Observable effects of the quantum adiabatic phase for noncyclic evolution

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It is pointed out that, contrary to naive expectation, the gauge structure or Berry connection recently found in slowly varying quantum systems gives rise to observable effects even for noncyclic evolutions corresponding to open paths in parameter space. We propose to test such effects in muon spin resonance and in level-crossing resonance in muon-spin-rotation spectroscopy. In our proposals either the probe or the system itself has a lifetime much shorter than the period of one adiabatic cycle.

In recent years the adiabatic evolution of a quantum system has been receiving a great deal of renewed attention.[1-12] This was initiated by Berry's remarkable discovery[1] of a geometrical (or topological) phase named after him in the adiabatic cyclic evolution of a nondegenerate energy eigenstate. It was immediately realized[1-3] that Berry's phase actually implies the appearance of a gauge structure in the evolution of slowly varying systems, whether the eigenstate is degenerate or not. This quantum adiabatic phase has shed light on important theoretical issues such as gauge anomalies,[13] Wess-Zumino terms,[14] and fractional statistics.[15] Also it has been verified in several experiments.[8-12] Usually Berry's phase is thought to make sense only when the adiabatic evolution is *cyclic*, i.e., when the Hamiltonian completes a *closed* path in parameter space.

However, according to our experience in gauge theories, nonintegrable phase factors make sense for open paths as well. Historically Yang[16] has used the nonintegrable phase factors for all paths satisfying certain properties as an alternative definition of gauge fields or connections. In this Brief Report we address ourselves to the following problems: Should the Berry connection give rise to observable effects for *noncyclic* adiabatic evolutions corresponding to *open* paths in parameter space? If the answer is yes, is there a convincing way to test or to verify such effects?

An objection against any significance of quantum adiabatic phases for open paths would be that for a given open path in parameter space, one can always choose the phases of instantaneous eigenstates on the path such that the geometrical phase for the evoluting state disappears.[17] Yes, indeed this is true, exactly the same as in gauge theory where one can always choose a gauge such that the nonintegrable phase along a *given* open path vanishes. But the point is that one cannot make nonintegrable phases for *all* open paths vanish simultaneously. In the context of adiabatic evolution, according to Berry's analysis,[1] the nonintegrable phase along an open path $\lambda(t)$ in the parameter λ space is given by

$$\exp[i\beta_n(t)]=\exp\left[-\int_0^t dt'\left\langle n,\lambda(t')\left|\frac{\partial}{\partial\lambda}\right|n,\lambda(t')\right\rangle\frac{d\lambda}{dt'}\right], \tag{1}$$

where $|n,\lambda\rangle$ is a nondegenerate eigenvector of $H(\lambda)$ with arbitrary phase choice. We note that if one changes $|n,\lambda\rangle\rightarrow|n,\lambda\rangle'=\exp[if(\lambda)]\,|n,\lambda\rangle$, then

$$\exp[i\beta_n'(t)]\,|n,\lambda(t)\rangle'=\exp[if(\lambda(0))]\exp[i\beta_n(t)]\,|n,\lambda(t)\rangle\,. \tag{2}$$

Therefore, the total wave function in the adiabatic approximation

$$|n,t\rangle=\exp\left[-i\int_0^t dt'\,\varepsilon_n[\lambda(t')]/\hbar\right]\exp[i\beta_n(t)]\,|n,\lambda(t)\rangle \tag{2'}$$

is independent of the phase arbitrariness of $|n,\lambda(t')\rangle$ for $0<t'\leq t$. This is hardly surprising, since the evoluting state $|n,t\rangle$ is determined completely by the time-dependent Schrödinger equation and the initial state up to the initial phase. In short, adiabatic phases associated with Berry connection make sense even for noncyclic evolutions; they tell us about how the phases of adiabatically transported states (apart from the dynamical phases) evolve in an arbitrary basis.

