Some geometrical considerations of Berry's phase

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A group-theoretic treatment is given of the new phase found by Berry in the adiabatic evolution of a quantum-mechanical system in a finite-dimensional Hilbert space. It is shown how the Berry phases for the various eigenstates of the Hamiltonian are obtained from a set of angles associated with a group element. For the special case of a two-level system there is just one such angle which corresponds to the holonomy transformation associated with parallel transport around a closed curve on a sphere.

Berry[1] has made the interesting observation that there is a phase factor $\exp(i\gamma_n)$ in addition to the familiar dynamical phase factor $\exp[-(i/\hbar)\int E_n dt]$ in the evolution of a system which remains in an eigenstate of a slowly varying nondegenerate Hamiltonian $H(t)$ with eigenvalue $E_n(t)$. It was shown by Simon[2] that this phase can be obtained from the holonomy in the line bundle corresponding to the eigenspace of the eigenvalue $E_n(t)$. Generalization to a degenerate Hamiltonian of the Berry phase was made by Wilczek and Zee.[3]

In the previous papers,[1–3] the Berry phase and its generalization have been treated for a given eigenspace of the $H(t)$. In this paper we give a group-theoretical treatment of this phenomenon and show that the Berry phases for the various subspaces can be obtained from the action of a common group element on each of the subspaces. This not only provides a geometrical meaning to Berry's phase, it also gives a simple prescription for evaluating it at least in the case of a particle with an arbitrary spin interacting with a magnetic field. In this case, the group element mentioned above is the holonomy transformation associated with parallel transport around a closed curve on a sphere which can be easily evaluated. Experimental implications of this result will also be briefly discussed.

Let $\{|n(0)\rangle\}$ be a complete, orthonormal set of eigenstates of $H(0)$ with eigenvalues $E_n(0)$. Suppose also that the unitary operator $U(t)$ diagonalizes $H(t)$ in this basis:

$$U^\dagger(t)H(t)U(t)=H_D(t)=\mathrm{diag}(E_1(t),\ldots,E_N(t)) \tag{1}$$

with $U(0)=I$. Then the Schrödinger equation

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

can be written as

$$H_D(t)\,|\,\psi'(t)\rangle=i\hbar\frac{\partial}{\partial t}\,|\,\psi'(t)\rangle+i\hbar U^\dagger\dot U\,|\,\psi'(t)\rangle\;, \tag{2}$$

where $|\,\psi'(t)\rangle=U^\dagger(t)\,|\,\psi(t)\rangle$ and the dot denotes time derivative. On defining $|\,n(t)\rangle=U(t)\,|\,n(0)\rangle$,

$$H(t)\,|\,n(t)\rangle=E_n(t)\,|\,n(t)\rangle\;. \tag{3}$$

Clearly (1) does not determine U uniquely. But another restriction on U may be imposed by requiring that for every n, $\langle n\,|\,\dot n\rangle=0$ or equivalently

$$\langle n(0)\,|\,U^\dagger(t)\dot U(t)\,|\,n(0)\rangle=0\;. \tag{4}$$

If $H(t)$ is nondegenerate then (1) can be satisfied by a unitary $\tilde U(t)$ if and only if

$$\tilde U(t)=U(t)\mathrm{diag}(e^{i\theta_1(t)},e^{i\theta_2(t)},\ldots,e^{i\theta_N(t)})\;.$$

Also $\tilde U$ satisfies (4) if and only if $\dot\theta_n(t)=-i\langle n(0)\,|\,U^\dagger\dot U\,|\,n(0)\rangle$ which determines θ_n up to a constant which is zero on requiring that $\tilde U(0)=U(0)=I$. This proves that (1), (4), and $U(0)=I$ can be satisfied by a unique $U(t)$. Now in the adiabatic approximation the system remains in an instantaneous eigenstate of $H(t)$ once it starts there. Writing

$$|\,\psi'(t)\rangle=\sum_n a_n(t)\,|\,n(0)\rangle$$

in (2), this implies that the off-diagonal matrix elements of the last term in (2) may be neglected compared to the first term. Therefore with the condition (4), we can neglect the last term entirely and write

$$H_D(t)\,|\,\psi'(t)\rangle=i\hbar\frac{\partial}{\partial t}\,|\,\psi'(t)\rangle \tag{5}$$

which has the solution

$$|\psi(t)\rangle = U(t)\,|\psi'(t)\rangle = U(t)\mathrm{diag}\left[\exp\left[-\frac{i}{\hbar}\int E_1 dt\right],\ldots,\exp\left[-\frac{i}{\hbar}\int E_N dt\right]\right]|\psi(0)\rangle \ . \tag{6}$$

