] and condition (b) will guarantee that

$$\lim_{T \to \infty} \int_0^s K_T^{(1)}(s') ds' = \int_0^s \lim_{T \to \infty} K_T^{(1)}(s') ds' = \sum_k \int_0^s \left\langle k(s') \right| \frac{\partial}{\partial s'} \left| k(s') \right\rangle \left| k(0) \right\rangle \left\langle k(0) \right| ds'.$$
(7)

Therefore, using equations (6) and (7), we have

$$\lim_{T \to \infty} W_T(s) = \exp\left[-\lim_{T \to \infty} \int_0^s K_T(s') ds'\right] = \sum_k \exp\left[-\int_0^s \left\langle k(s') | \frac{\partial}{\partial s'} | k(s') \right\rangle ds'\right] |k(0)\rangle \langle k(0)|$$

The proof is complete. \Box

Clearly, the theorem 3.2 has shown that $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger integral equation (5). Moreover, it is notable that if we use equation, $\langle j(sT)|\frac{\partial}{\partial s}|k(sT)\rangle = 0$ $(j \neq k)$, rather than the condition (d), then we can also obtain the equation (6). However, the equation, $\langle j(sT)|\frac{\partial}{\partial s}|k(sT)\rangle = 0$ $(j \neq k)$, will give rise to MS inconsistency [10,17]. Fortunately, condition (c) can remove this case. Moreover, it is easy to check that the MS counterexample in reference [8] does not fulfill the condition (d). That means, the condition (c) and (d) have clearly removed the MS inconsistency and MS counterexample.

4. Origin of inconsistency of quantum adiabatic theorem

In this section, we attempt to rigorously prove that if $\langle j(sT) | \frac{\partial}{\partial s} | k(sT) \rangle \neq 0$ $(j \neq k)$, then

 $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, does not satisfy the Schrödinger differential equation,

$$\frac{\partial}{\partial s}W_{T}(s) = -K_{T}(s)W_{T}(s). \tag{8}$$

Proof. If we carefully check $K_T^{(2)}(s)$, then we will note that if $\langle j(sT) | \frac{\partial}{\partial s} | k(sT) \rangle \neq 0$ $(j \neq k)$, the limit $\lim_{T \to \infty} K_T(s)$ will not exist. It implies that the limit $\lim_{T \to \infty} \frac{\partial}{\partial s} W_T(s)$ will not also exist.

On the one hand, the theorem 3.2 has shown that the limit $\lim_{T\to\infty} W_T(s)$ exists. On the other

hand, the condition (b) guarantees that $\lim_{T\to\infty} W_T(s)$ is differentiable. That is to say,

$$\frac{\partial}{\partial s} \lim_{T \to \infty} W_T(s) \text{ exists.}$$

Therefore, above discussions imply that
$$\lim_{T \to \infty} \frac{\partial}{\partial s} W_T(s) \neq \frac{\partial}{\partial s} \lim_{T \to \infty} W_T(s). \tag{9}$$

Reference [17] has shown that $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger

differential equation (8) if and only if $\lim_{T\to\infty} \frac{\partial}{\partial s} W_T(s) = \frac{\partial}{\partial s} \lim_{T\to\infty} W_T(s)$. Clearly, it is contrary to the inequality (9); therefore, the proof is complete. \Box

Conversely, if $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger differential equation, there will hold, $\langle j(sT)|\frac{\partial}{\partial s}|k(sT)\rangle = 0$ $(j \neq k)$. It would give rise to the MS inconsistency [17]. In reference [8], MS require that $\lim_{T\to\infty} W_T(s)$ satisfies the Schrödinger differential equation (8), that is the reason why there exists MS inconsistency in their derivation.

5. Conclusion

So far, we have rigorously proved that $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger integral equation (5) rather than the Schrödinger differential equation (8). Moreover, if $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger differential equation (8), then there will exist the MS inconsistency. In reference [8], MS require that $\lim_{T\to\infty} W_T(s)$ satisfies the Schrödinger differential equation (8), that is the reason why there exists MS inconsistency in their derivation. On the other hand, to guarantee that $\lim_{T\to\infty} W_T(s)$, in the adiabatic limit, satisfies the Schrödinger integral equation (5), there need to be a sufficient condition. Nevertheless, the traditional adiabatic condition, $\langle n(t) | \frac{\partial}{\partial t} | m(t) \rangle = 0$ $(n \neq m)$, is insufficient. That is the reason why these exists the MS counterexample in reference [8]. Fortunately, we give a sufficient condition, which can remove the MS counterexample. More specifically, the condition (d) of guaranteeing the validity of theorem 3.2 can remove the MS counterexample. Finally, we need to point out that the condition (c) of guaranteeing the validity of theorem 3.2 can remove the MS counterexample. Finally, we need to point out that the condition (c) of guaranteeing the validity of theorem 3.2 can remove the MS counterexample. Finally, we need to point out that the condition (c) of guaranteeing the validity of theorem 3.2 can remove the MS counterexample.

