Phase Change during a Cyclic Quantum Evolution

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A new geometric phase factor is defined for any cyclic evolution of a quantum system. This is independent of the phase factor relating the initial- and final-state vectors and the Hamiltonian, for a given projection of the evolution on the projective space of rays of the Hilbert space. Some applications, including the Aharonov-Bohm effect, are considered. For the special case of adiabatic evolution, this phase factor is a gauge-invariant generalization of the one found by Berry.

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A type of evolution of a physical system which is often of interest in physics is one in which the state of the system returns to its original state after an evolution. We shall call this a cyclic evolution. An example is periodic motion, such as the precession of a particle with intrinsic spin and magnetic moment in a constant magnetic field. Another example is the adiabatic evolution of a quantum system whose Hamiltonian H returns to its original value and the state evolves as an eigenstate of the Hamiltonian and returns to its original state. A third example is the splitting and recombination of a beam so that the system may be regarded as going backwards in time along one beam and returning along the other beam to its original state at the same time.

Now, in quantum mechanics, the initial- and final-state vectors of a cyclic evolution are related by a phase factor $e^{i\phi}$, which can have observable consequences. An example, which belongs to the second category mentioned above, is the rotation of a fermion wave function by 2π rad by adiabatic rotation of a magnetic field[1] through 2π rad so that $\phi=\pm\pi$. Recently, Berry[2] has shown that when H, which is a function of a set of parameters R^i, undergoes adiabatic evolution along a closed curve Γ in the parameter space, then a state that remains an eigenstate of $H(\mathbf{R})$ corresponding to a simple eigenvalue $E_n(\mathbf{R})$ develops a geometrical phase γ_n which depends only on Γ. Simon[3] has given an interpretation of this phase as due to holonomy in a line bundle over the parameter space. Anandan and Stodolsky[4] have shown how the Berry phases for the various eigenspaces can be obtained from the holonomy in a vector bundle. For the adiabatic motion of spin, this is determined by a rotation angle α, due to the parallel transport of a Cartesian frame with one axis along the spin direction, which contains the above-mentioned rotation by 2π radians as a special case. The result of a recent experiment[5] to observe Berry's phase for light can also be understood as a rotation of the plane of polarization by this angle α.

In this Letter, we consider the phase change for *all* cyclic evolutions which contain the three examples above as special cases. We show the existence of a phase associated with cyclic evolution, which is universal in the sense that it is the same for the infinite number of possible motions along the curves in the Hilbert space $\mathcal{H}$ which project to a given closed curve $\hat{C}$ in the projective Hilbert space $\mathcal{P}$ of rays of $\mathcal{H}$ and the possible Hamiltonians $H(t)$ which propagate the state along these curves. This phase tends to the Berry phase in the adiabatic limit if $H(t)\equiv H[\mathbf{R}(t)]$ is chosen accordingly. For an electrically charged system, we formulate this phase gauge invariantly and show that the Aharonov-Bohm (AB) phase[6] due to the electromagnetic field may be regarded as a special case. This generalizes the gauge-noninvariant result of Berry that the AB phase due to a static magnetic field is a special case of his phase. This also removes the mystery of why the AB phase, even in this special case, should emerge from Berry's expression even though the former is independent of this adiabatic approximation.

Suppose that the normalized state $|\psi(t)\rangle\in\mathcal{H}$ evolves according to the Schrödinger equation

$$H(t)\,|\psi(t)\rangle=i\hbar(d/dt)\,|\psi(t)\rangle, \tag{1}$$

such that $|\psi(\tau)\rangle=e^{i\phi}|\psi(0)\rangle$, ϕ real. Let $\Pi:\mathcal{H}\to\mathcal{P}$ be the projection map defined by $\Pi(|\psi\rangle)=\{|\psi'\rangle:|\psi'\rangle=c\,|\psi\rangle$, c is a complex number$\}$. Then $|\psi(t)\rangle$ defines a curve C: $[0,\tau]\to\mathcal{H}$ with $\hat{C}\equiv\Pi(C)$ being a closed curve in $\mathcal{P}$. Conversely given any such curve C, we can define a Hamiltonian function $H(t)$ so that (1) is satisfied for the corresponding normalized $|\psi(t)\rangle$. Now define $|\tilde{\psi}(t)\rangle=e^{-if(t)}|\psi(t)\rangle$ such that $f(\tau)-f(0)=\phi$. Then $|\tilde{\psi}(\tau)\rangle=|\tilde{\psi}(0)\rangle$ and from (1),

$$-\frac{df}{dt}=\frac{1}{\hbar}\langle\psi(t)\,|H|\,\psi(t)\rangle-\langle\tilde{\psi}(t)\,|\,i\frac{d}{dt}\,|\,\tilde{\psi}(t)\rangle. \tag{2}$$

