BERRY’S PHASE

Berry’s phase [1] is a quantum phase effect arising in systems that undergo a slow, cyclic evolution. It is a remarkable correction to the quantum adiabatic theorem and to the closely related Born-Oppenheimer approximation [2]. Berry’s elegant and general analysis has found application to such diverse fields as atomic, condensed matter, nuclear and elementary particle physics, and optics. In this brief review, we first derive Berry’s phase in the context of the quantum adiabatic theorem and then in the context of the Born-Oppenheimer approximation. We mention generalizations of Berry’s phase and analyze its relation to the →Aharonov-Bohm effect.

Consider a Hamiltonian $H_f(R)$ that depends on parameters $R_1, R_2, \ldots, R_N$, components of a vector $R$. Let us assume that $H_f(R)$ has at least one discrete and nondegenerate eigenvalue $E_i(R)$ with $|\Psi_i(R)\rangle$ its eigenstate; $E_i(R)$ and $|\Psi_i(R)\rangle$ inherit their dependence on $R$ from $H(R)$. If the vector $R$ changes in time, then $|\Psi_i(R(t))\rangle$ is not an exact solution to the time-dependent Schrödinger equation. But if $R$ changes slowly enough, the system will not →jump to another eigenstate. Instead, it adjusts itself to the changing Hamiltonian. A heavy weight hanging on a string illustrates such adiabaticity. Pull the string quickly—it snaps and the weight falls. Pull the string slowly—the weight comes up with it.

“Slowly enough” has the following formal sense. Let $R[t/T]$ evolve over a time interval $0 \leq t \leq T$; the larger $T$, the slower the evolution. If at time $t = 0$ the system is in the state $|\Psi_i(R[0])\rangle$, then at time $t = T$ the state is $e^{i\phi_i(T)}|\Psi_i(R[1])\rangle$ with probability approaching 1 as $T$ approaches infinity, according to the quantum adiabatic theorem [10]. We obtain the phase $\phi_i(t)$ by substituting $e^{i\phi_i(t)}|\Psi_i(R)\rangle$ into the time-dependent →Schrödinger equation,

$$i\hbar \frac{d}{dt} e^{i\phi_i(t)}|\Psi_i(R)\rangle = H_f(R[t/T]) e^{i\phi_i(t)}|\Psi_i(R)\rangle,$$

and projecting both sides of the equation onto $e^{i\phi_i(t)}|\Psi_i(R)\rangle$:

$$\frac{d}{dt} \phi_i(t) = i \langle \Psi_i(R)|\nabla_R|\Psi_i(R)\rangle \cdot \frac{dR}{dt} - \frac{1}{\hbar}E_i(R).$$

Thus

$$\phi_i(t) - \phi_i(0) = \int_0^t dt' \left[ i \langle \Psi_i(R)|\nabla_R|\Psi_i(R)\rangle \cdot \frac{dR}{dt'} - \frac{1}{\hbar}E_i(R) \right]$$

$$= \int_{R[0]}^{R[t]} \langle \Psi_i(R)|i\nabla_R|\Psi_i(R)\rangle \cdot dR - \frac{1}{\hbar} \int_0^t dt' E_i(R).$$

The integrand $A_B \equiv \langle \Psi_i(R)|i\nabla_R|\Psi_i(R)\rangle$ is Berry’s connection for the state $|\Psi_i(R)\rangle$. The integral $- \int_0^t E_i dt'/\hbar$ is called the dynamical phase.

The overall phase of a quantum state is not observable. But a quantum system may be in a →superposition of states; the relative phase of these states is observable. Consider two paths $R[t/T]$ and $R'[t/T]$ with the same endpoints $R[0] = R'[0]$. The integrand $A_B \equiv \langle \Psi_i(R)|i\nabla_R|\Psi_i(R)\rangle$ is Berry’s connection for the state $|\Psi_i(R)\rangle$. The integral $- \int_0^t E_i dt'/\hbar$ is called the dynamical phase.
and $R[1] = R'[1]$, and suppose that the system evolves in a superposition of states $|\Psi_i(R(t/T))\rangle$ and $|\Psi_i(R'(t/T))\rangle$. At time $t = T$ the relative phase of this superposition contains two parts. One part is the relative dynamical phase. The other part is Berry’s phase, the difference between $A_B$ integrated along $R$ and $A_B$ integrated along $R'$, i.e. it is the circular integral of $A_B$ along the closed path comprising $R$ and $R'$ with opposite senses. This phase is well defined, because it is →gauge invariant: If we multiply $|\Psi_i(R)\rangle$ by a phase factor $e^{i\Lambda(R)}$, it remains the same instantaneous eigenstate of $H_f(R)$, but $A_B$ changes by $-\nabla_R \Lambda(R)$. Since the change in $A_B$ is a gradient, the integral of $A_B$ around a closed loop is unchanged, hence well defined.

