Cyclic Evolution in quantal systems
and the Adiabatic Approximation:

The "Physics" versus the "Math" point of view

Suzanne Malitz
Math 1899, Prof. Marsden
Dec. 14, 1990
Abstract


Berry considers adiabatic evolutions in parameter space while Aharonov-Anandan consider cyclic evolution in the state space of the system.

The two formulations correspond under the appropriate limit (the adiabatic approximation).
Introduction

In quantum mechanics geometric phases can be used to explain diverse phenomena, from the rotation of spins by a magnetic field to the Aharonov-Bohm effect. The nature of these geometric phases generated in quantum systems can be explained in two fundamentally different yet related ways. One method assumes that the phase results from a cyclic evolution in the parameter space of the system. Berry uses this approach to study the geometric phase due to the adiabatic change of a system's environment. Aharonov and Anandan derive this same geometric phase as a limiting case of the phase acquired by a state in a general cyclic evolution. This general cyclic evolution occurs in a reduced state space of the system rather than in its "parameter" space. The relationship between
the two formulations is considered.

**Berry's Phase**

Consider a state \( |\psi(r)\rangle \) which is in an eigenstate of \( H(R) \), so \( |\psi(r)\rangle = |n(R)\rangle \) where \( |n(R)\rangle \) is one of the basis states of \( H(R) \) and \( |n(R)\rangle \) obey the Schrödinger equation:

\[
H(R) |n(R)\rangle = E_n(R) |n(R)\rangle.
\]  

(1)

If we change \( H(R) \) adiabatically by varying the parameters \( R \), then \( |n(R)\rangle \) will still describe the state of the system when \( R(t) \neq R(0) \).

An adiabatic change in \( H(R) \) means that

\[
\Delta t \gg \frac{\Delta}{\Delta E},
\]

where \( \Delta t \) is the time scale of the system and \( \Delta E = E_n - E_m \).

The energy change \( \frac{dH}{dt} \) of the system is provided the change occurs slow enough. Berry considers a closed circuit \( C \) in what he calls the parameter space of \( H(R) \).
such that \( R(T) = R(0) \). In a general sense, we can consider \( \langle \Psi(t) | n(R) \rangle \) as a point in a manifold \( \mathcal{M} \) (= Hilbert space for the system at fixed parameters \( R \)). Then \( T\mathcal{M} \) at \( \langle \Psi | n(R) \rangle \), the tangent space at \( \langle \Psi | n(R) \rangle \), contains tangent vectors which represent adiabatic variations in the parameters \( R \) of \( H(R) \). The change in \( H(R) \) must be adiabatic or else the circuit would not remain in \( T\mathcal{M} \) of \( \langle \Psi | n(R) \rangle \).

\[ \Phi = \mathcal{H} \]

So at time \( t = T \), \( R(T) = R(0) \)

and

\[ \langle \Psi(t) | n(R) \rangle = \exp \left\{ \frac{-i}{\hbar} \int_0^T dt \mathcal{E}_n(R(t)) \right\} \exp \left( i \mathcal{H}_n(t) \right) \langle n(R(t)) | n(R(0)) \rangle \quad (2) \]

However, in writing \( \langle \Psi(t) | n(R) \rangle \), we have assumed that \( \langle \Psi | n(R) \rangle \) is single valued in \( T\mathcal{M} \), and that \( \mathcal{H}_n(t) \) is differentiable. The first phase factor in \( \langle \Psi(t) | n(R) \rangle \)
is just the dynamical phase, which expresses the passage of time for the system. It has no effect on the energy $\mathcal{E}_n\left(\psi(t)\right)$. The second phase factor $\exp(i\psi_n(t))$, as we will see, results from the geometry of the circuit $C$ in $\mathbb{T}_Q$. It has two important properties:

1) It is coordinate independent, so it is a global rather than a local property of the circuit $C$ in $\mathbb{T}_Q$.

2) It is not (generally) single valued.

$$\psi_n(T) \neq \psi_n(0) \quad (3)$$

The second property implies that this phase is observable.

