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1988 J. Phys. A: Math. Gen. 21 1595

(http://iopscience.iop.org/0305-4470/21/7/023)

J. Phys. A: Math. Gen. 21 (1988) 1595-1599. Printed in the UK

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

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Received 2 June 1987, in final form 22 September 1987

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 aproximation [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

$$\hat{H} = \hat{H}[R_1(t), R_2(t), \ldots, R_N(t)] \equiv \hat{H}[R(t)] \tag{1}$$

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

$$|\psi(t_1)\rangle = \exp\left(\frac{1}{i\hbar}\int_{t_0}^{t_1} E_n[R(t')]\,dt'\right)\exp[i\nu_n(c)]|\phi_n[R(t)]\rangle \tag{2}$$

where

$$\exp[i\nu_n(c)] = \exp\left(-\oint_c \left\langle \phi_n[R] \middle| \sum_{i=1}^{n} \frac{\partial}{\partial R_i}\phi_n[R]\right\rangle dR_i\right) \tag{3}$$

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 paramter 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

$$U(t, t_0)=\sum_{m,k=0}^{N}\exp\left(\frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}E_m[R']\,\mathrm{d}t'\right)C_{mk}(t)|\phi_m[R(t)]\rangle\langle\phi_k[R(t_0)]| \tag{4}$$

where

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

Substituting (4) into the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}U(t, t_0)=\hat{H}[R(t)]U(t, t_0) \tag{5}$$

we obtain the motion equation in the changing representation:

$$\dot{C}_{mk}(t)+\langle\phi_m[R]|\dot{\phi}_m[R]\rangle C_{mk}(t)$$
$$=-\sum_{n\neq k}C_{nk}(t)\exp\left(\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}(E_m[R']-E_n[R'])\mathrm{d}t'\right)\langle\phi_m[R]|\dot{\phi}_n[R]\rangle. \tag{6}$$

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

$$\begin{aligned} &T=t_1-t_0 \qquad && S=t/T\\ &b_{mk}(S)=C_{mk}(TS) \qquad && R=R(TS)\end{aligned} \tag{7}$$

and rewrite (6) as

$$\frac{\mathrm{d}}{\mathrm{d}s}b_{mk}(S)+\left\langle\phi_m[R]\left|\frac{\partial}{\partial s}\phi_m[R]\right.\right\rangle b_{mk}(S)$$
$$=-\sum_{n\neq m}b_{nk}(S)\exp\left(\frac{\mathrm{i}T}{\hbar}\int_{S_0}^{S}(E_m[R']-E_n[R']\,\mathrm{d}S'\right)\left\langle\phi_m[R]\left|\frac{\partial}{\partial S}\phi_n[R]\right.\right\rangle. \tag{8}$$

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

$$b_{mk}(t)+\int_{S_0}^{S}\left\langle\phi_m[R]\left|\frac{\partial}{\partial S}\phi_m[R]\right.\right\rangle b_{mk}(S)\,\mathrm{d}S$$
$$=\delta_{mk}-\sum_{n\neq m}\int_{S_0}^{S}b_{nk}(S')\left\langle\phi_m[R']\left|\frac{\partial}{\partial S}\phi_n[R']\right.\right\rangle$$
$$\times\exp\left(\frac{\mathrm{i}T}{\hbar}\int_{0}^{S'}(E_m[R'']-E_n[R''])\,\mathrm{d}S''\right)\mathrm{d}S'. \tag{9}$$

3. High-order adiabatic approximate method

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

$$I_{mn}=\int_0^S b_{nk}(S')\left\langle \phi_m[R']\left|\frac{\partial}{\partial S}\phi_n[R']\right.\right\rangle \exp\left(\frac{\mathrm{i}T}{\hbar}\int_0^{S'}(E_m[R'']-E_n[R''])\,\mathrm{d}S''\right)\mathrm{d}S' \quad (10)$$

by parts, we have

$$I_{mn}=\frac{-\mathrm{i}\hbar}{T}\exp(\mathrm{i}\alpha_{mn}(S)T)\frac{F(S)}{E_m-E_n}+\left(\frac{-\mathrm{i}\hbar}{T}\right)^2\exp(\mathrm{i}\alpha_{mn}(S)T)\frac{1}{E_m-E_n}\frac{\mathrm{d}}{\mathrm{d}s}\frac{1}{E_m-E_n}F(S)$$
$$+\left(\frac{-\mathrm{i}\hbar}{T}\right)^3\exp(\mathrm{i}\alpha_{mn}(S)T)\frac{I}{E_m-E_n}\frac{\mathrm{d}}{\mathrm{d}S}\frac{1}{E_m-E_n}\frac{\mathrm{d}}{\mathrm{d}s}\frac{1}{E_m-E_n}F(S)+\dots \quad (11)$$

where

$$\alpha_{mn}(S)=\hbar^{-1}\int_0^S(E_m[R']-E_n[R'])\mathrm{d}S'$$
$$F(S)=b_{mk}(S)\left\langle \phi_m[R]\left|\frac{\partial}{\partial S}\phi_n[R]\right.\right\rangle \quad (12)$$
$$E_m=E_m[R].$$

By defining an operator

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

(11) can be written as

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

Then, differentiating (9), we have

$$\frac{\mathrm{d}}{\mathrm{d}S}b_{mk}(S)+\left\langle \phi_m[R]\left|\frac{\partial}{\partial S}\phi_m[R]\right.\right\rangle b_{mk}(S)$$
$$=-\sum_{n\neq m}\sum_{l=0}^{\infty}\left(\frac{-\mathrm{i}\hbar}{T}\right)^{l+1}\frac{\partial}{\partial s}$$
$$\times\left(\frac{\exp(\mathrm{i}T\alpha_{mn}(S))}{E_m-E_n}(\hat{O}_{mn})^l\left\langle \phi_m[R]\left|\frac{\partial}{\partial S}\phi_n[R]\right.\right\rangle b_{nk}(S)\right). \quad (15)$$

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.