Hence, if we remove the dynamical part from the phase ϕ by defining

$$\beta\equiv\phi+\hbar^{-1}\int_0^\tau\langle\psi(t)\,|H|\,\psi(t)\rangle dt, \tag{3}$$

it follows from (2) that

$$\beta=\int_0^\tau\langle\tilde{\psi}\,|\,i(d\,|\,\tilde{\psi}\rangle/dt)dt. \tag{4}$$

Now, clearly, the same $|\tilde{\psi}(t)\rangle$ can be chosen for every curve C for which $\Pi(C)=\hat{C}$, by appropriate choice of

$f(t)$. Hence β, defined by (3), is independent of ϕ and H for a given closed curve $\hat{C}$. Indeed, for a given $\hat{C}$, $H(t)$ can be chosen so that the second term in (3) is zero, which may be regarded as an alternative definition of β. Also, from (4), β is independent of the parameter t of $\hat{C}$, and is uniquely defined up to $2\pi n$ (n = integer). Hence $e^{i\beta}$ is a geometric property of the unparametrized image of $\hat{C}$ in $\mathcal{P}$ only.

Consider now a slowly varying $H(t)$, with $H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$, for a complete set $\{|n(t)\rangle\}$. If we write

$$|\psi(t)\rangle = \sum_n a_n(t)\exp\left[-\frac{i}{\hbar}\int E_n\,dt\right]|n(t)\rangle,$$

and use (1) and the time derivative of the eigenvector equation,[7] we have

$$\dot{a}_m = -a_m\langle m|\dot{m}\rangle - \sum_{n\neq m} a_n \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m}\exp\left[\frac{i}{\hbar}\int (E_m - E_n)\,dt\right], \quad (5)$$

where the dot denotes time derivative. Suppose that

$$\sum_{n\neq m}\left|\frac{\hbar\langle m|\dot{H}|n\rangle}{(E_n - E_m)^2}\right| \ll 1. \quad (6)$$

Then if $a_n(0) = \delta_{nm}$, the last term in (5) is negligible and the system would therefore continue as an eigenstate of $H(t)$, to a good approximation.

In this adiabatic approximation, (5) yields

$$a_m(t) \simeq \exp\left[-\int\langle m|\dot{m}\rangle dt\right] a_m(0).$$

For a cyclic adiabatic evolution, the phase $i\int_0^\tau\langle m|\dot{m}\rangle\,dt$ is independent of the chosen $|m(t)\rangle$ and Berry[2] regarded this as a geometrical property of the parameter space of which H is a function. But this phase is the same as (4) on our choosing $|\tilde{\psi}(t)\rangle \simeq |m(t)\rangle$ in the present approximation. But β, defined by (3), does not depend on any approximation; so (4) is exactly valid. Moreover, $|\psi(t)\rangle$ need not be an eigenstate of $H(t)$, unlike in the limiting case studied by Berry. Also, the two examples below will show respectively that it is neither necessary nor sufficient to go around a (nontrivial) closed curve in parameter space in order to have a cyclic evolution, with our associated geometric phase β. For these reasons, we regard β as a geometric phase associated with a closed curve in the projective Hilbert space and not the parameter space, even in the special case considered by Berry. But given a cyclic evolution, an $H(t)$ which generated this evolution can be found so that the adiabatic approximation is valid. Then β can be computed with the use of the expression given by Berry in terms of the eigenstates of this Hamiltonian.

