Validity of the quantum adiabatic theorem

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The consistency of the quantum adiabatic theorem has been doubted recently. It is shown in the present paper that the difference between the adiabatic solution and the exact solution to the Schrödinger equation with a slowly changing driving Hamiltonian is small; while the difference between their time derivatives is not small. This explains why substituting the adiabatic solution back into the Schrödinger equation leads to "inconsistency" of the adiabatic theorem. Physics is determined completely by the state vector, and not by its time derivative. Therefore the quantum adiabatic theorem is physically correct.

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I. INTRODUCTION

Quantum adiabatic theorem (QAT) dates back to the early years of quantum mechanics [1]. It has important applications within and beyond quantum physics. In 1984, Berry found there is a geometrical phase in the adiabatically evolving wave function besides the dynamic phase [2]. Simon pointed out Berry's phase factor is the holonomy of a Hermitian line bundle [3]. This started a rush for geometrical phases in quantum physics [4], which helped people to get deeper insight into many physical phenomena, such as Bohm-Aharanov effect, quantum Hall effect, etc. Recently, the quantum adiabatic theorem has renewed its importance in the context of quantum control and quantum computation [5–9]. More recently, however, the consistency of the QAT has been doubted [10]. In their paper entitled "Inconsistency in the application of the adiabatic theorem," Marzlin and Sanders gave a proof of inconsistency implied by the QAT (MS inconsistency), and declared that the standard statetment of the QAT alone does not ensure that a formal application of it results in correct results. This interesting suggestion has attracted attention from the physics circle [11–13]. However, it has also caused confusion about the validity of the QAT. In view of the importance of the QAT, the purpose of this paper is to point out that the QAT does give approximate state vectors when there is no resonance in the Schrödinger equation in the rotating axis representation, but not necessarily the approximate time derivatives of state vectors. While physics is completely determined by the state vector, it has nothing to do with its time derivative. Therefore the QAT is physically completely correct, provided there is no resonance in the Schrödinger equation in the rotating axis representation. What leads to MS inconsistency of the QAT is neglect of the fact that the adiabatic approximate state vector does not necessarily give the approximate time derivative of state vector ($\|\psi_{AT}(t)-\psi_{EX}(t)\| \ll 1 \not\Rightarrow \|\dot{\psi}_{AT}(t)-\dot{\psi}_{EX}(t)\| \ll 1$, where $\|\varphi\| \equiv \sqrt{\langle\varphi|\varphi\rangle}$ denotes the norm of state vector φ).

II. STANDARD TREATMENT OF THE QAT

Suppose that the Hamiltonian depends on N real parameters $R^1,\ldots,R^N$:

$$H = H(R^1,\ldots,R^N) = H(R). \tag{1}$$

When the representing point of the Hamiltonian describes slowly a finite curve C on the N-dimensional parameter manifold $\mathcal{M}$

$$C{:}R^\sigma = R^\sigma(t), \quad \forall\, t \in [0,T], \quad 1 \leqslant \sigma \leqslant N, \tag{2}$$

where T is the evolution time, let us study the evolution of the system. The instantaneous Hamiltonian's eigenequation is

$$H(R)u_n(R) = E_n(R)u_n(R). \tag{3}$$

Getting to the rotating axis representation

$$\psi(t) = \sum_{n\geqslant 0} c_n(t)u_n(R(t))\exp\left[\frac{-i}{\hbar}\int_0^t E_n(R(t'))dt'\right] \tag{4}$$

we get the Schrödinger equation

$$\dot{c}_m(t) = -\sum_{n\geqslant 0}\langle u_m(R(t))|\dot{u}_n(R(t))\rangle \times \exp\left\{\frac{i}{\hbar}\int_0^t [E_m(R(t'))-E_n(R(t'))]dt'\right\}c_n(t). \tag{5}$$

To avoid confusion of infinitesimals of different orders and to show what "rapidly oscillating" means, let us change to the dimensionless time $\tau = t/T$

$$\frac{d}{d\tau}\check{c}_m(\tau) = -\sum_{n\geqslant 0}\left\langle u_m(\check{R}(\tau))\middle|\frac{d}{d\tau}u_n(\check{R}(\tau))\right\rangle \times \exp\left\{\frac{i}{\hbar}T\int_0^\tau [E_m(\check{R}(\tau'))-E_n(\check{R}(\tau'))]d\tau'\right\}\check{c}_n(\tau), \tag{6}$$

where

$$\check{c}_m(\tau) = c_m(T\tau) = c_m(t), \quad \check{R}(\tau) = R(T\tau) = R(t). \tag{7}$$