So if $|\psi(0)\rangle = |n(0)\rangle$ then

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\int E_n dt\right]U(t)\,|n(0)\rangle \ .$$

Suppose now that the Hamiltonian is a function of a set of parameters $\mathbf{B}$ and that its time dependence is due to the variation of $\mathbf{B}(t)$ with time. Suppose that $\mathbf{B}(\tau)=\mathbf{B}(0)$ so that $H(\tau)=H(\mathbf{B}(\tau))=H(\mathbf{B}(0))=H(0)$. If H is nondegenerate then $|\psi(\tau)\rangle \propto |n(0)\rangle$. Hence

$$U(\tau)\,|n(0)\rangle = e^{i\gamma_n}\,|n(0)\rangle \ , \tag{7}$$

where γ_n is Berry's phase. So γ_n can be evaluated from $U(\tau)$ which is uniquely determined by (1) and (4). More generally, if $|\psi(0)\rangle = \sum_n b_n\,|n(0)\rangle$, where b_n are constants, then

$$|\psi(\tau)\rangle = \sum_n b_n \exp\left[-\frac{i}{\hbar}\int_0^\tau E_n dt\right]|n(\tau)\rangle$$
$$= \sum_n b_n \exp\left[-\frac{i}{\hbar}\int_0^\tau E_n dt\right]e^{i\gamma_n}\,|n(0)\rangle \ .$$

Thus $|\psi(t)\rangle$ undergoes the usual dynamical evolution with respect to the basis $\{|n(t)\rangle\}$ which are parallel transported according to (4) and acquire the Berry phases when transported around a closed curve in parameter space.

We now give a geometrical interpretation for $U(t)$ in the special case when H is the Hamiltonian of a particle with an arbitrary spin interacting with a magnetic field $\mathbf{B}$. In the rest frame of the particle, we may take the Hamiltonian to be

$$H = \mu\mathbf{J}\cdot\mathbf{B}(t) \ ,$$

where $\mathbf{J}=(J_x,J_y,J_z)$ are the generators of rotation in this representation. (For the special case of a spin-$\frac{1}{2}$ particle, $2J_i=\sigma_i$, the Pauli spin matrices.) Since $U(t)$ satisfies (1), (4), and $U(0)=I$, $U(t)$ must belong to the SU(2) group generated by J_i and it does not rotate about the instantaneous direction of $\mathbf{B}(t)$. This can be proved by noting that a $U(t)\in$ U(2) group, satisfying (1), can be found for a spin-$\frac{1}{2}$ particle (fundamental representation) for which H is a 2×2 Hermitian matrix. Then, (4), written as $\langle n\,|\,\dot{n}\rangle=0$, implies that the diagonal elements of the generator of $U(t)$ at time t has no diagonal elements in the basis $\{|n(t)\rangle\}$. For an arbitrary spin, the same form of $U(t)$, with J^i generating the corresponding representation, will then satisfy (1) and (4) for the same $\mathbf{B}(t)$. So, $U(t)\in$ SU(2) can be regarded as a rotation.

A rotation can be completely specified by giving the orientation of a triad (e_x,e_y,e_z) relative to some starting position. Let us consider the triad representing U. We take it initially to be oriented parallel to the fixed external coordinate system. We also take $\mathbf{B}$ to be initially pointing along the external z axis. The condition (1) obviously means that the triad representing U always has $\mathbf{e}_z$ pointing along $\mathbf{B}(t)$ as $\mathbf{B}$ moves. The condition (4) means that the triad, as it moves, does not rotate around $\mathbf{e}_z$. This may be seen from the condition (4) $\langle n\,|\,\dot{n}\rangle=0$ and from the fact that since $|n(t)\rangle$ is the eigenstate with respect to quantization along $\mathbf{e}_z$, a rotation around $\mathbf{e}_z$ would mean $|n\rangle\rightarrow\exp(i\theta_n)\,|n\rangle$, θ_n is some phase.