We now consider two examples in which the phase β emerges naturally and is observable, in principle, even though the adiabatic approximation is not valid. Suppose that a spin-$\frac{1}{2}$ particle with a magnetic moment is in a homogeneous magnetic field $\mathbf{B}$ along the z axis. Then the Hamiltonian in the rest frame is $H_1 = -\mu B\sigma_z$, where

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Also,

$$|\psi(0)\rangle = \begin{bmatrix}\cos(\theta/2) \\ \sin(\theta/2)\end{bmatrix}$$

so that

$$|\psi(t)\rangle = \exp(i\mu Bt\sigma_z/\hbar)|\psi(0)\rangle = \begin{bmatrix}\exp(i\mu Bt/\hbar)\cos(\theta/2) \\ \exp(-i\mu Bt/\hbar)\sin(\theta/2)\end{bmatrix},$$

which corresponds to the spin direction being always at an angle θ to the z axis. This evolution is periodic with period $\tau = \pi\hbar/\mu B$. Then from (3), for each cycle, $\beta = \pi(1-\cos\theta)$, up to the ambiguity of adding $2\pi n$. Hence, β is $\frac{1}{2}$ of the solid angle subtended by a curve traced on a sphere, by the direction of the spin state, at the center. This is like the Berry phase except that in the latter case (1) the solid angle is subtended by a curve traced by the magnetic field $\mathbf{B}'(t)$ which is large [i.e., $\mu B'/\hbar \gg \omega$, the frequency of the orbit of $\mathbf{B}'(t)$] so that the adiabatic approximation is valid, and (2) $|\psi(t)\rangle$ is assumed to be an eigenstate of this Hamiltonian. Indeed, we may substitute such a Hamiltonian for the above H_1 or add it to H_1 with $\omega = 2\mu B/\hbar$, without changing β, in this approximation. The spin state will also move through the same closed curve in the projective Hilbert space as above if the magnetic field $\mathbf{B} = (B_0\cos\omega t,\ B_0\sin\omega t,\ B_3)$ with $\cot\theta = (B_3 - \hbar\omega/2\mu)/B_0$, where $B_0 \neq 0$.[8] And β is the same for all such Hamiltonians. This illustrates the statement earlier that β is the same for all curves C in H with the same $\hat{C} \equiv \Pi(C)$. Also, β may be interpreted as arising from the holonomy transformation, around the closed curve on the above sphere traced by the direction of the spin state, due to the curvature on this sphere,[4] which is a rotation. By varying appropriately a magnetic field applied to the two arms of a neutron interferometer with polarized neutrons, it is possible to make the dynamical part of β [the last term in (3)] the same for the two beams.[2,4] Then the phase difference between the two beams is just the geometrical phase, which is observable in principle, from the interference pattern, even when the magnetic field is varied nonadiabatically. In particular, a phase difference of $\pm\pi$ rad would correspond to a 2π-rad rotation of the fermion wave function, which is thus observable.

As our second example, suppose that the magnetic field is $\mathbf{B}(t) = \mathbf{B}_0 + \mathbf{B}_1(t)$, where $\mathbf{B}_0$ is constant and $\mathbf{B}_1(t)$ rotates slowly in a plane containing $\mathbf{B}_0$ with $|\mathbf{B}_1(t)|$

$=|\mathbf{B}_0|$. Suppose that at time t the angle between $\mathbf{B}_1$ and $\mathbf{B}_0$ is $\pi-\theta(t)$ and the spin state $|\psi(t)\rangle$ is in an approximate eigenstate of $H(t)=\mu\mathbf{B}\cdot\boldsymbol{\sigma}$, where σ^i are the Pauli spin matrices. For $0\le\theta\ll 1$, the adiabatic condition (6) gives $0\le -\hbar\dot{\theta}/\mu B_0\theta\ll 1$, assuming $\dot{\theta}\le 0$. Hence $\theta\gg\theta_0\exp(-\mu B_0 t/\hbar)>0$. So θ can never become zero. That is, if $\mathbf{B}(T)=\mathbf{0}$ for some T then the adiabatic approximation, as defined above, cannot be satisfied, regardless of how slowly $\mathbf{B}_1(t)$ rotates. However, because of conservation of angular momentum, $|\psi(t)\rangle$ remains an eigenstate of $H(t)$ even at $t=T$. But if θ changes monotonically then a level crossing occurs at the point of degeneracy ($\mathbf{B}=\mathbf{0}$) so that the energy eigenvalue corresponding to $|\psi(t)\rangle$ changes sign at $t=T$. For each rotation of $\mathbf{B}_1$ by 2π rad, $|\psi\rangle$ rotates by π rad, so that the system returns to its original state after two rotations of $\mathbf{B}(t)$. For this cyclic evolution, our $\beta=\pi$ which can be seen from the fact that a spin-$\frac{1}{2}$ particle acquires a phase π during a rotation, or that the curve $\hat{C}$ on the projective Hilbert space, which is a sphere, is a great circle, subtending a solid angle 2π at the center. This example is similar to Berry's phase in that $|\psi(t)\rangle$ is always an eigenstate of $H(t)$, even though Berry's prescription cannot be applied here because of the crossing of the point of degeneracy at which the adiabatic approximation breaks down.