The initial value problem of the above differential equations is equivalent to the following integral equation:

$$\check{c}_m(\tau) = \check{c}_m(0) - \sum_{n\geq 0}\int_0^{\tau}\left\langle u_m(\check{R}(\tau_1))\left|\frac{d}{d\tau}u_n(\check{R}(\tau_1))\right.\right\rangle \times \exp\left\{\frac{i}{\hbar}T\int_0^{\tau_1}[E_m(\check{R}(\tau')) - E_n(\check{R}(\tau'))]d\tau'\right\}\check{c}_n(\tau_1)d\tau_1. \quad (8)$$

Let us slow down evenly the changing speed of the Hamiltonian while keeping the finite curve C fixed. Mathematically, that is to let $T\rightarrow\infty$, while keeping the function form of $\check{R}(\tau)$ unchanged. The oscillating factors in the integrand ensure vanishing of the corresponding integrals, provided there is no resonance. For the practical physical problem, slowly changing of the Hamiltonian means T is such a long time that

$$\left|\frac{\langle u_m(R(t))|\dot{u}_n(R(t))\rangle\hbar}{E_m(R(t)) - E_n(R(t))}\right| \ll 1. \quad (9)$$

The integral equation (8) can be approximately rewritten as

$$\check{c}_m^A(\tau) = \check{c}_m(0) - \int_0^{\tau}\left\langle u_m(\check{R}(\tau_1))\left|\frac{d}{d\tau}u_m(\check{R}(\tau_1))\right.\right\rangle\check{c}_m^A(\tau_1)d\tau_1. \quad (10)$$

Solving this equation by using iteration gives

$$\check{c}_m^A(\tau) = \exp\left\{-\int_0^{\tau}\left\langle u_m(\check{R}(\tau_1))\left|\frac{d}{d\tau}u_m(\check{R}(\tau_1))\right.\right\rangle d\tau_1\right\}\check{c}_m(0). \quad (11)$$

This proves the QAT.

III. ANALYSIS OF "INCONSISTENCY" OF THE QAT

When we substitute the adiabatic approximate solution (11) back into the integral equations (8), the equations approximately hold.

$$0 \approx -\sum_{n(\neq m)}\int_0^{\tau}\left\langle u_m(\check{R}(\tau_1))\left|\frac{d}{d\tau}u_n(\check{R}(\tau_1))\right.\right\rangle \times \exp\left\{\frac{i}{\hbar}T\int_0^{\tau_1}[E_m(\check{R}(\tau')) - E_n(\check{R}(\tau'))]d\tau'\right\}\check{c}_n^A(\tau_1)d\tau_1. \quad (12)$$

However, when we substitute the adiabatic approximate solution (11) back into the differential equations (6) whose initial value problem is equivalent to the integral equations (8), we obtain

$$0 \approx -\sum_{n(\neq m)}\left\langle u_m(\check{R}(\tau))\left|\frac{d}{d\tau}u_n(\check{R}(\tau))\right.\right\rangle \times \exp\left\{\frac{i}{\hbar}T\int_0^{\tau}[E_m(\check{R}(\tau')) - E_n(\check{R}(\tau'))]d\tau'\right\}\check{c}_n(\tau). \quad (13)$$

Considering that $\psi(0)$ [hence $\psi(t)$] can be an arbitrary state vector, we have

$$0 \approx \left\langle u_m(\check{R}(\tau))\left|\frac{d}{d\tau}u_n(\check{R}(\tau))\right.\right\rangle, \quad \forall\, m \neq n, \quad (14)$$

which is false.