As an example of Berry’s phase, consider the spin-1/2 Hamiltonian $H_f = \mu R \cdot \sigma$, where $\sigma_x$, $\sigma_y$ and $\sigma_z$ are the →Pauli spin matrices. The eigenstate corresponding to the positive eigenvalue $E_+ = \mu R$ is

$$\left( \begin{array}{c} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{array} \right),$$

where $R_z = R \cos \theta$ and $R_x + iR_y = Re^{i\phi} \sin \theta$. The Berry connection, expressed as a function of $\theta$ and $\phi$, is $(A_B)_\theta = 0$, $(A_B)_\phi = (\cos \theta - 1)/2$ and matches the vector potential of a Dirac monopole of strength 1/2 located at the origin $R = 0$. The integral of $A_B$ along any loop in $R$ equals $-1/2$ times the solid angle subtended by the loop at the origin (as an application of Stokes’s theorem shows). This example is generic because wherever two nondegenerate energy levels cross at a point in a space of parameters, the Hamiltonian near the point reduces to an effective two-level Hamiltonian proportional to $R \cdot \sigma$, with the degeneracy at $R = 0$. Hence an effective magnetic monopole can arise wherever two discrete, nondegenerate levels become degenerate.

The spin-1/2 example also illustrates how Berry’s phase can be topological. A loop in $R$ defines two solid angles, just as a loop on the surface of a sphere cuts the surface into two parts. Why, then, is Berry’s phase not ambiguous? The answer is that the difference between the two solid angles is equal to $\pm 4\pi$. (The two solid angles have opposite signs because their orientations, or the directions of integration of $A_B$, are opposite.) But a $\pm 4\pi$ difference of solid angle corresponds to a $\mp 2\pi$ difference in phase, which is unobservable. Here Berry’s phase obeys a constraint arising from the topology of a sphere.

In the Born-Oppenheimer approximation, the $R_1, R_2, \ldots$ are quantum observables and may not even commute. They evolve according to their own “slow” Hamiltonian $H_s$, and the overall Hamiltonian is the sum $H = H_f + H_s$. The eigenvalues of $H_f$ must be discrete, and the adiabatic limit applies if $H_s$ is an arbitrarily weak perturbation on $H_f$. The weaker the perturbation, the smaller the probability of transitions (quantum jumps) among the eigenstates of $H_f$. The unperturbed Hilbert space for $H$ divides into subspaces, one for each eigenvalue $E_i$ of $H_f$. In the adiabatic limit, the “fast” variables remain in an eigenstate $|\Psi_i(R)\rangle$ of $H_f$, with $i$ fixed, while dynamical and Berry phases of $|\Psi_i(R)\rangle$ show up in $H$ as induced scalar and vector potentials.
Born and Oppenheimer multiplied \(|\Psi_i(R)\rangle\) by a function \(\Phi(R, t)\) and obtained an effective Hamiltonian for \(\Phi(R, t)\). Here we obtain and simplify their effective Hamiltonian algebraically. Let \(\Pi_i\) denote the →operator of projection onto the subspace corresponding to \(E_i\). The subspaces are disjoint and form a complete set: \(\sum_i \Pi_i = 1\). In the adiabatic limit, we can replace \(H_s\) by \(\sum_i \Pi_i H_s \Pi_i\) to obtain the effective Hamiltonian of Born and Oppenheimer:

\[
H_{\text{eff}} = H_f + \sum_i \Pi_i H_s \Pi_i .
\]

In \(H_{\text{eff}}\) there are induced potentials. If

\[
H_s = P^2/2M + V(R) ,
\]

where \(P_i = -i\hbar \partial /\partial R_i\), the sum \(\sum_i \Pi_i H_s \Pi_i\) in \(H_{\text{eff}}\) contains products of the form

\[
\Pi_i P^2 \Pi_i = \sum_j \Pi_i \Pi_j P \Pi_i .
\]

We simplify them by decomposing \(P\) into two parts, \(P = (P - A) + A\). The first part acts only within subspaces; that is, \([P - A, \Pi_i] = 0\) for all \(i\). Only the second part, \(A\), causes transitions among the subspaces. Like a vector potential, \(A\) is somewhat arbitrary: we can add to \(A\) any term that commutes with the \(\Pi_i\). Let us remove this arbitrariness by requiring \(\Pi_i A \Pi_i = 0\) for each \(i\). The effective Hamiltonian for the \(R\) is then [3]

\[
H_{\text{eff}} = H_f + \frac{1}{2M} (P - A)^2 + \frac{1}{2M} \sum_i \Pi_i A^2 \Pi_i + V(R) .
\]