Consider now a system with electric charge q for which $H=H_k(\mathbf{p}-(q/c)\hat{\mathbf{A}}(t),R_i)+q\hat{A}_0(t)$ in (1). Here, $\langle\mathbf{x}|\hat{A}_\mu(t)|\psi(t')\rangle=A_\mu(\mathbf{x},t)\psi(\mathbf{x},t')$, where $A_\mu(\mathbf{x},t)$ is the usual electromagnetic four-potential, and R_i are some parameters. Under a gauge transformation,

$$|\psi(t)\rangle\to\exp[i(q/c)\hat{\Lambda}(t)]\,|\psi(t)\rangle,$$

$$\hat{A}_0(t)\to\hat{A}_0(t)-c^{-1}\partial\hat{\Lambda}(t)/\partial t,$$

and

$$H_k(t)\to\exp[i(q/c)\hat{\Lambda}(t)]H_k(t)\exp[-i(q/c)\hat{\Lambda}(t)].$$

As before, define $|\tilde{\psi}(t)\rangle=e^{-if(t)}|\psi(t)\rangle$. If we require that $|\tilde{\psi}\rangle$ undergo the same gauge transformation as $|\psi(t)\rangle$, $f(t)$ is gauge invariant. Then, from (1),

$$\frac{df}{dt}(t)=\langle\tilde{\psi}(t)|\frac{d}{dt}-\frac{q}{\hbar}\hat{A}_0(t)|\tilde{\psi}(t)\rangle-\frac{1}{\hbar}\langle\psi(t)|H_k(t)|\psi(t)\rangle. \tag{7}$$

We consider now a cyclic evolution so that

$$|\psi(\tau)\rangle=e^{i\phi}\exp\left[-\frac{iq}{\hbar}\int_0^\tau\hat{A}_0\,dt\right]|\psi(0)\rangle.$$

Choose $f(t)$ so that $\phi=f(\tau)-f(0)$. Then

$$|\tilde{\psi}(\tau)\rangle=\exp\left[-i\frac{q}{\hbar}\int_0^\tau\hat{A}_0\,dt\right]|\tilde{\psi}(0)\rangle.$$

So we now define the gauge-invariant generalization of (3) as

$$\beta\equiv\phi+\frac{1}{\hbar}\int_0^\tau\langle\psi(t)|H_k(t)|\psi(t)\rangle dt, \tag{8}$$

which on use of (7) gives

$$\beta=\int_0^\tau\langle\tilde{\psi}(t)|i\frac{d}{dt}-\frac{q}{\hbar}\hat{A}_0(t)|\tilde{\psi}(t)\rangle dt. \tag{9}$$

Here, $|\tilde{\psi}(\tau)\rangle$ is obtained by parallel transport of $|\tilde{\psi}(0)\rangle$, with respect to the electromagnetic connection, along the congruence of lines parallel to the time axis. We could have chosen, instead, any other congruence of paths from $t=0$ to $t=\tau$ in our definition of ϕ and therefore $|\tilde{\psi}(\tau)\rangle$. This would correspondingly change β, which therefore depends on the chosen congruence. But, again, β is independent of ϕ and $H(t)$ for all the motions in $\mathcal{H}$ that project to the same closed curve $\hat{C}$ in $\mathcal{P}$, for a given chosen congruence. Both β and ϕ, which satisfies

$$e^{-i\phi}=\langle\psi(\tau)|\exp\left[-\frac{iq}{c}\int_0^\tau\hat{A}_0\,dt\right]|\psi(0)\rangle,$$

are gauge invariant. In the adiabatic limit, $|\tilde{\psi}(t)\rangle$ can be chosen to be an eigenstate of $H_k(t)$ and (9) is then a gauge-invariant generalization of the Berry phase.

We illustrate this by means of the AB effect.[6] Berry has obtained the AB phase from the gauge-noninvariant expression (4) with $|\tilde{\psi}(t)\rangle$ an eigenstate of $H(t)$, for a stationary magnetic field, in a special gauge.[9] But a gauge can be chosen so that the AB phase is included in the dynamical phase instead of the geometrical phase (4). Also, in general, there is no cyclic evolution in an AB experiment. But our β defined by Eq. (8) or (9) is gauge invariant and includes the AB phase in the special case to be described now.