Do these phases give rise to observable effects? The latter should be looked for in phenomena that crucially depend on the evolution phase difference of two adiabatically transported states. The resonance phenomenon belongs to such a category. Before discussing noncyclic situations, let us first describe the general principles[18] underlying the nuclear-magnetic-resonance (NMR) or nuclear-quadrupole-resonance (NQR) experiments[11,12] designed for verifying Berry's phase. Consider a quantum (e.g., spin) system with a time-independent Hamiltonian H_0. Let it be subject to a slowly but periodically changing external field, whose coupling is described by a Hamiltonian $H_1(t)$ characterized by an angular frequency $\omega = 2\pi/T$ (T being the period). Suppose that H_1 cannot be considered as a small perturbation to H_0. When $\omega \ll \omega_0$ ($\hbar\omega_0$ being the typical energy scale in H_0), one can apply the adiabatic approximation. Since $H_0+H_1(t)$ is periodic in time, there exists[19] a complete set of the so-called quasistationary states $|n,t\rangle$ each of which return to itself after the period T with an extra phase factor: $|n,t+T\rangle = \exp(-i\alpha_n)|n,t\rangle$. For the periodic Hamiltonian, the quasistationary state and quasienergy $E_n \equiv \hbar\alpha_n/T$ play similar roles as the stationary state and energy do for a time-independent Hamiltonian.[20] In particular, any solution to the time-dependent Schrödinger equation is a linear combination of the quasistationary states with constant coefficients. In the adiabatic approximation, the quasistationary states of $H_0+H_1(t)$ are just the adiabatically transported states and the quasienergies are related to Berry's phases by $E_n = \varepsilon_n - \hbar\beta_n(T)/T$. Here ε_n are the instantaneous energies of $H_0+H_1(t)$ that we assume to be constant in time, as in NMR or NQR experiments. Now let us apply periodic perturbation $H_2(t)$ to the system; it will induce transitions between the quasistationary states. According to the time-dependent perturbation theory, when the angular frequency ω_2 of the probing Hamiltonian $H_2(t)$ is close to the difference of any two quasienergies, resonance phenomena will occur. But the resonance peak deviates from the value $(\varepsilon_m-\varepsilon_n)/\hbar$ by an amount $-[\beta_m(T)-\beta_n(T)]/T$ plus possibly $N\omega$ (N is some integer which Berry's phases cannot fix on). Alternatively, we can couple the system with another (probing) quantum system that may or may not be influenced by the previous slowing varying environment. When there is an energy or quasienergy level crossing between the two systems, the transition caused by the interactions between them will be greatly enhanced. Again the resonance peak is shifted by an amount which is related to Berry's phases for the involving levels.

The above discussion applies when the detection duration t is much longer than the period T of one adiabatic cycle. To exhibit the effects of adiabatic phases for noncyclic evolution, one may use a short-lived probe or deal with a short-lived system, with a lifetime τ much shorter than T. In these situations, the detection duration t is of the order of τ. Then what is under test becomes the adiabatic phases for short open paths rather than Berry's phases for cyclic evolution. The latter certainly do not make sense during the lifetime of the system or the probe which is, say, one thousand times shorter than the period T of one adiabatic cycle.

For a resonance-type experiment, if at time t_i when the detection begins the system is in the nth quasistationary state, the probability for the system to be in the mth one at time t_i+t is given by first-order perturbation theory as (for ω near resonance)

$$|c_m(t)|^2 = \left| -(i/\hbar)\int_{t_i}^{t+t_i} dt' \langle m,t'|H_2(t')|n,t'\rangle \right|^2 \approx \frac{4|(h_2)_{mn}|^2}{(\varepsilon_m-\varepsilon_n+\Delta E \mp \hbar\omega_2)^2}\sin^2\left(\frac{\varepsilon_m-\varepsilon_n+\Delta E\mp\hbar\omega_2}{2\hbar}\right)t \tag{3}$$

with the shift of the resonance peak given as

$$\Delta E/\hbar = \bar\beta_n - \bar\beta_m \pm N_{mn}\omega,$$
$$\bar\beta_n \equiv \bar\beta_n(t_i) = -\left\langle n,\lambda(t')\left|\frac{\partial}{\partial\lambda}\right|n,\lambda(t')\right\rangle \frac{d\lambda}{dt'}\bigg|_{t'=t_i}, \tag{4}$$

$$\langle m,\lambda(t')|h_2|n,\lambda(t')\rangle = (h_2)_{mn}\exp(iN_{mn}\omega t'),$$
$$H_2(t') = h_2\exp(-i\omega_2 t') + \text{c.c.} \tag{5}$$

