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J.Y. Zeng

Y.A. Lei

P.O.Box 2735, Beijing 100080, The People's Republic of China

Telefax : (86)-1-2562587 Telephone : 2568348

Telex : 22040 BAOAS CN Cable : 6158

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J. Y. Zeng[a,b,c] and Y. A. Lei[b]

[a]China Center of Advanced Science and Technology (World Laboratory),

Center of Theoretical Physics, P. O. Box 8730, Beijing 100080

[b]Department of Physics, Peking University, Beijing 100871

[c]Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080

Abstract

It is shown that the Berry phase β appears for any nonstationary state of a quantum system. For time-independent H there may exist stationary state, for which β vanishes. For time-dependent H there exists no exactly stationary state (even in adiabatic case) and the Berry phase always appears. The Berry phase by exact calculation is different from the adiabatic one.

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The concept of Berry adiabatic phase [1] has been a subject of considerable interest during the last ten years in different areas of modern physics [2–6]. Simon [7] gave a geometric interpretation of Berry phase. Aharonov and Anandan [8] generalized Berry's results by giving up the assumption of adiabaticity. The key step in this work is their identification of the integral of the expectation value of the Hamiltonian as the "dynamical" phase. For any cyclic evolution of a quantum system once this dynamical phase is removed, the evolution of the phase recovers to the Berry phase. Samuel and Bhandari [9] made a further generalization that the evolution of the system need be neither unitary (norm conserving) nor cyclic. However, it seems that most of these generalization are from mathematical points of view with emphasis on the geometric aspect of Berry phase. In this letter, it will be shown that both the Berry phase and "dynamical" phase observed in nature are of dynamical origin in the final analysis, and the Berry phase is intimately connected with the nonstationarity of a quantum state.

Firstly let us consider a quantum system with time-independent Hamiltonian, which may be considered as a limiting case of adiabatic variation. In this case the energy of the system is conserved and there may exist exactly stationary states. Let $|\psi_m\rangle$ be an eigenstate of a complete set of observables including H,

$$H|\psi_m\rangle = E_m|\psi_m\rangle, \quad \langle\psi_m|\psi_n\rangle = \delta_{mn}. \tag{1}$$

Assuming the initial state of the system $|\psi(0)\rangle = |\psi_n\rangle$, it is easily to verify that

$$|\psi(t)\rangle = e^{-iE_nt/\hbar}|\psi_n\rangle = e^{-iE_nt/\hbar}|\psi(0)\rangle \tag{2}$$

satisfies the Schrödinger dynamical equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{3}$$

and $-E_nt/\hbar$ in (2) is usually called the dynamical phase. The general solution of the Schrödinger equation can be expressed as

$$|\psi(t)\rangle = \sum_m a_m e^{-iE_mt/\hbar}|\psi_m\rangle, \tag{4}$$

where a_m is time-independent and determined by the initial state $a_m = \langle\psi_m|\psi(0)\rangle$.

Now we consider the system with time-dependent Hamiltonian $H(t)$, e.g. the Hamiltonian $H(\mathbf{R}(t))$ involving some time-dependent parameters $\mathbf{R}(t)$. In this case the energy of the system is not conserved and *there exists no exactly stationary state*. However, we may consider the instaneous eigenstate $|\psi_m(\mathbf{R}(t))\rangle$

$$H(\mathbf{R}(t))|\psi_m(\mathbf{R}(t))\rangle = E_m(\mathbf{R}(t))|\psi_m(\mathbf{R}(t))\rangle, \qquad (5)$$
$$\langle\psi_m(\mathbf{R}(t))|\psi_n(\mathbf{R}(t))\rangle = \delta_{mn}.$$

Let us assume

$$|\psi(0)\rangle = |\psi_n(\mathbf{R}(t))\rangle, \qquad (6)$$

it seems naive that the state of the system at time t may be expressed as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt' E_n(\mathbf{R}(t'))}|\psi_n(\mathbf{R}(t))\rangle. \qquad (7)$$