In order to understand the situation we are facing, let us study the following basic mathematical fact. Let $|\psi(t)\rangle \equiv |0\rangle e^{-i\omega t} + \varepsilon|1\rangle e^{-it/(\varepsilon^2)}$, $(0<\varepsilon\ll 1)$, $|\varphi(t)\rangle \equiv |0\rangle e^{-i\omega t}$, where $|0\rangle$, $|1\rangle$ are eigenvectors of the one-dimensional harmonic oscillator energy.

$$\because \||\psi(t)\rangle - |\varphi(t)\rangle\| = \varepsilon \ll 1, \quad \therefore |\psi(t)\rangle \approx |\varphi(t)\rangle. \quad (15)$$

While

$$\because \||\dot{\psi}(t)\rangle - |\dot{\varphi}(t)\rangle\| = 1/\varepsilon \gg 1, \ \because |\dot{\psi}(t)\rangle \neq |\dot{\varphi}(t)\rangle. \quad (16)$$

The above example shows that two approximately equal time-dependent state vectors do not necessarily have approximately equal time derivatives. Therefore the approximate solution to integral equations (8) does not ensure that the equivalent differential equations (6) approximately hold. It is neglect of this basic mathematical fact that leads to "inconsistency" of the QAT in [10].

MS inconsistency in [10] is one of the many contradictions obtained by combining the QAT with wrong reasoning such as Eq. (14). Reference [11] gives a simpler way of deriving MS inconsistency. We can derive MS inconsistency from contradiction (14) easily.

$$\because 0 \approx \left\langle u_m(R(t))\left|\frac{d}{dt}u_n(R(t))\right.\right\rangle, \quad \forall\, m \neq n, \quad (17)$$

$$\therefore \left|\frac{d}{dt}u_n(R(t))\right\rangle \approx |u_n(R(t))\rangle\left\langle u_n(R(t))\left|\frac{d}{dt}u_n(R(t))\right.\right\rangle. \quad (18)$$

Taking the inner product of $|u_n(R(t_0))\rangle$ with both sides of Eq. (17), we obtain

$$\frac{d}{dt}\langle u_n(R(t_0))|u_n(R(t))\rangle \approx \langle u_n(R(t_0))|u_n(R(t))\rangle\left\langle u_n(R(t))\left|\frac{d}{dt}u_n(R(t))\right.\right\rangle. \quad (19)$$

Solving this differential equation, we obtain

$$\langle u_n(R(t_0))|u_n(R(t))\rangle \approx \exp \int_{t_0}^{t} \left\langle u_n(R(t')) \middle| \frac{d}{dt'} u_n(R(t'))dt' \right\rangle, \tag{20}$$

$$\langle u_n(R(t_0))|u_n(R(t))\rangle \approx \exp(-i\beta_n(t)). \tag{21}$$

That is the MS inconsistency.

When we say, "$\psi_{AP}(\tau)$ is an approximate solution to an initial problem of a differential equation," it only means $\|\psi_{AP}(\tau)-\psi_{EX}(\tau)\|\approx 0$, where $\psi_{EX}(\tau)$ is the exact solution and $\|\psi(\tau)\|$ denotes the norm of $\psi(\tau)$. It does not necessarily mean $\|\dot{\psi}_{AP}(\tau)-\dot{\psi}_{EX}(\tau)\|\approx 0$. Therefore the approximate solution does not ensure that the differential equations approximately hold. It is neglect of this basic mathematical fact that leads to "Inconsistency" of AT. In fact, that the Schrödinger equation (6) does not even approximately hold for $\psi_{AP}(\tau)$ means that

$$i\hbar \frac{\partial}{\partial \tau} \breve{U}_{AT}(\tau,\tau_0) \neq TH(\tau)\breve{U}_{AT}(\tau,\tau_0).$$

Therefore

$$i\hbar \frac{\partial}{\partial \tau} \breve{U}_{AT}(\tau,\tau_0)^{\dagger}|E_0(\tau_0)\rangle \neq -T\breve{U}_{AT}(\tau,\tau_0)^{\dagger}H(\tau) \times \breve{U}_{AT}(\tau,\tau_0)\breve{U}_{AT}(\tau,\tau_0)^{\dagger}|E_0(\tau_0)\rangle.$$

We see the minor premise of the proof of "inconsistency" in [10] is invalid. Here we have used the variable $\tau = t/T$ to avoid infinitely large variable t. The above reasoning is equivalent to the one given in [14], which is for the case when the infinitely large variable t is used.