Here we have separated out a harmonic t' dependence in Eq. (5) so that the remaining matrix element $(h_2)_{mn}$ is constant or slowly varying in time, as quite often the case is in NMR or NQR experiments; so an integer N_{mn} may appear whose value depends on the phase choice of the basis, but ΔE is independent of this choice. [Note that according to Eqs. (2) and (2′), the first line of Eq. (3) is independent of the phase choice for $|m,\lambda(t')\rangle$ and $|n,\lambda(t')\rangle$.] In some situations, a basis can be chosen such that $\bar\beta_n(t_i) = \beta_n(T)/T$ is constant along the adiabatic path. So the position of the resonance peak is shifted by the same amount as for the cyclic case; but the peak is now broadened by an amount $\approx \hbar/\tau$ due to the finiteness of the detection time or that of the lifetime of the system. The more interesting cases are when $\bar\beta_n(t_i)$ varies along an open adiabatic path; then the position of the resonance peak will vary depending on the detection time t_i. In this way, one can see more explicitly the t_i-dependent effects due to the adiabatic phases $\beta_n(t) \approx \bar\beta(t_i)t$ for a small open path. For level-crossing resonance, one has similar results.

To propose realistic experiments, let us consider muon-spin resonance and level-crossing resonance (LSR) techniques in muon-spin-rotation (μSR) spectroscopy. μSR is well known and well developed as an important tool in material research and condensed matter science. For a recent review, see Ref. 21. The use of LSR in μSR is quite new. It was first suggested by Abragam in 1984[22] and the first successful experiments were reported only very recently.[23,24] It is needless to say that we are going to take advantage of the short lifetime of muon ($\tau_\mu = 2.2$ μs).

(1) *Muon-spin resonance.* In this type of experiment, a pulsed beam of highly polarized ($\geq 80\%$) positively charged muons μ^+ from $\pi^+ \to \mu^+ + \nu_\mu$ are injected into nonmagnetic bulk material. They are thermalized and then stopped in the sample. An external longitudinal magnetic field $\mathbf{B}_0$ along the direction of muon polarization is applied to the sample. The presence of $\mathbf{B}_0$ leads to the splitting of μ-spin states. To generate adiabatic phases for these states, add to $\mathbf{B}_0$ a transverse rotating field $\mathbf{B}_\perp(t)$ with angular frequency $\omega \ll 1/\tau_\mu$. Then

$$\varepsilon_\pm = \mp\hbar\gamma_\mu B, \quad \bar\beta_+ - \bar\beta_- = -\omega(1-\cos\theta), \tag{6}$$

where B is the magnitude of the total magnetic field $\mathbf{B}(t)=\mathbf{B}_0+\mathbf{B}_\perp(t)=(B\sin\theta\cos\omega t,\ B\sin\theta\sin\omega t,\ B\cos\theta)$. To detect the adiabatic phases one can apply a pulsed rf field after the arrival of muons. The measurement of the shift of resonance peak should give us a test of Eq. (6). This experiment would be similar to the NMR one that verifies Berry's phase,[12] but the system (muon) does not live long enough to complete one adiabatic cycle. Also, if $B_\perp(t)$ rotates not with a uniform angular velocity, one can test whether the shift of resonance peak depends on the detection time t_i.

(2) *Level-crossing resonance in muon-spin rotation.* The principles of LCR-μSR were described in Refs. 22 and 23. Here a beam of highly polarized muons μ^+ are used as a probe to the splitting of spin states of nuclei with nonvanishing quadrupole moment near which the muons are stopped.

