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High-order quantum adiabatic approximation and Berry's phase factor

Chang-Pu Sun
Physics Department, Northeast Normal University, Changchun, Jilin Province, People's Republic of China

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Abstract. In this paper high-order adiabatic approximate solutions of the Schrödinger equation for a quantum system with a slowly changing Hamiltonian are presented. We not only obtain Berry's phase factor and strictly prove the quantum adiabatic theorem in the first-order approximation, but also discuss an observable effect of the second adiabatic approximation.

1. Introduction

Recently it has been recognised that in quantum mechanics there exists a new topological phase factor, namely Berry's phase factor [1]. This phase factor is not only used to explain the Aharonov-Bohm effect and Aharonov-Susskind effect [2], but has also been verified in more recent experiments [3-6].

In theoretical aspects, the concept of Berry's phase has appeared in many areas of physics, e.g. anomalies in gauge field theories [7], the quantum Hall effect [8], the Born-Oppenheimer approximation [9], and so on. Berry and other authors have also discussed the classical counterparts of the quantum Berry phase [10].

Berry's phase factor was discovered by Berry in investigating the quantum adiabatic theorem [11]. Let

\[ \hat{H} = \hat{H}[R_1(t), R_2(t), \ldots, R_N(t)] = \hat{H}[R(t)] \]

be the Hamiltonian of a quantum system, which varies with the parameters \( R_1(t), R_2(t), \ldots, R_N(t) \) depending on time \( t \). When the Hamiltonian changes from a certain initial value \( \hat{H}[R(t_0)] \) at time \( t_0 \) to a certain final value \( \hat{H}[R(t_1)] \) at time \( t_1 \), if the system is initially in an eigenstate \( \phi_n[R(t_0)] \) of \( \hat{H}[R(t_0)] \), then it will, under the adiabatic limit \( T \to \infty \), pass into the eigenstate \( \phi_n[R(t_1)] \) of \( \hat{H}[R(t_1)] \) at time \( t_1 \). This result is known as the quantum adiabatic theorem. According to it, when the Hamiltonian is transported round a closed path \( c \) in parameter space \( M: \{R\} \) from \( t_0 \) to \( t_1 \), for which \( R(t_0) = R(t_1) \), the wavefunction at time \( t_1 \) is

\[ \psi(t_1) = \exp \left( \frac{1}{i\hbar} \int_{t_0}^{t_1} E_n[R(t')] dt' \right) \exp[i\nu_n(c)] \phi_n[R(t)] \]

where

\[ \exp[i\nu_n(c)] = \exp \left( -\oint_c \left( \phi_n[R] \left| \sum_{i=1}^{n} \frac{\partial}{\partial R_i} \phi_n[R] \right> \right) dR_i \right) \]
is a geometrical phase factor in addition to the familiar dynamical phase factor, which is called Berry's phase factor. Berry's phase $\nu_n(c)$ is mathematically interpreted as a holonomy of a Hermitian line bundle over the parameter manifold by Simon [1].

In this paper we will pay attention to the high-order adiabatic approximation and the manifestation of the second term in an observable quantum process.

2. Motion equation in the changing representation

The changing representation is a state space spanned by all the eigenstates $\phi_m[R](m = 1, 2, \ldots, N)$ of the Hamiltonian $\hat{H}[R]$ at time $t$ for the eigenvalues $E_m(R)$. The evolution operator $U(t, t_0)$ of this system in this representation is expressed as

$$U(t, t_0) = \sum_{m,k=0}^{N} \exp\left(\frac{i}{\hbar} \int_{t_0}^{t} E_m[R'] \, dt'\right) C_{mk}(t) |\phi_m[R(t)]\rangle\langle\phi_k[R(t_0)]|$$

where

$$C_{mk}(0) = \delta_{mk}, \quad R' \equiv R(t').$$

Substituting (4) into the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = \hat{H}[R(t)] U(t, t_0)$$

we obtain the motion equation in the changing representation:

$$\dot{C}_{mk}(t) + \left(\phi_m[R]\dot{\phi}_m[R]\right) C_{mk}(t) = -\sum_{n \neq k} C_{nk}(t) \exp\left(\frac{i}{\hbar} \int_{t_0}^{t} (E_m[R'] - E_n[R']) \, dt'\right) \langle\phi_m[R]|\phi_n[R]\rangle.$$

In order to study the influence of the changing rate of $\hat{H}[R(t)]$ on the behaviour of the solution of (6), we define

$$T = t - t_0, \quad S = t/T$$

and rewrite (6) as

$$\frac{d}{ds} b_{mk}(S) + \left(\phi_m[R]\frac{\partial}{\partial S} \phi_m[R]\right) b_{mk}(S) = -\sum_{n \neq m} b_{nk}(S) \exp\left(\frac{iT}{\hbar} \int_{S_0}^{S} (E_m[R'] - E_n[R']) \, dS'\right) \langle\phi_m[R]\frac{\partial}{\partial S} \phi_n[R]\rangle.$$