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[21]. In this paper, we define Berry phase as

$$\gamma(C) = \lim_{T \to \infty} i \oint \langle n(sT) | d | n(sT) \rangle = i \oint \lim_{T \to \infty} \langle n(sT) | d | n(sT) \rangle = i \oint \langle n(s) | d | n(s) \rangle,$$

which is different from that of Berry [6] who defines the Berry phase as

$$\gamma'(C) = i \oint \langle n(sT) | d | n(sT) \rangle$$

where d denotes differential operator. Here we have applied the conditions of theorem 3.1 and the bounded convergence theorem of Lebesgue [23].

[22]. In this paper, we suppose that $|n(sT)\rangle$ and $\frac{\partial}{\partial s}|n(sT)\rangle$ are uniform convergence to

$$|n(s)\rangle$$
 and $\frac{\partial}{\partial s}|n(s)\rangle$ respectively,

that is,
$$\lim_{T \to \infty} \sup_{s \in [0,1]} \left| n(sT) \right\rangle - \left| n(s) \right\rangle = 0 \text{ and } \lim_{T \to \infty} \sup_{s \in [0,1]} \left| \frac{\partial}{\partial s} \left| n(sT) \right\rangle - \frac{\partial}{\partial s} \left| n(s) \right\rangle \right| = 0,$$

where $|n(s)\rangle$ is independent of the total evolution time T and the symbol $\sup_{x\in[a,b]}|f(x)|$

denotes the super bound of function |f(x)| on the interval $x \in [a, b]$.

[23]. J. Franks, Notes on Measure and Integration, arXiv:0802.4076v3, p59.

[24]. The general Riemann-Lebesgue lemma states that: If $\{g_n(x)\}\$ are sequence of measurable

functions on the interval [a,b] and satisfy two conditions:

- (A) $|g_n(x)| \le M$ with $x \in [a, b]$, where *M* is a constant;
- (B) For any $c \in [a,b]$, there holds $\lim_{n \to \infty} \int_a^c g_n(x) dx = 0$;

then there would be, for any function f(x) which is Lebesgue integrable, that $\lim_{n\to\infty}\int_a^b g_n(x)f(x)dx = 0$. The proof sees Appendix .

Appendix

The proof of general Riemann-Lebesgue lemma [24]

Proof. For any $\varepsilon > 0$, we can construct the step function

$$\begin{split} \varphi(x) &= \sum_{i=1}^{p} y_{i} \chi_{[x_{i-1}, x_{i})}(x) \text{ with } x \in [a, b], \text{ so that} \\ \int_{a}^{b} |f(x) - \varphi(x)| dx &< \frac{\varepsilon}{2M}, \\ \text{where, } \chi_{[x_{i-1}, x_{i})}(x) &= \begin{cases} 1, x \in [x_{i-1}, x_{i}) \\ 0, x \notin [x_{i-1}, x_{i}) \end{cases} \text{ with } a = x_{0} < x_{1} < \dots < x_{p} = b, \end{split}$$

and y_i is constant.

If we use the condition (B) and the inequality $\left| \int_{a}^{b} \varphi(x) g_{n}(x) dx \right| \leq \sum_{i=1}^{p} \left| y_{i} \int_{x_{i-1}}^{x_{i}} g_{n}(x) dx \right|$

then there holds,

$$\left|\int_{a}^{b} \varphi(x) g_{n}(x) dx\right| \leq \frac{\varepsilon}{2} \quad \text{as} \quad n \geq N,$$

where N is sufficiently large.

Thus, if $n \ge N$ and if we use the condition (A), then there holds

$$\left| \int_{a}^{b} f(x)g_{n}(x)dx \right| \leq \left| \int_{a}^{b} [f(x) - \varphi(x)]g_{n}(x)dx \right| + \left| \int_{a}^{b} \varphi(x)g_{n}(x)dx \right|$$

$$\leq M \int_{a}^{b} |f(x) - \varphi(x)|dx + \frac{\varepsilon}{2} < \varepsilon$$

that is,
$$\lim_{n \to \infty} \int_{a}^{b} g_{n}(x)f(x)dx = 0. \Box$$