Again a longitudinal magnetic field $\mathbf{B}_0$ and a transverse rotating field $\mathbf{B}_\perp(t)$ with angular frequency $\omega \ll 1/\tau_\mu$ are applied as before. The adiabatic phases for μ-spin states are generated as given in Eq. (6) as well. To generate adiabatic effects for nuclear spin states, we rotate the sample. In addition to the nuclear Zeeman effect in the applied field $\mathbf{B}_0+\mathbf{B}_\perp(t)$, there is an interaction of the nuclear quadrupole moment with either an intrinsic field gradient or the local field whose appearance is due to the distortion of lattice by the presence of muons. To avoid complications, it is desirable to synchronize the rotation of the gradient axis of the quadrupolar interaction so that the gradient axis remains parallel to the total magnetic field. Then the nuclear Hamiltonian

$$H_N=\tfrac{1}{2}\omega_Q[I_z(t)]^2-\omega_N I_z(t)=\tfrac{1}{2}\omega_Q\left(I_z(t)-\frac{\omega_N}{\omega_Q}\right)^2+\text{const} \tag{7}$$

(with $\omega_N=\gamma_N B$) has a very simple structure. Depending on the ratio ω_N/ω we have to distinguish between two situations:

(i) $\omega \ll \omega_N \simeq \omega_Q$. In this case, the Hamiltonian (7) does not have degenerate eigenstates at the $O(\omega^0)$ order. Assuming $I=\frac{3}{2}$, the adiabatic quantum phases generated in the nuclear $I_z(t)$ eigenstates $|-\frac{3}{2}\rangle$, $|-\frac{1}{2}\rangle$, $|\frac{1}{2}\rangle$, and $|\frac{3}{2}\rangle$ are given by

$$\begin{aligned}\bar\beta_{\pm 3/2}&=\pm 3\omega(\cos\theta-1)/2\,,\\ \bar\beta_{\pm 1/2}&=\pm\omega(\cos\theta-1)/2\,.\end{aligned} \tag{8}$$

(ii) $\omega \simeq \omega_N \ll \omega_Q$. In this case, the eigenstates of the Hamiltonian (7) are doubly degenerate at the $O(\omega^0)$ order; therefore, there are mixing of the states $|\pm\frac{1}{2}\rangle$ and intertwining of the Zeeman and adiabatic phases at the $O(\omega)$ order. The adiabatic quantum phases are given by

$$\begin{aligned}\bar\beta_{\pm 3/2}&=\pm\tfrac{3}{2}\omega(\cos\theta-1)\,,\\ \bar\beta_{\pm}&=\pm\tfrac{1}{2}\omega\{[(\cos\theta+\omega_N/\omega)^2+4\sin^2\theta]^{1/2}-1\}\,,\end{aligned} \tag{8$'$}$$

where $|+\rangle$ and $|-\rangle$ are orthonormal mixing of the $I_z(t)$ eigenstates $|\pm\frac{1}{2}\rangle$.

A way to test these phases is to exploit the level-crossing resonance caused by direct dipolar interactions between muon and nuclear spins

$$H_D=-S_+D_{+-}I_- - S_-D_{-+}I_+ + \cdots\,, \tag{9}$$

where D_{kj} denotes the coefficient matrix. When the muon Zeeman splitting is made to match the splitting of any two nuclear levels by adjusting the magnitude B of the applied field, the effect H_D is much enhanced and gives rise to a quite big depolarization of muons. Compared to the situation in which only a longitudinal field B is applied on a nonrotating sample, the shift of the resonance peak will give us a test of Eqs. (6) and (8).

Here our probe (muon) has a short lifetime and, therefore, is detecting adiabatic phases during short noncyclic evolutions ($t\approx\tau\approx 0.001$ T when, say, $\omega\approx 1$ kHz). Similarly, one may use a pulsed rf field in usual NQR (Ref.10) or NMR (Ref. 12) experiments that verify Berry's phase. The more interesting cases are when, e.g., the sample in NQR or the transverse magnetic field in NMR rotates nonuniformly and the rf pulses are synchronized so that they are applied at a fixed segment of each adiabatic cycle. The variation of the rotational effects can then be monitored segment by segment along the cycle.

To conclude we remark that there are also observable effects from nonintegrable (path-dependent) adiabatic phases for finite noncyclic evolutions. An example is the rotation of the polarization of a linearly polarized light traveling down a helically wound optical fiber. A discussion using Berry's phase for the cyclic case has been given in Ref. 8. Using adiabatic phases for open paths one can discuss the noncyclic situations in which the tangents at the ends of the fiber are not necessarily parallel to each other. The results coincide with those obtained by classical parallel transport arguments.[25] The details will be presented elsewhere.

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