However, *this is totally wrong*, because the $|\psi(t)\rangle$ in (7) does *not* satisfy the Schrödinger equation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle &= H|\psi(t)\rangle + e^{-\frac{i}{\hbar}\int_0^t dt' E_n(\mathbf{R}(t'))} i\hbar\frac{\partial}{\partial t}|\psi_n(\mathbf{R}(t))\rangle \\ &\neq H|\psi(t)\rangle. \end{aligned} \qquad (8)$$

The reason is that in (7) *only* the time-dependence of the instaneous eigenenergy is considered. In general, the state of the system at time t can be formally expressed as

$$|\psi(t)\rangle = \sum_m a_m(t) e^{-\frac{i}{\hbar}\int_0^t dt' E_m(\mathbf{R}(t'))}|\psi_m(\mathbf{R}(t))\rangle, \qquad (9)$$

where

$$a_m(t) = \langle\psi_m(\mathbf{R}(t))|\psi(t)\rangle e^{\frac{i}{\hbar}\int_0^t dt' E_m(\mathbf{R}(t'))} \qquad (10)$$

is time-dependent. For the initial condition (6), $a_m(0) = \delta_{mn}$, but this does not imply $a_m(t) \propto \delta_{mn}$, which holds only in the adiabatic approximation [1]. Even in the adiabatic approximation, $a_m(t) \neq \delta_{mn}$, because such a solution does not satisfy the Schrödinger

equation, as shown in (8). To satisfy the Schrödinger dynamical equation, the correct adiabatic solution (norm conserving) should be expressed as

$$|\psi(t)\rangle = a_n(t) e^{-\frac{i}{\hbar}\int_0^t dt' E_n(\mathbf{R}(t'))}|\psi_n(\mathbf{R}(t))\rangle, \qquad (11)$$
$$|a_n(t)| = 1.$$

Let

$$a_n(t) = e^{i\beta_n(t)} \quad (\beta_n \text{ real}), \qquad (12)$$

substituting (11) and (12) into the Schrödinger equation and integrating, we get

$$\beta_n(t) = i\int_0^t dt' \left\langle \psi_n(\mathbf{R}(t')) \middle| \frac{\partial}{\partial t'} \middle| \psi_n(\mathbf{R}(t')) \right\rangle, \qquad (13)$$

which is just the Berry adiabatic phase and may be transformed into an integral in the parameter space [1]. Particularly, after a cycle $t = \tau$, $\mathbf{R}(t)$ changes by moving along a circuit C in parameter space returning to their original values $\mathbf{R}(\tau) = \mathbf{R}(0)$, the Berry phase acquired on such a circuit $\beta(\tau) - \beta(0) = \beta(C)$ is independent of deformations of C, thus is often called a geometric or topological phase. However, it is clearly seen that the *appearance of Berry phase in (11) and (12) is the result of the requirement that the evolution of a quantum system must follow the Schrödinger dynamical equation.*

In general, if the evolution with time of $|\phi(t)\rangle$ does not satisfy the Schrödinger equation, we may perform a (norm conserving) time-dependent phase transformation

$$|\psi(t)\rangle = e^{if(t)}|\phi(t)\rangle \qquad (14)$$

and require $|\psi(t)\rangle$ satisfying the Schrödinger equation, then we find

$$f(t) = \int_0^t dt' \left\langle \phi(t') \middle| i\frac{\partial}{\partial t'} - \frac{H(t')}{\hbar} \middle| \phi(t') \right\rangle, \qquad (15)$$

which is reminiscent of the Lewis phase for treating the time-dependent invariant [10]. Particularly, let $|\phi(t)\rangle$ be an instaneous eigenstate $|\psi_n(\mathbf{R}(t))\rangle$, the second term on the right-hand side of (15) turns out to be $-\int_0^t dt' E_n(\mathbf{R}(t'))/\hbar$ ("dynamical" phase) and the first term becomes $\int_0^t dt' \langle\psi_n(\mathbf{R}(t'))|i\frac{\partial}{\partial t'}|\psi_n(\mathbf{R}(t'))\rangle$ (Berry adiabatic phase).