As a matter of fact, the deviation of the adiabatic approximate solution $\psi_{AT}(t)$ from the exact solution $\psi_{EX}(t)$ is a small but rapidly oscillating (in terms of the scaled time) quantity, hence $\psi_{EX}(t)\approx\psi_{AT}(t)$ does not imply $\dot{\psi}_{EX}(t)\approx\dot{\psi}_{AT}(t)$. Substituting $\psi_{AT}(t)$ back into the Schrödinger equation (in terms of the scaled time) immediately leads to contradiction, no matter if the change in eigenstate is significant or not. "AT is valid" means "$\psi_{EX}(t)\approx\psi_{AT}(t)$." While "$\dot{\psi}_{EX}(t)\neq\dot{\psi}_{AT}(t)$" causes MS inconsistency. Since "$\dot{\psi}_{EX}(t)\neq\dot{\psi}_{AT}(t)$" does not imply "$\psi_{EX}(t)\neq\psi_{AT}(t)$," therefore MS inconsistency has nothing to do with the validity of AT. The factor that breaks the validity of AT is the resonance in Eq. (8). Whenever there is no such resonance, it is needless to check the validity of AT case by case just because of the MS inconsistency. All the physical information of the system at time t is contained in $\psi(t)$, and has nothing to do with $\dot{\psi}(t)$. In this context, we say the AT is physically completely correct, provided there is no resonance in Eq. (8).

IV. AN EXACTLY SOLVABLE EXAMPLE

Let us consider an exactly solvable example, the evolution of the spin wave function of an electron in a slowly rotating magnetic field $\vec{B}(t)=B_0(\vec{i}\cos 2\pi t/T+\vec{j}\sin 2\pi t/T)$. The instantaneous Hamiltonian is

$$H(t) = -\vec{\mu}\cdot\vec{B}(t) = \frac{e}{m}\vec{s}\cdot\vec{B}(t) = \frac{e\hbar}{2m}\vec{\sigma}\cdot\vec{B}(t) = \frac{e\hbar B_0}{2m}\begin{bmatrix} 0 & e^{-i2\pi t/T} \\ e^{i2\pi t/T} & 0 \end{bmatrix} = \varepsilon \begin{bmatrix} 0 & e^{-i2\pi t/T} \\ e^{i2\pi t/T} & 0 \end{bmatrix}. \tag{22}$$

Its eigenvalues are $E_{\pm}(t)=\pm\varepsilon$. And the corresponding eigenvectors are

$$u_{\pm}(t) = \frac{1}{\sqrt{2}}\begin{bmatrix} e^{-i\pi t/T} \\ \pm e^{i\pi t/T} \end{bmatrix}. \tag{23}$$

The exact general solution to the Schrodinger equation

$$i\hbar\frac{d}{dt}\psi(t) = H(t)\psi(t) \tag{24}$$

or

$$i\hbar\frac{d}{dt}\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \varepsilon\begin{bmatrix} 0 & e^{-i\pi t/T} \\ e^{i2\pi t/T} & 0 \end{bmatrix}\begin{bmatrix} x(t) \\ y(t) \end{bmatrix} \tag{25}$$

is

$$\psi(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix} = \begin{bmatrix} -A^{-1}[c_1(B+C)e^{iCt} + c_2(B-C)e^{-iCt}]e^{-iBt} \\ [c_1e^{iCt}+c_2e^{-iCt}]e^{iBt} \end{bmatrix}, \tag{26}$$

where $A=\varepsilon/\hbar$ $B=\pi/T$, $C=\sqrt{A^2+B^2}$, and c_1, c_2 are the integral constants. The specific solution determined by the initial condition

$$\psi(0) = \begin{bmatrix} x(0) \\ y(0) \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{27}$$

is

$$\psi(t) = \frac{1}{\sqrt{2}}\begin{bmatrix} \left(\cos Ct - i\frac{A-B}{C}\sin Ct\right)e^{-iBt} \\ \left(\cos Ct - i\frac{A+B}{C}\sin Ct\right)e^{iBt} \end{bmatrix}. \tag{28}$$

Let us get into the rotating axis representation.

$$\psi(t) = c_+(t)u_+(t)e^{-iAt} + c_-(t)u_-(t)e^{iAt}. \tag{29}$$

The exact Schrödinger equation becomes

$$\dot{c}_+(t) = iBe^{i2At}c_-(t), \qquad \dot{c}_-(t) = iBe^{-i2At}c_+(t). \tag{30}$$

Its general solution is

$$\begin{bmatrix} c_+(t) \\ c_-(t) \end{bmatrix} = \begin{bmatrix} e^{iAt}\left(\frac{C-A}{B}c'e^{iCt} - \frac{C+A}{B}c''e^{-iCt}\right) \\ e^{-iAt}(c'e^{iCt}+c''e^{-iCt}) \end{bmatrix}. \tag{31}$$

