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On removing Berry's phase

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ABSTRACT

The Berry phase can always be cancelled by a unitary transformation if the space of external parameters is appropriately restricted. But it simply reappears as part of the dynamical phase, and this shift can be regarded as a gauge transformation. The overall extra phase measured in experiments is unambiguous, and retains its geometrical character.

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When a Hamiltonian H depends on slowly-changing parameters, the quantum dynamics is approximately described by the instantaneous eigenstates of H , multiplied by a time-dependent phase. If H evolves in a cycle, so that $H(T) = H(0)$, this phase contains two parts: a dynamical phase, the integral of the instantaneous frequency $E_n(t)/\hbar$, and an additional phase, pointed out by Berry [1], which can be understood as the curvature of a Hilbert space bundle over the base space of parameters [2]. The Berry phase depends only on the path taken in parameter space and not on the rate of progress along that path. It is gauge invariant, in the sense that we can freely redefine the phases of the (time-independent) eigenstates, and the Berry phase is not affected. However, there is another freedom we have, due to the fact that different Hamiltonians can describe the same physical system. These Hamiltonians are related (classically) by canonical or (quantally) by unitary transformations depending generally on the 'external' parameters. It might seem that Berry's phase can be removed in this way. However, it is not removed: it can be shifted into the dynamical phase, but retains its geometrical character. The shift in fact reflects a wider gauge invariance than has been noted before.

A time-varying Hamiltonian can be written in the form

$$H(t) = U(t)H_D(t)U^\dagger(t) \quad (1)$$

where $U(t)$ is a unitary operator and $H_D(t)$ is diagonal in a (fixed) orthonormal basis $\{|n\rangle\}$. Assume that $U(t)$ depends on time only through cyclic, slowly-varying parameters $R_i(t)$. If the adiabatic approximation is applicable, we start from a state $|n\rangle$ at $t = 0$ and end up at time T with the same state and an overall phase

$$\Phi_n(T) = -\frac{i}{\hbar} \int_0^T E_n(t) dt + i \int_0^T \langle n | U^\dagger(t) \dot{U}(t) | n \rangle dt. \quad (2)$$

Besides the expected dynamical phase we have a contribution of purely geometric origin, Berry's phase. However, the splitting of the phase into a dynamical and a geometrical part is subject to reinterpretation in terms of a Hamiltonian unitarily equivalent to the one in Eq.(1). Let us subject $H(t)$ to a unitary transformation $H'(t) = W(t)H(t)W^\dagger(t)$, then the Schrödinger equation for the transformed states involves an effective Hamiltonian

$$H_{\text{eff}}(t) = H'(t) - i\hbar W(t) \dot{W}^\dagger(t). \quad (3)$$

The adiabatic assumption requires that $W(t)$ not induce transitions among the eigenstates

of $H'(t)$. Then only the diagonal part of Eq.(3) remains, so that

$$H_{\text{eff}}(t) \simeq H'(t) - i\hbar \sum_n P'_n(t) W(t) \dot{W}^\dagger(t) P'_n(t)$$

where $P'_n(t)$ is the projector onto the n -th state of $H'(t)$. If we also require that $W(t)$ depend on time only through the cyclic R_i , we obtain the analogue of Eq.(2) for $H_{\text{eff}}(t)$:

$$\Phi'_n(T) = -\frac{i}{\hbar} \int_0^T (E_n(t) + E_n^w(t)) dt + i \int_0^T \langle n | (W(t) U(t))^\dagger \frac{d}{dt} (W(t) U(t)) | n \rangle dt \quad (4)$$

where $E_n^w(t) = -i\hbar \langle n | U^\dagger(t) \dot{W}(t) W(t) U(t) | n \rangle$. Eq. (4) explicitly shows that a unitary transformation changes the balance between dynamical and geometrical parts of the phase. It is sufficient to choose $W(t) = U^\dagger(t)$ to cancel the second term and make the Berry phase in Φ'_n entirely dynamical. However $\Phi_n = \Phi'_n$, and the same phase will be measured in an experiment, whatever we call it. Since both U and W depend on time only via the parameters R_i , the integral of $E_n^w(t)$ over time can be rewritten as an integral over a closed loop in parameter space. Thus the extra phase measured in an experiment still keeps its geometrical meaning even if it appears as dynamical: it depends only on the connection on parameter space.

The issue of global removability of Berry's phase concerns the possibility of defining the operator $U(t)$ (which instantaneously diagonalizes $H(t)$) globally over the parameter space. If the Hilbert space bundle defined by the Berry connection in Eq.(2) involves a non trivial bundle, we cannot do this. But even if the bundle is trivial, the geometric phase cannot be removed. We now illustrate this point with reference to hypothetical or actual experiments.