In ref. [8], Aharonov and Anandan considered the cyclic evolution of quantum systems, for which no adiabatic variation was made. They assumed that $|\psi(t)\rangle$ satisfies the Schrödinger equation and after a cyclic evolution $t[0,\tau]$,

$$|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle, \tag{16}$$

ϕ is the total phase change. They performed a time-dependent phase transformation

$$|\psi(t)\rangle = e^{if(t)}|\tilde{\psi}(t)\rangle, \tag{17}$$

requiring $f(\tau) - f(0) = \phi$, i.e. no phase change occurs for $|\tilde{\psi}(t)\rangle$ during a cyclic evolution, $|\tilde{\psi}(\tau)\rangle = |\tilde{\psi}(0)\rangle$; then they found

$$\phi = \int_0^\tau dt \left\langle \psi(t) \left| \frac{-H(t)}{\hbar} \right| \psi(t) \right\rangle + \int_0^\tau dt \left\langle \tilde{\psi}(t) \left| i\frac{\partial}{\partial t} \right| \tilde{\psi}(t) \right\rangle \tag{18}$$

and the first term was identified as the "dynamical" phase

$$\alpha(\tau) - \alpha(0) = \int_0^\tau dt \left\langle \psi(t) \left| \frac{-H(t)}{\hbar} \right| \psi(t) \right\rangle. \tag{19}$$

and the second term was called the Berry phase

$$\beta(\tau) - \beta(0) = \int_0^\tau dt \left\langle \tilde{\psi}(t) \left| i\frac{\partial}{\partial t} \right| \tilde{\psi}(t) \right\rangle = \phi - (\alpha(\tau) - \alpha(0)). \tag{20}$$

To clarify the physical meaning of "dynamical" and Berry phases thus defined, firstly we may consider some examples, for which both the adiabatic and exact solutions have been found, and then give some general discussions.

Example 1, magnetic resonance. Consider a system with magnetic moment μ in the time-dependent magnetic field

$$\mathbf{B}(t) = (B_1 \cos 2\omega_0 t, B_1 \sin 2\omega_0 t, B_0), \quad \omega_0 = \mu B_0/\hbar. \tag{21}$$

In Pauli representation

$$H(t) = \begin{pmatrix} -\mu B_0 & -\mu B_1 e^{2i\omega_0 t} \\ -\mu B_1 e^{-2i\omega_0 t} & \mu B_0 \end{pmatrix}, \tag{22}$$

$$H(\tau) = H(0), \quad \tau = \pi/\omega_0.$$

The instaneous eigenenergies and orthonormal eigenstates are

$$\begin{aligned} E_\pm &= \pm\mu\sqrt{B_1^2 + B_0^2}, \\ |\psi_-(t)\rangle &= \begin{pmatrix} \cos\theta/2 \\ -\sin\theta/2 e^{-2i\omega_0 t} \end{pmatrix}, \quad |\psi_+(t)\rangle = \begin{pmatrix} \sin\theta/2 \\ \cos\theta/2 e^{-2i\omega_0 t} \end{pmatrix}, \\ \psi_\pm(\tau) &= \psi_\pm(0), \\ \tan\theta &= B_1/B_0 = \omega_1/\omega_0, \ \omega_1 = \mu B_1/\hbar. \end{aligned} \tag{23}$$

Assuming the initial state $|\psi(0)\rangle = |\psi_-\rangle$ and substituting the adiabatic solution $|\psi(t)\rangle_{adi} = a_-(t)e^{-\frac{i}{\hbar}\int_0^t dt' E_-(t')}|\psi_-(t)\rangle$ into the Schrödinger equation and integrating, one finds that $a_-(t) = e^{2i\omega_0 t \sin^2\theta/2}$, i.e., the Berry adiabatic phase is $\beta(t) = 2\omega_0 t \sin^2\theta/2$, and after a cyclic evolution,

$$\beta(\tau) - \beta(0) = (1 - \cos\theta)\pi = \Omega(C)/2, \tag{24}$$

$\Omega(C) = 2\pi(1 - \cos\theta)$ being the solid angle subtended in a space by the magnetic field.