The sum in \(i\) is an induced scalar potential, while \(A\) is an induced vector potential; \(A\) is Berry’s connection \(A_B\) in an off-diagonal gauge. For example, suppose \(H_f = \mu R \cdot \sigma\) as in the spin-1/2 example above. The operators of projection corresponding to \(E_\pm = \pm \mu R\) are

\[
\Pi_\pm = \frac{1}{2} (1 \pm R \cdot \sigma /R) ,
\]

and the vector potential

\[
A = \frac{\hbar R \times \sigma}{2R^2}
\]

solves the two conditions \([P - A, \Pi_\pm] = 0\) and \(\Pi_\pm A \Pi_\pm = 0\); \(A\) is off-diagonal. The field corresponding to \(A\),

\[
B_i = \frac{1}{2} \epsilon_{ijk} F_{jk} = \frac{1}{2} \epsilon_{ijk} (\partial_j A_k - \partial_k A_j - i[A_j, A_k]) = -\frac{\hbar R_i}{2R^4} (R \cdot \sigma) ,
\]

is a monopole field \(B = \mp \hbar R /2R^3\) since the eigenvalues of \(R \cdot \sigma /R\) are \(\pm 1\).
So far we have taken the eigenvalues of $H_f$ to be discrete and nondegenerate. If $H_f$ has a discrete and degenerate eigenvalue, Berry’s phase may be non-abelian [4]. The eigenstates belonging to this eigenvalue do not (in the adiabatic approximation) jump to eigenstates belonging to other eigenvalues, but they may mix among themselves. The mixing amounts to multiplication by a non-abelian phase, i.e. a unitary matrix.

Another generalization of Berry’s phase is the Aharonov-Anandan phase [5]. Suppose a system evolves according to Schrödinger’s equation, but the change in the Hamiltonian is neither adiabatic nor cyclic. Aharonov and Anandan showed that the system can still exhibit a Berry phase; all that is needed is cyclic evolution of the state of the system. Cyclic evolution of a state defines a closed path in the Hilbert space of the state. Whether or not this evolution is adiabatic, it leaves the system with a dynamical phase, which depends on the Hamiltonian of the system, and a geometrical phase—Berry’s phase—which depends only on the closed path of the state in its Hilbert space. Thus Berry’s phase need not be adiabatic (although it is still a correction to the adiabatic theorem).

We have considered evolution consistent with Schrödinger’s equation. But as Pancharatnam showed [6], geometric phases can emerge from nonunitary evolution. For example, let an ensemble be divided into two subensembles, one of which is subjected to a sequence of filtering measurements (projections). If the sub-subensemble that survives this filtering has returned to its initial state, it has a well defined phase (relative to the unfiltered subensemble) which equals a relative dynamical phase plus the Berry phase for this evolution.

Berry’s phase has a classical analogue: Hannay’s angle [7] is a phase effect in a classical periodic system that depends on adiabatically changing parameters. A canonical pair of variables for such a system is an “action” variable $I$, which is an adiabatic constant of the motion, and a conjugate “angle” variable $\phi$. Hannay’s angle is an extra shift in $\phi$ acquired by the system during a cyclic evolution in the space of parameters. When the Hannay angle of a system depends on its action $I$, the corresponding quantum system acquires a Berry phase during the same cyclic evolution [8].

Although the Aharonov-Bohm effect has no classical analogue, we may treat it as an example of Berry’s phase. More generally, however, the Aharonov-Bohm and Berry phases can combine in a topological phase [9]. For example, imagine a “semifluxon”, something like a straight, heavy, infinite solenoid enclosing flux $hc/2e$—exactly half a flux quantum—that moves perpendicular to itself. It interacts with an electron wave function that has support in two disjoint regions. If the semifluxon moves in a slow circuit, we can ask what phase the electron acquires from this adiabatic cyclic evolution. Figure 1 shows one of the two regions where the electron wave function has support, and two possible circuits for the semifluxon. If the semifluxon evolves along $C_1$, the electron acquires no relative Berry phase and also the Aharonov-Bohm phase vanishes. If the semifluxon evolves along $C_2$, the relative Berry phase is $\pi$ and it is entirely the Aharonov-Bohm phase. If the semifluxon does neither but plows through the electron wave function, we might expect the Berry phase to lie between 0 and $\pi$. However, it can be shown (using time-reversal symmetry) that the Berry phase can only be 0 or $\pi$. Since the path of
the semifluxon is arbitrary, at some point \( P \), the Berry phase must jump from 0 to \( \pi \), i.e. the electron wave function must become degenerate when the semifluxon is situated at \( P \). Here the Berry phase and the Aharonov-Bohm phase combine in a single topological phase that depends only on the winding number of the semifluxon path around the point \( P \).

**References**

[Primary]

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[Secondary]

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**Figure Caption**

Fig. 1. An electron cloud with support in a region \( S \) (and in disjoint region not shown) and two possible paths, \( C_1 \) and \( C_2 \), of a semifluxon. At the point \( P \), the semifluxon induces a degeneracy in the energy of the electron.