As a first example, consider the parametric harmonic oscillator [3]. The Hamiltonian is

$$H = \frac{1}{2}(\alpha p^2 + \beta(pq + qp) + \gamma q^2)$$

where α, β , and γ are slowly varying parameters, $\alpha\gamma > \beta^2$ and $\alpha > 0$. The energy levels are $E_n = (n + 1/2)\hbar(\alpha\gamma - \beta^2)^{1/2}$. The Berry phase for a closed circuit $\mathcal{C}$ in α, β and γ is [3]

$$\gamma_n(\mathcal{C}) = (n + \frac{1}{2}) \oint_{\mathcal{C}} \frac{\beta d\alpha - \alpha d\beta}{2\alpha(\alpha\gamma - \beta^2)^{1/2}}. \quad (5)$$

(The extra phase could perhaps be detected in an interference experiment similar to the one described in Ref. [4] but with a charged particle). Jackiw [5] and Gerbert [5] add

the total time derivative of $-\beta q^2/2\alpha$ to the classical Lagrangian; it induces a canonical transformation to a new Hamiltonian H_{eff} with no cross term in p and q and γ replaced by $\gamma - \beta^2/\alpha - (d/dt)(\beta/\alpha)$. At the quantum level, we obtain H_{eff} from H via a unitary transformation $W = \exp(i\beta q^2/2\alpha)$. By applying Eq.(5) we can verify [5] that no Berry phase arises from H_{eff} . The phase is present, however, in a new guise: the instantaneous energy levels are now

$$E'_n \simeq (n + \frac{1}{2}) \hbar(\alpha\gamma - \beta^2)^{1/2} \left(1 - \frac{\alpha}{2(\alpha\gamma - \beta^2)} \frac{d}{dt} \left(\frac{\beta}{\alpha} \right) + \dots \right)$$

where the dots refer to terms with two or more time derivatives of the slow parameters. The difference between E'_n and E_n , when integrated over time as part of the dynamical phase, is equivalent to the Berry phase in Eq. (5). Gerbert [5] notes this shift and suggests that the Berry phase loses its geometrical significance when it can be cancelled globally. But even though the extra phase is now dynamical, it retains its geometric character: it depends only on the path in parameter space and not on the rate of progress along the path. The adiabatic assumption is essential here; if we make the generalized phase of Aharonov and Anandan [6] dynamical, the terms with more than one time derivative cannot be neglected. Then it is more problematic to decide what is geometrical.

Among the papers reporting measurements of Berry's phase are several that note the freedom to change the form of the Hamiltonian. The Berry phase of a spinning particle in a magnetic field [1] was measured by Bitter and Dubbers [7] among others. They used beams of polarized neutrons in a twisting magnetic field. The twisting field represented an external parameter going through its adiabatic cycle, and the Berry phase is proportional to the solid angle swept out. This experiment does not quite fit Berry's definition since the neutrons were not polarized along the direction of the field. The geometrical principle is exactly the same, however, and the predicted phase shift was observed as an additional rotation of the precessing neutrons. The authors remark that, 'in its simplest manifestation, which we believe to have realized, the appearance of a topological phase seems to be trivial: it can be generated or transformed away by going to a rotating-reference frame....' It should be noted that their experimental set-up did not permit the magnetic field to point directly along the beam axis. By excluding a region from the parameter space, they allowed their experiment to probe only a local trivialization of the $U(1)$ phase bundle, which in this case was a monopole potential. This topological issue can be kept separate, however, for even if the bundle is trivial, the geometric phase cannot be transformed away. Explicitly, we

can consider the classical Lagrangian, written in terms of Grassmann variables [8],

$$\mathcal{L} = \frac{i}{2} \psi_k \dot{\psi}_k + \frac{i}{2} \varepsilon_{ijk} \psi_i \dot{\psi}_j B_k$$

where a sum is implied over repeated indices, which run from 1 to 3. Now suppose we go to a coordinate frame rotating with the azimuthal component of $\vec{B}$; the transformation is effected by a generating function

$$F_1(\psi_k, \psi'_k) = \frac{i}{2} [\psi_1(\psi'_1 \cos \varphi - \psi'_2 \sin \varphi) + \psi_2(\psi'_1 \sin \varphi + \psi'_2 \cos \varphi)]$$

where $\tan \varphi = B_2/B_1$. (Actually F_1 vanishes when ψ_1 and ψ_2 are evaluated in terms of the primed quantities.) The transformed Lagrangian is then

$$\mathcal{L}' = \frac{i}{2} \psi'_k \dot{\psi}'_k + \frac{i}{2} \psi'_2 \psi'_3 (B_1^2 + B_2^2)^{1/2} + i \psi'_1 \psi'_2 (B_3 - \dot{\varphi}),$$

missing one component of the magnetic field. Since in these coordinates $\vec{B}$ cannot sweep out a solid angle, there is no additional phase due to parallel transport. Note that the coordinate transformation is not well-defined for paths that intersect the B_3 -axis, but for the experiment we are discussing, this region of the parameter space is not relevant.