The exact solution of the Schrödinger equation for the Hamiltonian (22) can be easily found. Assuming

$$|\psi(0)\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \tag{25}$$

the result is

$$|\psi(t)\rangle = \begin{pmatrix} (a\cos\omega_1 t + ib\sin\omega_1 t)e^{i\omega_0 t} \\ (ia\sin\omega_1 t + b\cos\omega_1 t)e^{-i\omega_0 t} \end{pmatrix}. \tag{26}$$

Particularly, for the initial condition $|\psi(0)\rangle = |\psi_-(0)\rangle$,

$$\begin{aligned} |\psi(t)\rangle &= \begin{pmatrix} (\cos\theta/2\cos\omega_1 t - i\sin\theta/2\sin\omega_1 t)e^{i\omega_0 t} \\ (i\cos\theta/2\sin\omega_1 t - \sin\theta/2\cos\omega_1 t)e^{-i\omega_0 t} \end{pmatrix} \\ &= (\cos\omega_1 t - i\sin\theta\sin\omega_1 t)e^{i\omega_0 t}|\psi_-(t)\rangle + i\cos\theta\sin\omega_1 t e^{i\omega_0 t}|\psi_+(t)\rangle. \end{aligned} \tag{27}$$

Therefore, the probabilities of the system at time t found in the instaneous eigenstates $|\psi_\pm(t)\rangle$ are (see Fig. 1(a))

$$P_+(t) = \cos^2\theta\sin^2\omega_1 t, \quad P_-(t) = \cos^2\omega_1 t + \sin^2\theta\sin^2\omega_1 t. \tag{28}$$

When $\omega_1 t = n\pi$ $(n = 0, 1, 2, \cdots)$, $P_+(t) = 0$, and $|\psi(t)\rangle \propto |\psi_-(t)\rangle$. However, only for

$$\omega_1/\omega_0 = B_1/B_0 = \tan\theta = n, \quad n = 0, 1, 2, \cdots, \tag{29}$$

$|\psi(\tau)\rangle$ returns to the initial state apart from a phase change,

$$|\psi(\tau)\rangle = e^{i(n+1)\pi}|\psi(0)\rangle, \tag{30}$$

i.e., the total phase change $\phi = (n+1)\pi$. Using (27), (19) and (20), the "dynamical" and Berry phases are

$$\alpha(\tau) - \alpha(0) = \frac{\pi}{\cos\theta}, \qquad \beta(\tau) - \beta(0) = \left(1 - \frac{1 - \sin\theta}{\cos\theta}\right)\pi, \tag{31}$$

which are different from the adiabatic ones (eq. (24)). Only when $(1 - \sin\theta)/\cos\theta = \cos\theta$, i.e., $\sin\theta = 0$ ($B_1 = 0$, H time-independent) and $\sin\theta = 1$ ($\theta = \pi/2$, i.e., $\tan\theta = n \gg 1$, adiabatic limit), the exact Berry phase recovers to the adiabatic one (see Fig. 1(b)).

Example 2, harmonic oscillator. The Hamiltonian $H = p^2/2m + \frac{1}{2}m\omega^2 x^2$ is time-independent, and its eigenstate is denoted by $|\psi_n\rangle$ with eigenvalue $E_n = (n + \frac{1}{2})\hbar\omega$, $n = 0, 1, 2, \cdots$. Assume the initial state

$$|\psi(0)\rangle = \cos\theta/2|\psi_0\rangle + \sin\theta/2|\psi_1\rangle, \tag{32}$$

which is a pure stationary state for $\theta = 0$ ($|\psi(0)\rangle = |\psi_0\rangle$) and $\theta = \pi$ ($|\psi(0)\rangle = |\psi_1\rangle$), but for $\theta = \pi/2$, it is completely nonstationary (having equal probability to be in $|\psi_0\rangle$ and $|\psi_0\rangle$). The state at time t is

$$|\psi(t)\rangle = \cos\theta/2e^{-i\omega t/2}|\psi_0\rangle + \sin\theta/2e^{-i3\omega t/2}|\psi_1\rangle. \tag{33}$$