By considering $b_{mk}(t_0) = \delta_{mk}$, the Volterra integral equation of (8) is obtained as

$$b_{mk}(t) + \int_{S_0}^{S} \left(\phi_m[R]\frac{\partial}{\partial S} \phi_m[R]\right) b_{mk}(S) \, dS$$

$$= \delta_{mk} - \sum_{n \neq m} \int_{S_0}^{S} b_{nk}(S') \left(\phi_m[R']\frac{\partial}{\partial S} \phi_n[R']\right)$$

$$\times \exp\left(\frac{iT}{\hbar} \int_{0}^{S'} (E_m[R''] - E_n[R'']) \, dS''\right) \, dS'.$$
3. High-order adiabatic approximate method

For simplicity we let $S_0 = 0 = t_0$ in the following sections. Integrating

$$I_{mn} = \int_0^S b_{nk}(S') \left\langle \phi_m[R'] \right| \frac{\partial}{\partial S} \phi_n[R'] \right\rangle \exp \left( \frac{iT}{\hbar} \int_0^S (E_m[R'] - E_n[R']) \, dS' \right) \, dS'$$  \hspace{1cm} (10)

by parts, we have

$$I_{mn} = -\frac{i\hbar}{T} \exp(i\alpha_{mn}(S) T) \frac{F(S)}{E_m - E_n} + \left( \frac{-i\hbar}{T} \right)^2 \exp(i\alpha_{mn}(S) T) \frac{1}{E_m - E_n} \frac{d}{dS} \frac{1}{E_m - E_n} F(S)$$

$$+ \left( \frac{-i\hbar}{T} \right)^3 \exp(i\alpha_{mn}(S) T) \frac{1}{E_m - E_n} \frac{d}{dS} \frac{1}{E_m - E_n} \frac{d}{dS} \frac{1}{E_m - E_n} F(S) + \ldots$$  \hspace{1cm} (11)

where

$$\alpha_{mn}(S) = \hbar^{-1} \int_0^S (E_m[R'] - E_n[R']) \, dS'$$

$$F(S) = b_{mk}(S) \left\langle \phi_m[R] \right| \frac{\partial}{\partial S} \phi_n[R] \right\rangle$$  \hspace{1cm} (12)

$$E_m = E_m[R].$$

By defining an operator

$$\hat{O}_{mn} = \frac{\partial}{\partial S} \left( \frac{1}{E_m - E_n} \right) + \frac{1}{E_m - E_n} \frac{\partial}{\partial S}$$  \hspace{1cm} (13)

(11) can be written as

$$I_{mn} = \sum_{i=0}^{\infty} \left( \frac{-i\hbar}{T} \right)^{i+1} \exp(i\alpha_{mn}(S) T) (E_m - E_n)^{-1} (\hat{O}_{mn})^i \left\langle \phi_m[R] \right| \phi_n[R] \right\rangle.$$  \hspace{1cm} (14)

Then, differentiating (9), we have

$$\frac{d}{dS} b_{mk}(S) + \left\langle \phi_m[R] \right| \frac{\partial}{\partial S} \phi_n[R] \right\rangle b_{mk}(S)$$

$$= - \sum_{n \neq m} \sum_{i=0}^{\infty} \left( \frac{-i\hbar}{T} \right)^{i+1} \frac{\partial}{\partial S}$$

$$\times \left( \frac{\exp(iT\alpha_{mn}(S))}{E_m - E_n} (\hat{O}_{mn})^i \left\langle \phi_m[R] \right| \frac{\partial}{\partial S} \phi_n[R] \right\rangle b_{nk}(S) \right).$$  \hspace{1cm} (15)

If $1/T$ is sufficiently small, it is reasonable to assume that $b_{mk}(S)$ can be expanded into a rapidly converging power series in $1/T$, i.e.

$$b_{mk}(S) = \sum_n \left( \frac{-i\hbar}{T} \right)^n b_{mk}^{[n]}(S).$$  \hspace{1cm} (16)

We substitute the expression (16) into both sides of (15) and obtain an equality between two power series in $1/T$. In order that this equality be satisfied, the coefficients of each power of $1/T$ must be separately equal, giving

$$\frac{d}{ds} b_{mk}^{[0]}(S) + \left\langle \phi_m[R] \right| \frac{\partial}{\partial S} \phi_m[R] \right\rangle b_{mk}^{[0]}(S) = 0$$
\[
\frac{d}{dS}b_{mk}^{(1)} + \left( \phi_m[R] \left| \frac{\partial}{\partial S} \phi_m[R] \right| \right) b_{mk}^{(1)}(S) \\
= f_{(S)}^{(1)} = - \sum_{h=0}^{(i-1)} \sum_n \frac{\partial}{\partial S} \left( \frac{\exp(iT\alpha_{mn}(S))}{E_m - E_n} (\hat{O}_{mn})^h b_{mk}^{(1-h-1)}(S) \right) \\
\times \left( \phi_m[R] \left| \frac{\partial}{\partial S} \phi_m[R] \right| \hbar^{h+1} \right).
\]