The specific solution determined by the initial condition

$$\begin{bmatrix} c_+(0) \\ c_-(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{32}$$

is

$$\begin{bmatrix} c_+(t) \\ c_-(t) \end{bmatrix} = \begin{bmatrix} \left(\cos Ct - i\frac{A}{C}\sin Ct\right)e^{iAt} \\ \left(i\frac{B}{C}\sin Ct\right)e^{-iAt} \end{bmatrix}. \tag{33}$$

The adiabatic approximation means neglecting the nondiagonal ($n \neq m$) terms, which contain oscillating factors, on the right-hand side of differential equations (30). The adiabatic approximate solution determind by the initial condition (32) is

$$\begin{bmatrix} c_+^A(t) \\ c_-^A(t) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \tag{34}$$

Getting to the dimensionless time $\tau = t/T$, we rewrite Eqs. (33) and (34) as

$$\begin{bmatrix} \check{c}_+(\tau) \\ \check{c}_-(\tau) \end{bmatrix} = \begin{bmatrix} \left(\cos\sqrt{(\varepsilon T/\hbar)^2+\pi^2}\,\tau - i\frac{\varepsilon T/\hbar}{\sqrt{(\varepsilon T/\hbar)^2+\pi^2}}\sin\sqrt{(\varepsilon T/\hbar)^2+\pi^2}\,\tau\right)e^{i\varepsilon T\tau/\hbar} \\ \left(i\frac{\pi}{\sqrt{(\varepsilon T/\hbar)^2+\pi^2}}\sin\sqrt{(\varepsilon T/\hbar)^2+\pi^2}\,\tau\right)e^{-i\varepsilon T\tau/\hbar} \end{bmatrix}, \tag{35}$$

$$\begin{bmatrix} \check{c}_+^A(\tau) \\ \check{c}_-^A(\tau) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \tag{36}$$

It is easy to see that

$$\begin{bmatrix} \check{c}_+(\tau) \\ \check{c}_-(\tau) \end{bmatrix} \xrightarrow[T\to\infty]{} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \check{c}_+^A(\tau) \\ \check{c}_-^A(\tau) \end{bmatrix}. \tag{37}$$

The difference between Eqs. (35) and (36) is small, but rapidly oscillates with dimensionless time τ. Therefore it is to be expected that the derivative with τ of the difference is no longer small. (Let $F \equiv \sqrt{(\varepsilon T/\hbar)^2+\pi^2}$),

$$\begin{bmatrix} \frac{d}{d\tau}\check{c}_+(\tau) \\ \frac{d}{d\tau}\check{c}_-(\tau) \end{bmatrix} = \begin{bmatrix} \left(\frac{-\pi^2}{F}\sin F\tau\right)e^{i\varepsilon T\tau/\hbar} \\ \left(\frac{\pi\varepsilon T/\hbar}{F}\sin F\tau + i\pi\cos F\tau\right)e^{-i\varepsilon T\tau/\hbar} \end{bmatrix} \xrightarrow[T\to\infty]{} \begin{bmatrix} 0 \\ i\pi e^{-i2\varepsilon T\tau/\hbar} \end{bmatrix} \neq \begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{d}{d\tau}\check{c}_+^A(\tau) \\ \frac{d}{d\tau}\check{c}_-^A(\tau) \end{bmatrix}. \tag{38}$$

V. CONCLUSION

The above discussion shows that the QAT is completely correct physically, provided there is no resonance in Eq. (8). This is ensured by $\|\psi_{EX}(t)-\psi_{AT}(t)\| \ll 1$. But it is not necessarily true that $\|\dot{\psi}_{EX}(t)-\dot{\psi}_{AT}(t)\| \ll 1$. Taking $\dot{\psi}_{AT}(t)$ for $\dot{\psi}_{EX}(t)$ will possibly lead to contradiction. MS inconsistency is only a result from invalid reasoning; we need not test the validity of the QAT case by case, provided there is no resonance in Eq. (8).

Even though we do not agree with [10], we still think it is an interesting work because it has raised an important question: In all theoretical reasoning, one has to bear in mind that approximately equal functions do not have to have approximately equal derivatives.

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