After a cyclic evolution (period $\tau = 2\pi/\omega$), $|\psi(\tau)\rangle = -|\psi(0)\rangle$, so the total phase change $\phi = \pi$. From (19), (20), and (33), the "dynamical" and Berry phases are

$$\alpha(\tau) - \alpha(0) = -\pi(1 + 2\sin^2\theta/2), \quad \beta(\tau) - \beta(0) = \pi(1 - \cos\theta). \tag{34}$$

Particularly, for $\theta = 0$ or π (stationary state), $\alpha(\tau) - \alpha(0) = \pi$, $\beta(\tau) - \beta(0) = 0$, and for $\theta = \pi/2$ (completely nonstationary), $\alpha(\tau) - \alpha(0) = 0$, $\beta(\tau) - \beta(0) = \pi$. It is clearly seen that the "dynamical" phase characterizes the stationarity of a quantum system and would be better to be referred to as ***stationary phase***, and the Berry phase describes the nonstationarity and would be referred to as ***nonstationary phase***.

Another interesting case is the initial state being the coherent state

$$\langle x|\psi(0)\rangle = \psi_0(x - x_0) = e^{-\delta^2/2}\sum_{n=0}^{\infty}\frac{\delta^n}{\sqrt{n!}}\psi_n(x), \qquad \delta = x_0/l\sqrt{2}, \quad l = \sqrt{\hbar/m\omega}. \tag{35}$$

It is easily found that after a cyclic evolution ($\tau = 2\pi/\omega$) $\phi = \pi$, $\alpha(\tau) - \alpha(0) = -2\pi(\delta^2 + 1/2)$, $\beta(\tau) - \beta(0) = 2\pi\delta^2$. Therefore, for $\delta = 0$ ($|\psi(0)\rangle = |\psi_0\rangle$, pure stationary state), $\beta(\tau) - \beta(0) = 0$, and for $\delta^2 = 1/2$ ($x_0 = l$, characteristic length of harmonic oscillator) the Berry phase achieves its maximum value $\beta(\tau) - \beta(0) = \pi$, which implies that in this case the coherent state is completely non-stationary.

The discussion given above may be extended to any two-state system. The two stationary states with $E = \pm|E|$ are labelled by $|\psi_\pm\rangle$. Assume the initial state

$$|\psi(0)\rangle = \cos\theta/2|\psi_-\rangle + \sin\theta/2|\psi_+\rangle, \tag{36}$$

which is stationary for $\theta = 0$ or π, and completely nonstationary for $\theta = \pi/2$. The state at time t is

$$|\psi(t)\rangle = \cos\theta/2e^{i|E|t/\hbar}|\psi_-\rangle + \sin\theta/2e^{-i|E|t/\hbar}|\psi_+\rangle. \tag{37}$$

After a cyclic evolution ($\tau = \pi\hbar/|E|$), $|\psi(\tau)\rangle = -|\psi(0)\rangle$, the total phase change $\phi = -\pi$. From (19), (20) and (37), $\alpha(\tau) - \alpha(0) = -\pi\cos\theta$, $\beta(\tau) - \beta(0) = -\pi(1 - \cos\theta)$. Therefore, $\beta(\tau) - \beta(0) = 0$ for stationary state ($\theta = 0$, or π) and achieves its maximum value $\beta(\tau) - \beta(0) = \pi$ for completely nonstationary state ($\theta = \pi/2$).