Suppose that a charged-particle beam is split into two beams at $t=0$ which, after traveling in field-free regions, are recombined so that they have the same state at $t=\tau$. It is assumed here that the splitting and the subsequent evolution of the two beams occur under the action of two separate Hamiltonians. This is possible if we restrict ourselves to the Hilbert space of a subset of the degrees of freedom of a given system, as in the example considered by Aharonov and Vardi.[10] This belongs to the third example of a cyclic evolution mentioned at the beginning of this Letter. The wave function of each beam at $t=\tau$, assuming that it has a fairly well defined momentum, is

$$\psi_i(\mathbf{x},\tau)=\exp\left[-\frac{i}{\hbar}\int_0^\tau E_i\,dt\right]\exp\left[-\frac{iq}{c}\int_{\gamma_i}A_\mu dx^\mu\right]\exp\left[\frac{i}{\hbar}\int_{\gamma_i}\mathbf{p}\cdot d\mathbf{x}\right]\psi(\mathbf{x},0),\quad i=1\text{ or }2,$$

where γ_i is a space-time curve through the beam and $\mathbf{p}$ represents the approximate kinetic momentum of the beam. Hence on using (8), we have

$$\beta=-\frac{q}{c}\oint_\gamma A_\mu dx^\mu+\frac{1}{\hbar}\oint_\gamma \mathbf{p}\cdot d\mathbf{x}, \tag{10}$$

where γ is the closed curve formed from γ_1 and γ_2. But this is only an approximate treatment and a more careful investigation of this problem is needed.

In conclusion, we note that $\mathcal{H}^*=\mathcal{H}-\{0\}$ is a principal fiber bundle over $\mathcal{P}$ with structure group C^* (the group of nonzero complex numbers), and the disjoint union of the rays in $\mathcal{H}$ is the natural line bundle over $\mathcal{P}$ whose fiber above any $p\in\mathcal{P}$ is p itself. Then, clearly, β, given by (4), arises from the holonomy due to a connection in either bundle such that $|\psi(t)\rangle$ is parallel transported if

$$\langle\psi(t)|(d/dt)|\psi(t)\rangle=0, \tag{11}$$

i.e., the horizontal spaces are perpendicular to the fibers with respect to the Hilbert space inner product. Condition (11) was used by Simon[3] to define a connection on a line bundle over parameter space, which is different from the above bundles. The real part of (11) says that $\langle\psi(t)|\psi(t)\rangle$ is constant during parallel transport. Since this is true also during any time evolution determined by (1), we may restrict consideration to the subbundle $\mathcal{S}=\{|\psi\rangle\in\mathcal{H}:\langle\psi|\psi\rangle=1\}$ of $\mathcal{H}^*$. This $\mathcal{S}$ is the Hopf bundle[11] over $\mathcal{P}$. Then the imaginary part of (11) defines the horizontal spaces in $\mathcal{S}$ which determine a connection. This is the usual connection in $\mathcal{S}$ and $e^{i\beta}$ is the holonomy transformation associated with it. If $\mathcal{H}$ has finite dimension N then $\mathcal{P}$ has dimension $N-1$. For $N=2$, $\mathcal{P}$ is the complex projective space $P_1(C)$ which is a sphere with the Fubini-study metric[11] on $\mathcal{P}$ being the usual metric on the sphere. Opposite points on this sphere represent rays containing orthogonal states. Our geometric phase can then be obtained from the holonomy angle α associated with parallel transport around a closed curve on this sphere like in Ref. 4.

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[8]An experiment of this type has been done to measure Berry's phase ($\omega\rightarrow 0$) using nuclear magnetic resonance by D. Suter, G. Chingas, R. A. Harris, and A. Pines, to be published. One of us (J.A.) wishes to thank A. Pines for a discussion during which it was realized that the same type of experiment can be used to measure the geometric phase β introduced in the present Letter for nonadiabatic cyclic evolutions as well.

[9]In this proof, in Ref. 2, the eigenfunctions, in the absence of the electromagnetic field, are in effect assumed to be real, in order that Eq. (34) is valid. Since the coefficients of the stationary Schrödinger equation are then real, it is always possible to find real solutions. Then, for any eigenfunction belonging to a given eigenvalue to be necessarily a real function multiplied by $e^{i\lambda}$ ($\lambda=$const), it is necessary and sufficient that the eigenvalue is simple. But in our treatment of the AB effect, it is not necessary to make this assumption.

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