The visualization of the motion of the triad is aided by the following construction: Take a sphere S and consider the triad placed on its surface with $\mathbf{e}_z$ perpendicular to the surface. As $\mathbf{B}(t)$ varies, the triad moves on the sphere with its origin at the point of S representing the direction of $\mathbf{B}(t)$ such that it does not rotate about the local direction of $\mathbf{e}_z$. In other words, $\mathbf{e}_x,\mathbf{e}_y$ are *parallel transported* on S. Now let $\mathbf{B}$ return to the external z axis. The triad has gone around a closed curve C on S traced out by $\mathbf{B}(t)$ and so has rotated about the original direction of $\mathbf{e}_z$, because of the curvature on S, by an angle α. U will be rotation around the external z axis giving a Berry phase to each of the original eigenstates:

$$U(\tau)=e^{i\alpha J_z} \ . \tag{8}$$

It is well known that $\alpha=\int_\Sigma R\,d\Sigma$, where R is the Gaussian curvature on the surface and Σ is the part of the surface of S bounded by C defined as follows: If we walk along on the sphere in the direction determined by increasing time then the surface Σ lies to the left. If this direction is reversed then α is changed to $4\pi-\alpha$ which corresponds to taking the Hermitian conjugate of the $U(\tau)$ given by (8). This is to be expected because time reversal involves complex conjugation. We emphasize that the above arguments do not depend on the particular representation of J_i. Since for a sphere $R=(\text{radius})^{-2}$, α is the solid angle subtended by Σ at the center. The phases γ_n, which are then obtained from (7) and (8), are in agreement with the result of Berry.[1]

We now consider the experimental implications of the above purely geometric angle α. Consider the interference of the two coherent beams in a neutron interferometer passing through a slowly spatially varying magnetic field, which can be time independent in the laboratory, and in this respect is somewhat different from the experiment considered by Berry.[1] In the rest frame of the neutron, however, the magnetic field is time dependent and the polarizations of the two beams in the interference region are related by an extra rotation by the angle α defined above, assuming the adiabatic approximation to be valid. Since both eigenstates of σ_z undergo the rotation by the angle α, the experiment can be done even with unpolarized neutrons—the neutron "interferes with itself."

In particular, when $\alpha=2\pi$ there is a phase shift of $\pm\pi$

between the interfering beams for the two eigenstates even though classically there should be no difference between the two spins.[4] Such an experiment would therefore truly demonstrate that a rotation of a fermion by 2π radians is observable. This is different from the experiment of Rauch *et al.* and Werner *et al.*[5] in which there is a phase shift $\pm\pi$ due to the passage of one neutron beam through a suitably chosen homogeneous magnetic field. In the adiabatic method one literally "sees" the spin being rotated, independent of the detailed properties of the neutron, while in the other method one must use the experimental value of the neutron magnetic moment and the time spent in the field to calculate the 2π rotation. Hence the two methods are on a rather different footing, and it would not be *a priori* impossible for them to give different answers, although this would be very surprising. A measurement of the 2π rotation effect by the adiabatic method would therefore be an independent test of the overall consistency of our usual methods for handling spin.

Consider now an arbitrary Hamiltonian H describing an N-level system. Then H may be regarded as an element of the Lie algebra of the unitary group U(N). Since $U(N)=U(1)\times SU(N)$, $H=B_0J_0+\mathbf{B}\cdot\mathbf{J}$, where J_0 generates U(1) and J_i $(i=1,\ldots,N^2-1)$ generate SU(N). But the effect of B_0J_0 on the eigenstates of H is to give just the dynamical phase factor and there is no Berry phase associated with it. Therefore, we shall consider just $H=\mathbf{B}\cdot\mathbf{J}$ where $\mathbf{B}$ are time-dependent parameters. Then there exists $U(t)\in SU(N)$, such that (1) is valid with H_D belonging to the Cartan subalgebra of the Lie algebra of SU(N), generated by $J_1,\ldots,J_{n-1}$, i.e.,