In fact, one of the fundamental assumptions of quantum mechanics is that the state of a quantum system in the nature evolves with time according to the Schrödinger dynamical equation, and the state at time t can be formally expressed as

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt' H(t')}|\psi(0)\rangle. \tag{38}$$

Assuming after a cyclic evolution t $[0,\tau]$, $|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle$, the total phase change can be formally expressed as

$$e^{i\phi} = \langle\psi(0)|e^{-\frac{i}{\hbar}\int_0^\tau dt H(t)}|\psi(0)\rangle, \tag{39}$$

which is obviously of dynamical origin. According to Aharonov and Anandan, ϕ is divided into two parts, $\phi = [\alpha(\tau) - \alpha(0)] + [\beta(\tau) - \beta(0)]$ (see (19) and (20)). From the discussions above, it is seen that only the stationary part of the total phase change is involved in α, and the remaining part β characterizes the nonstationarity of a quantum state. For time-independent H, there exists exactly stationary state. If the initial state is stationary, $|\psi(0)\rangle = |\psi_n\rangle$, we have $\phi = -E_n\tau/\hbar = \alpha(\tau) - \alpha(0)$, and $[\beta(\tau) - \beta(0)] = 0$. But if the initial state is nonstationary,

$$|\psi(0)\rangle = \sum_m a_m|\psi_m\rangle, \tag{40}$$

then

$$|\psi(t)\rangle = \sum_m a_m e^{-iE_m t/\hbar}|\psi_m\rangle. \tag{41}$$

From (19) and (39)

$$\alpha(\tau) - \alpha(0) = -\sum_m |a_m|^2 E_m\tau/\hbar, \tag{42}$$

$$e^{i\phi} = \sum_m |a_m|^2 e^{-iE_m\tau/\hbar}. \tag{43}$$

Obviously, $\phi \neq \alpha(\tau) - \alpha(0)$, $\beta(\tau) - \beta(0) \neq 0$, and only for $a_m = \delta_{mn}$ (stationary state), $\phi = \alpha(\tau) - \alpha(0) = -E_n\tau/\hbar$, $\beta(\tau) - \beta(0) = 0$. For time-dependent H, there exist no exact stationary state (even in the adiabatic case) and the Berry phase always appears. Moreover, calculation shows that the Berry phase obtained in the adiabatic approximation is different from the exact one.

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Figure caption

Fig. 1 (a) Probabilities of the magnetic resonance system found in the instaneous eigenstates $|\psi_\pm\rangle$ for the initial condition $|\psi(0)\rangle = |\psi_-\rangle$ (see (28)). $n = \tan\theta = 2$ and 4. (b) Variation with $n = \tan\theta = B_1/B_0$ of the exact and adiabatic Berry phases for each cycle (see (24) and (31)).

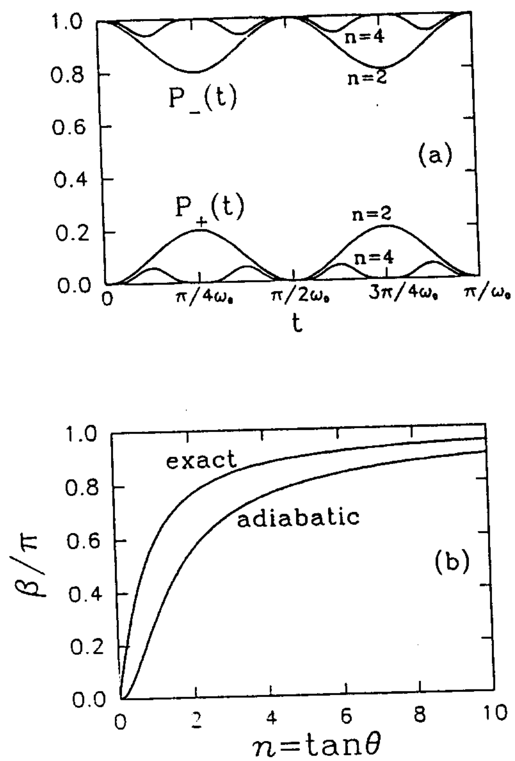

Fig. 1