In the rotating frame, the apparent magnitude of the magnetic field is

$$B' = [B_1^2 + B_2^2 + (B_3 - \dot{\varphi})^2]^{1/2} \simeq B - \cos \theta \dot{\varphi}$$

where θ and φ indicate the direction of the field and $B = |\vec{B}|$. The precession of the neutrons is proportional to the field, and the extra term reproduces the Berry connection; the anholonomy is still present and is accounted for by an extra precession of the polarization vector. (The experiment was not sensitive to the additional $\dot{\varphi}$ which is normally part of the Berry connection, so a classical calculation suffices.)

Other measurements of this phase have been reported using NMR interferometry [9, 10] and polarization states in lasers [11]. Ref. [10] discusses unitary transformations in general, showing that geometric phases can appear as 'fictitious' dynamical phases. (In rotating reference frames, which are non-inertial, the extra dynamical phases are indeed fictitious.) Berry [1, 12] suggested a split-beam experiment to measure the spin phase effect. Imagine a double-slit experiment with neutrons, in a magnetic field

$$\vec{B}(z) = B[\hat{x} \sin \theta_0 \cos \varepsilon z + \hat{y} \sin \theta_0 \sin \varepsilon z + \hat{z} \cos \theta_0].$$

$\vec{B}$ rotates slowly with z since ε is small. Let polarized neutrons, moving in the $\hat{x}$ -direction, pass through slits lying along the z -axis. (We can neglect the $\hat{y}$ -direction). In addition

to the usual interference pattern due to path length, there will be interference because they have been rotated different amounts by the field, depending on the $\hat{z}$ -component of their path. If we arrange the distance Δz between the slits so that $\varepsilon \Delta z = 2\pi$, then the different rotations of the beams correspond to one closed loop in parameter space. Berry's phase will appear as a shift in the pattern of fringes. Although the geometrical phase is unambiguous, here too it can appear as dynamical. The combined Hamiltonian is

$$H = \frac{1}{2m}(p_z^2 + p_z^2) + \frac{\hbar}{2} \vec{\sigma} \cdot \vec{B}(z). \quad (6)$$

If we consider only one beam and treat the spatial dependence of $\vec{B}$ as an adiabatic time dependence, the Hamiltonian is $H = \hbar \vec{\sigma} \cdot \vec{B}(t)/2$. Let $\phi(t)$ represent the azimuthal angle of $\vec{B}$, and define a Hamiltonian $H' = WHW^\dagger$ in terms of the unitary transformation $W = \exp\{i\phi(1 + \sigma_z)/2\}$. The combination $1 + \sigma_z$ (rather than σ_z alone) in W is chosen to make the states invariant under a 2π rotation about the z -axis, so that no spurious factors of -1 will arise from the change of coordinates. The energy eigenvalues, in the adiabatic approximation, are now

$$E'_\pm \simeq \frac{\hbar}{2} \left[\phi \left(1 \pm \frac{B_3}{B} \right) \pm B \right].$$

The integral of $\frac{1}{2}\phi(1 \pm B_3/B)$ yields Berry's phase, now appearing as dynamical.

We can also shift the phase in both beams simultaneously. Simply by making W depend on z , so that $W = \exp\{i(1 + \sigma_z)\varepsilon z/2\}$, and referring back to Eq. (6), we find that the apparent magnetic field does not twist at all. Thus the geometric phase difference between the two beams has become a dynamical one. However we stress once more that the phase difference can be measured experimentally and still has geometrical meaning.

We have seen that Berry's phase can always be cancelled by a unitary transformation, once the parameter space has been suitably restricted (if necessary). The phase reappears as dynamical and can in principle be measured unambiguously. The example of a spin in a magnetic field is one where the Berry phase cannot be removed globally, since the phase bundle is non-trivial [13]. Yet in all the experiments discussed above, the bundle became trivial by virtue of restrictions on the parameter space. One might imagine an experiment, for example with optical fibers [14], that would make the whole sphere of directions available. However, since a single measurement can probe only a local trivialization of the monopole bundle, it is hard to imagine how any experiment could verify that a bundle is indeed non-trivial.