To find an explicit formula for $\psi_n(t)$, Berry substitutes $14(t)$ in (2) into

$$H(\psi(t)) = \text{Im} \frac{d}{dt} 14(t) \quad (4)$$
the Schrödinger equation. Then
\[
\mathcal{T}_n(c) = i \int_0^T dt \langle n(c(t)) | \partial_t n(c(t)) \rangle - \frac{dR}{dt} \\
= i \oint c \partial_R - \langle n(c) | \partial_R n(c) \rangle ,
\]
\[\tag{5}\]

Clearly \( \mathcal{T}_n(c) \) is real because \( \partial_R \langle n | n \rangle = \partial_R 1 = 0 \), and \( c \) is the circuit in \( T\Phi \). In this form, \( \mathcal{T}_n(c) \) is independent \( \Phi \) the parametrization of the circuit \( c \) (as long as \( H(c) \) still changes adiabatically).

To gain some physical intuition into the expression for \( \mathcal{T}_n(c) \), Berry considers the case where \( T\Phi \) is 3-dimensional. Then Stokes' theorem says:
\[
\mathcal{T}_n(c) = - \text{Im} \oint_c dS \cdot \partial_R \times \langle n(c) | \partial_R n(c) \rangle \\
= - \oint_c dS \cdot V_n(R) ,
\]
\[\tag{6}\]
\[\tag{7}\]
where \( V_n(R) \equiv \text{Im} \sum_{m \neq n} \frac{\langle n(c) | \partial_R H(c) | m(c) \rangle \times \langle m(c) | \partial_R H(c) | n(c) \rangle}{(E_m(R) - E_n(R))^2} \)
\[\tag{8}\]

If \( T\Phi \) is 3-dimensional, \( V_n(R) \) becomes a 2-form
and $\mathcal{F}_n(c)$ is the integral of this two form over a surface in $\mathcal{T}\mathcal{Q}$ bounded by $C$. This two form, however, may not be symplectic, if the manifold $\mathcal{T}\mathcal{Q}$ does not have a symplectic structure.

Moreover, $V_n(R)$ is independent of the phase relationship between different vectors $\mathcal{I}\mathcal{N}(c_R)\rangle$ in $\mathcal{T}\mathcal{Q} \mathcal{I}\mathcal{N}(c_R)\rangle$, thus, any basis of $\mathcal{I}\mathcal{N}(c)\rangle$ which satisfy

$$H(c)\mathcal{I}\mathcal{N}(c)\rangle = E_n(c)\mathcal{I}\mathcal{N}(c)\rangle$$

may be used to compute $\mathcal{F}_n(c)$. Nor is single-valuedness of $\mathcal{I}\mathcal{N}(c)\rangle$ required since $\mathcal{F}_n(c)$ does not depend on $\mathcal{I}\mathcal{N}(c)\rangle$ being differentiable. Instead, only $H(R)$ must be differentiable. In 3 dimensions (i.e., $\mathcal{T}\mathcal{Q}$ in 3-dimensional) $\mathcal{F}_n(c)$ can be interpreted as the "flux" through a surface in $\mathcal{T}\mathcal{Q}$ bounded by $C$ where $V_n(R)$ is analogous to a magnetic field. This description is valid
in higher dimensions except for the analogy of $V_4(r)$ with a magnetic field.

Berry then goes on to give several examples of how $\gamma_n(c)$ can be calculated. The first two examples study the effect of a circuit around a degeneracy in $T_4$. In these examples, the connection between parameter space and the state space of the system is less clear.

Simplest Case: a two-state system (spinor system)

Suppose $T_4 = \mathbb{R}^3$, then for

$$H(r) = \frac{1}{2} \begin{bmatrix} z & x-i\chi \\ x+i\chi & -z \end{bmatrix},$$

(10)

there is a degeneracy (due to symmetry) at the origin. Then

$$\nabla H(r) = \frac{1}{2} \hat{\sigma},$$

(11)

where $\hat{\sigma} =$ Pauli Spin Matrices, and $\{\ket{1}, \ket{-1}\}.$
is a natural choice of eigenstates.

Calculating $V_+(R) = \frac{1}{2R^2}$ for $k$ along $R$

$$= \frac{\hat{R}}{2R^2} \text{ for } \hat{k} \text{ in a general direction}$$

So

$$\sigma_+(C) = -\int_C dS \cdot \frac{\hat{R}}{2R^2} = -\frac{1}{2} \sigma(C), \quad (12)$$

where $\sigma(C)$ is the solid angle subtended by the circuit in $\mathbb{R}^3$.