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

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

$$\frac{\mathrm{d}}{\mathrm{d}s}b_{mk}^{[0]}(S)+\left\langle \phi_m[R]\left|\frac{\partial}{\partial S}\phi_m[R]\right.\right\rangle b_{mk}^{[0]}(S)=0$$

$$\frac{\mathrm{d}}{\mathrm{d}S} b_{mk}^{[l]} + \left\langle \phi_m[R] \left| \frac{\partial}{\partial S} \phi_m[R] \right\rangle b_{mk}^{[l]}(S) \right.$$
$$= f_{(S)}^{[l]} = -\sum_{h=0}^{l-1} \sum_{n \neq m} \frac{\partial}{\partial S} \left(\frac{\exp(\mathrm{i} T \alpha_{mn}(S))}{E_m - E_n} (\hat{O}_{mn})^h b_{mk}^{(l-h-1)}(S) \right.$$
$$\left. \times \left\langle \phi_m[R] \left| \frac{\partial}{\partial S} \phi_n[R] \right\rangle \hbar^{h+1} \right). \right. \tag{17}$$

Considering the initial conditions

$$b_{mk}^{[0]} = \delta_{mk} \qquad b_{mk}^{[i]} = 0 \qquad i = 1, 2, 3, \ldots$$

we successively solve equation (17), obtaining

$$b_{mk}^{[0]}(S) = \delta_{mk} \exp\left(- \int_0^S \left\langle \phi_m[R'] \left| \frac{\partial}{\partial S} \phi_m[R'] \right\rangle \mathrm{d}S' \right) \right.$$
$$b_{mk}^{[l]}(S) = \exp\left(- \int_0^S \left\langle \phi_m[R'] \left| \frac{\partial}{\partial S} \phi_m[R'] \right\rangle \mathrm{d}S' \right) \right.$$
$$\times \int_0^S f_{(S')}^{[l]} \exp\left(\int_0^{S'} \left\langle \phi_m[R''] \left| \frac{\partial}{\partial S'} \phi_m[R''] \right\rangle \mathrm{d}S'' \right) \mathrm{d}S'. \right. \tag{18}$$

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

$$U_{(t,t_0)}^{[0]} = \sum_{m=0}^{N} \exp\left(- \int_0^t \left\langle \phi_m[R'] \left| \frac{\partial}{\partial t} \phi_m[R'] \right\rangle \mathrm{d}t' \right. \right.$$
$$\left. \times \exp\left(\frac{1}{\mathrm{i}\hbar} \int_0^t E_m[R'] \, \mathrm{d}t' \right) |\phi_m[R(t)]\rangle\langle\phi_m[R(t_0)]| \right. \tag{19}$$

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 $B_0 \boldsymbol{e}_z$, while the other passes through a varying magnetic field

$$\boldsymbol{B}(t) = B_0(\sin\theta \cos\beta(t) \boldsymbol{e}_x + \sin\theta \sin\beta(t) \boldsymbol{e}_y + \cos\theta \boldsymbol{e}_z) \tag{20}$$

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

$$\hat{H}[\boldsymbol{B}(t)] = g\boldsymbol{S} \cdot \boldsymbol{B} = \hbar\omega_0 \begin{bmatrix} \cos\theta & \sin\theta \exp(-\mathrm{i}\beta(t)) \\ \sin\theta \exp(\mathrm{i}\beta(t)) & -\cos\theta \end{bmatrix} \tag{21}$$

where $\omega_0 = \frac{1}{2} g B_0$ is the dynamical frequency.

From (4) and (7), we see that the wavefunction at time t_1 is

$$|\psi(T)\rangle = [\exp(-\sin^2 \tfrac{1}{2}\theta 2\pi \mathrm{i}) + 1]\exp(-\mathrm{i}\omega t)|\phi_+[\boldsymbol{B}(0)]\rangle + \frac{f(T)}{T}\exp(-\mathrm{i}\pi\cos^2 \tfrac{1}{2}\theta)|\phi_-[B(0)]\rangle \tag{22}$$

when the particle is initially in an eigenstate $|\phi_+[\boldsymbol{B}(0)]$ of $\hat{H}[\boldsymbol{B}(0)]$ with eigenvalue $\hbar\omega_0$, where

$$f(t) = \frac{\mathrm{i}\hbar \sin\theta}{4\omega_0}\int_0^t \frac{\partial}{\partial t'}[B(t')\exp(2\mathrm{i}\omega_0 t' - \mathrm{i}\tfrac{1}{2}\sin^2 \tfrac{1}{2}\theta\beta(t'))]\exp(\mathrm{i}\tfrac{1}{2}\cos^2 \tfrac{1}{2}\theta\beta(t'))\,\mathrm{d}t'. \tag{23}$$

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

$$I_{(\theta)} = I_0 \cos^2[\tfrac{1}{2}\pi(1-\cos\theta)] + f^2(T)/T^2 \tag{24}$$

which leads to an extra term f^2/T^2 in Berry's result

$$I'_{(\theta)} = I_0 \cos^2[\tfrac{1}{2}\pi(1-\cos\theta)]. \tag{25}$$

It would be interesting to see the above prediction experimentally verified.

Acknowledgment

The author is grateful to Professors Zhao-Yan Wu and De-Huai Luan for their interest in the problem and for useful discussions.

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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