Considering the initial conditions

\[
b_{mk}^{(1)}(0) = \delta_{mk} \quad b_{mk}^{(1)} = 0 \quad i = 1, 2, 3, \ldots
\]

we successively solve equation (17), obtaining

\[
b_{mk}^{(1)}(S) = \delta_{mk} \exp \left( - \int_0^S \left( \phi_m[R'] \left| \frac{\partial}{\partial S} \phi_m[R'] \right| \right) dS' \right) \\
b_{mk}^{(1)}(S) = \exp \left( - \int_0^S \left( \phi_m[R'] \left| \frac{\partial}{\partial S} \phi_m[R'] \right| \right) dS' \right) \\
\times \int_0^S f_{(S)}^{(1)} \exp \left( \int_0^S \left( \phi_m[R'] \left| \frac{\partial}{\partial S} \phi_m[R'] \right| \right) dS'' \right) dS'.
\]

4. Manifestation of first- and second-order approximate solutions

According to (4) and (18), under the adiabatic limit \( T \to \infty \), the first-order evolution operator is

\[
U_{(t,t_0)}^{(1)} = \sum_{m=0}^{N} \exp \left( - \int_0^t \left( \phi_m[R'] \left| \frac{\partial}{\partial t} \phi_m[R'] \right| \right) dt' \right) \\
\times \exp \left( \frac{1}{i\hbar} \int_0^t E_m[R'] dt' \right) |\phi_m[R(t_0)]\rangle \langle \phi_m[R(t_0)]| 
\]

which just gives the known quantum adiabatic theorem and the results obtained by Berry.

When the adiabatic condition does not hold, we consider the second-order approximation in an experiment of a spinning particle in a magnetic field, which has been considered under adiabatic conditions by Berry. A polarised beam of spin-\( \frac{1}{2} \) particles along a magnetic field splits into two beams, one of which passes through a constant magnetic field \( B_0\mathbf{e}_z \), while the other passes through a varying magnetic field

\[
\mathbf{B}(t) = B_0(\sin \theta \cos \beta(t)\mathbf{e}_x + \sin \theta \sin \beta(t)\mathbf{e}_y + \cos \theta \mathbf{e}_z)
\]

where \( \dot{\beta}(t) \) need not be uniform along a closed path in the parameter space \( M: \{B_x, B_y, B_z\} \) and \( \beta(t) \) satisfies \( \beta(0) = 0, \beta(T) = 2\pi \). The Hamiltonian is

\[
\hat{H}[\mathbf{B}(t)] = g\mathbf{S} \cdot \mathbf{B} = \hbar\omega_0 \begin{bmatrix} \cos \theta & \sin \theta \exp(-i\beta(t)) \\ -\sin \theta \exp(i\beta(t)) & -\cos \theta \end{bmatrix}
\]

where \( \omega_0 = \frac{1}{2}gB_0 \) is the dynamical frequency.
From (4) and (7), we see that the wavefunction at time $t_r$ is
\[
|\psi(T)\rangle = [\exp(-\sin^2 \frac{1}{2} \theta 2 \pi i) + 1] \exp(-i\omega t) |\phi_+[B(0)]\rangle
+ \frac{f(T)}{T} \exp(-i\pi \cos^2 \frac{1}{2} \theta) |\phi_-[B(0)]\rangle
\] (22)
when the particle is initially in an eigenstate $|\phi_+[B(0)]\rangle$ of $\hat{H}[B(0)]$ with eigenvalue $\hbar \omega_0$, where
\[
f(t) = \frac{i \hbar \sin \theta}{4\omega_0} \int_0^t \frac{\partial}{\partial t'} [B(t') \exp(2i\omega_0 t' - i\frac{1}{2} \sin^2 \frac{1}{2} \theta \beta(t')) \exp(i\frac{1}{2} \cos^2 \frac{1}{2} \theta \beta(t')) \, dt'.
\] (23)
If we adjust the path length of the beams such that the dynamical phases for both beams are the same when beams are combined in a detector at time $T$, the predicted intensity contrast is
\[
I_{(\phi)} = I_0 \cos^2 \left[ \frac{1}{2} \pi (1 - \cos \theta) \right] + f^2(T)/T^2
\] (24)
which leads to an extra term $f^2/T^2$ in Berry's result
\[
I'_{(\phi)} = I_0 \cos^2 \left[ \frac{1}{2} \pi (1 - \cos \theta) \right].
\] (25)
It would be interesting to see the above prediction experimentally verified.

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Note added. After this paper was written, from a paper by Aharonov and Anndan [12] and the referee's report on my paper, I discovered that the experiment I propose, bridging the gap between small and large $T$, has now been carried out by D Suter, G Chingas, R A Hariss and A Pine.

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