$$U^\dagger(t)H(t)U(t)=\sum_{i=1}^{n-1}B_i'J_i \; .$$

This can be proved[6] by choosing a representation in which $J_1,\ldots,J_{n-1}$ generate the set of real traceless diagonal matrices and U then merely diagonalizes the traceless Hermitian matrix H. Condition (4) may be viewed as follows. Let $U(t+\delta t)$ be written as $U(t)(1+iJ\delta t)$. J is in the Lie algebra, and $1+iJ\delta t$ can be interpreted as the infinitesimal rotation with respect to the local coordinate system, as established by $U(t)$. Then (4) says that J has no diagonal elements, i.e., lies outside of the Cartan subalgebra. Hence (1) and (4) have the following geometrical interpretation: consider an orthonormal frame in a (N^2-1) dimensional parameter space to which we give a Euclidean metric. At $t=0$, the axes are oriented so that $B_i=0$ for $i=N, N+1,\ldots,N^2-1$. Then $U(t)$ corresponds to transporting this frame so that for every t, the $i=N,\ldots,N^2-1$ components of $\mathbf{B}(t)$, with respect to this frame, are zero. Moreover, U is a product of infinitesimal SU(N) transformations such that in each such transformation there is no contribution to the corresponding rotation of this frame from the Cartan subalgebra in the instantaneous basis.

But when $\mathbf{B}(t)$ returns to its original value at $t=\tau$,

$$U(\tau)=\exp\left[i\sum_{j=1}^{N-1}\alpha_jJ_j\right] \tag{9}$$

if H is nondegenerate so that for each eigenstate, $|n(\tau)\rangle$ and $|n(0)\rangle$ are related by a phase factor. Hence, there are $N-1$ angles α_i, which are purely geometric in the sense of being determined by a group-theoretic prescription just from the time dependence of $\mathbf{B}(t)$, that determine the Berry phases γ_n for the various eigenvectors $|n\rangle$ of H according to

$$\exp\left[i\sum_{j=1}^{N-1}\alpha_jJ_j\right]|n\rangle=e^{i\gamma_n}|n\rangle\;,\quad n=1,\ldots,N\;. \tag{10}$$

In general, the variation of $\mathbf{B}(t)$ would be such that $\{H(t)\colon t\in[0,\tau]\}$ generate a subalgebra of the Lie algebra of SU(N). If this subalgebra is compact and connected then there are as many independent angles α_i as the rank of this subalgebra.[6] In principle these angles can be determined by obtaining $U(\tau)$ according to the above prescription.

The transformation (9) can be regarded as the holonomy transformation in a vector bundle, with the parameter space as the base manifold, and each fiber being isomorphic to the N-dimensional Hilbert space. The connection here is determined by condition (4), similar to the connection on the complex line bundle considered by Simon[2] by focusing on just one eigensubspace. In our approach, we also have the associated principal fiber bundle with SU(N), or the subgroup generated by the above-mentioned Lie subalgebra, as the structure group. The holonomy group is then a subgroup of the subgroup generated by the Cartan subalgebra. Since each holonomy transformation and the associated angles α_j are the same for all the representations (associated vector bundles) and for all the eigensubspaces in any given representation, this makes our treatment more geometrical. Moreover, for the SU(2) case, we were able to determine the single angle α from the holonomy of the usual Riemannian connection on a sphere, unlike the holonomy in the line bundle over the parameter space of Simon. An interesting problem is to find similar Riemannian spaces for more general Hamiltonians.

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[1]M. V. Berry, Proc. R. Soc. London **A392**, 45 (1984).
[2]B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).
[3]F. Wilczek and A. Zee, Phys. Rev. Lett. **52**, 2111 (1984).
[4]Y. Aharonov and L. Susskind, Phys. Rev. **158**, 1237 (1967) have also considered the rotation by 2π radians of an electron wave function by adiabatically rotating a magnetic field applied in the z direction along the spin, with the corresponding rotation operator being $R_x = e^{i2\pi J_x} = -I$. In our treatment, which is valid for arbitrary variation of the magnetic field, the rotation operator is $e^{i\alpha J_z}$ for a closed orbit. But for the above special case, $\alpha = 2\pi$ and the two results are in agreement.
[5]H. Rauch *et al.*, Phys. Lett. **54A**, 425 (1975); S. A. Werner *et al.*, Phys. Rev. Lett. **35**, 1053 (1975).
[6]This property is valid for any connected compact group of which SU(N) is a special case. See, for example, P. Goddard, J. Nuyts, and D. Olive, Nucl. Phys. **B125**, 1 (1977), pp. 2 and 7 and W. Greub, S. Halperin, and R. Vanstone, *Connections, Curvature and Cohomology II: Lie Groups Principal Bundles and Characteristic Classes* (Academic, New York, 1973), p. 92. It follows that the present treatment is valid more generally when SU(N) is replaced by a compact, connected Lie group.