Our analysis of the geometric phase can be summarized very simply by the statement that a shift of Berry's phase into the dynamical phase represents a time-dependent gauge transformation. The gauge invariance of Berry's phase has so far been discussed only for time-independent redefinitions of the eigenstates. However, Eq. (4) implies invariance over 'space-time': the space of the parameters and time as well. Let a Hamiltonian depend on 'fast' variables $\vec{r}$ and 'slow' variables $\vec{R}$ and consist of two parts, $H_f(\vec{R}, \vec{p}, \vec{r})$ and $H_s(\vec{P}, \vec{R})$. The trial solution, in the Born-Oppenheimer approximation, is $\phi(\vec{R}, t)\psi_n(\vec{R}, \vec{r})$, in which $\psi_n(\vec{R}, \vec{r})$ is an instantaneous eigenstate of $H_f(\vec{R}, \vec{p}, \vec{r})$. It leads to an effective Schrödinger equation for $\phi(\vec{R}, t)$ [15]

$$-\frac{\hbar^2}{2M} D_{\vec{R}}^2 \phi + [E_n(\vec{R}) + V(\vec{R})]\phi = i\hbar \frac{\partial}{\partial t} \phi, \quad (7)$$

where

$$D_{\vec{R}} \equiv \nabla_{\vec{R}} + \langle \psi_n | \nabla_{\vec{R}} \psi_n \rangle \equiv \nabla_{\vec{R}} + i\vec{A}_n(\vec{R}). \quad (8)$$

If we redefine ψ_n by an $\vec{R}$ -dependent phase, then $\vec{A}_n$ transforms as a vector potential; ϕ must acquire the opposite phase for $D_{\vec{R}}$ to transform covariantly (and for $\Psi(\vec{R}, \vec{r}, t)$ to be invariant). The fast variables have induced a gauge covariance in the effective Schrödinger equation for the slow variables. So far, however, the only gauge transformations are time-independent ones.

The path integral for this system is [15, 16]

$$K(\vec{R}_T, \vec{r}_T; \vec{R}_0, \vec{r}_0; T) = \int [d\vec{R}] [d\vec{r}] \exp \left[\frac{i}{\hbar} \int_0^T (M \dot{\vec{R}}^2 / 2 - V(\vec{R}) + \vec{p} \cdot \dot{\vec{r}} - H_f) dt \right]. \quad (9)$$

In the adiabatic approximation, the system is in an eigenstate ψ_n of $H_f(\vec{R}, \vec{p}, \vec{r})$; the path integral in then $K_n(\vec{R}_T, \vec{R}_0; T)$ and the part of the path integral involving the fast variables can be written

$$\psi_n^*(\vec{R}_T, \vec{r}_T) \exp \left[-\frac{i}{\hbar} \int_0^T (E_n - i\hbar(\psi_n | \nabla_{\vec{R}} \psi_n) \cdot \dot{\vec{R}}) dt \right] \psi_n(\vec{R}_0, \vec{r}_0). \quad (10)$$

The path integral for the slow variables now has an effective Lagrangian with a contribution from (10). Eqs. (7-9) show that the effective Lagrangian leads directly to the Schrödinger equation for $\phi(\vec{R}, t)$ in the Born-Oppenheimer approximation. But the fast part of the

path integral could just as well have been written with the Berry phase absorbed into the dynamical phase, and we would have removed the induced vector potential $\vec{A}_n$. As noted earlier, Eq. (4) gives us the freedom to shift the geometric phase between the Berry connection and the dynamical part, for any given path in $\vec{R}$ -space. This freedom can be regarded as a time-dependent gauge invariance. Time-dependent gauge transformations need not affect the integral of the vector potential around a closed loop; those that do generally introduce singularities into $\vec{A}_n$. ($\vec{A}_n$ can be removed from an arbitrary loop in $\vec{R}$ -space, but around other loops it is usually non-zero.) In terms of the effective Schrödinger equation for the slow variables, the implication is that we can transform between a scalar potential $V_n(t) = E_n^w(t)/\hbar$ and a vector potential $\vec{A}_n = -i\langle\psi_n|W^\dagger\nabla_{\vec{R}}W|\psi_n\rangle$. Here, as in Eq. (4), the unitary operator W depends on time only through $\vec{R}$. That the geometrical phase Φ_n is invariant, even if the Berry phase becomes dynamical, is now expressed compactly as $\Phi_n = \int \vec{A}_n(\vec{R}) \cdot d\vec{R} - \int V_n(t)dt$, showing that the effective Schrödinger equation is covariant under (adiabatic) time-dependent gauge transformations as well as time-independent ones. Indeed, the Berry phase retains its geometrical significance; the adiabatic gauge invariance induced by the fast variables extends to time-dependent gauge transformations, and the geometrical phase indicates the curvature of a bundle defined over time as well as the space of parameters.

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