General Case: Spin Rotation by a $B$-field

Parameter space $= (B_x, B_y, B_z)$

and $\hat{A}(B) = k \cdot B \cdot \hat{S}$, \quad (13)

where $\hat{A}(B) |n, s\rangle = k |n, s\rangle$. \quad (14)
so, once again the point of degeneracy occurs at the origin of parameter space. This time the degeneracy is 2S + 1-fold where S = integer or half integer (for $S = \frac{1}{2}$, this reduces to the previous example).

A similar analysis, using

$$\nabla_{\vec{b}} H(\vec{B}) = k \hat{\vec{b}} \vec{S},$$

with $
\vec{S} = (S_+, S_-, S_z) = (S_x + iS_y, S_x - iS_y, S_z)$

gives the analogous results

$$V_n(\vec{B}) = \frac{n \hat{\vec{b}}}{B^2} \quad \text{for } \vec{B} \text{ along a general direction},$$

and

$$\varphi_n(\vec{c}) = -n \varphi(\vec{c}),$$

where $n$ is the eigenvalue of the component of the spin along $\vec{B}$. What is surprising (and the reason for not made very clear in Berry's paper) is that $\varphi_n(\vec{c})$ is independent of the amount of degeneracy in the system, i.e., $\varphi_n(\vec{c})$ is independent
of $g$. The point of degeneracy can be seen as a "point" $g$ intersection of the tangent spaces of the degenerate states for a particular value of $g$. That is, the amount of degeneracy does not contribute to the phase $\delta \tau(g)$ must correspond to these tangent spaces being somehow distinct.

The last example Berry discusses is the Aharonov-Bohm effect, which shows the physical significance of the vector potential in quantum mechanics even in a region where $B = 0$. In this case $B$ is static, so there is no cyclic evolution in parameter space. This raises the question: what are the necessary (and sufficient) conditions on $\Psi(R)$ and/or $H(R)$ for a cyclic evolution to occur? Is there an underlying structure to such cyclic evolutions?
In 1987, Aharonov and Anandan published a paper which attempts to answer these questions. Rather than consider a cyclic evolution as occurring in the parameter space of HCR, they consider general cyclic evolutions of $|\Psi(t)\rangle$ in state space (projective Hilbert space). They show that a cyclic evolution in parameter space is neither a necessary nor a sufficient condition for a cyclic evolution in state space. Berry's phase comes out of taking the limiting case where $H(\tau)$ changes adiabatically.

**Derivation:**

Consider a state $|\Psi(t)\rangle$ in Hilbert space ($\equiv \mathcal{H}$) such that $\langle \Psi(t) | \Psi(t) \rangle = 1$.

and $H(\tau)|\Psi(t)\rangle = i\hbar \frac{d}{dt} |\Psi(t)\rangle$.

(18)

The Schrödinger equation determines the evolution
of the state \( |\psi(t)\rangle \). After some time \( T \)

\[
|\psi(T)\rangle = e^{i\Phi} |\psi(0)\rangle,
\]

where \( \Phi = \text{total phase} = \text{dynamical + geometric phases} \).

In general, the curve \( C \) defined in Hilbert space by \( C : [0, T] \to H \) does not define a closed circuit in \( H \). To consider a cyclic evolution of \( |\psi(t)\rangle \), make the projection:

\[
\Pi : H \to \Phi
\]

\[
|\psi\rangle \rightarrow \frac{|\psi\rangle}{\phi}, \quad |\psi\rangle = e^{i\Phi} |\psi\rangle, \quad \phi \text{ complex}.
\]

That is, quotient \( C \) out of \( H \) by \( \frac{|1\psi\rangle}{\phi} \times \phi_{\geq 0} \)

\[
\frac{|1\psi\rangle}{\phi} = \frac{|\psi\rangle}{\phi}.
\]

(Thus is an example of reductio.) Then \( \Pi(C) = \hat{C} \)

where \( \hat{C} \) is a closed curve in \( \Phi = \text{projective Hilbert space} \) (the quotient space).
Pictorially:

\[ |\psi(t)\rangle = e^{i\phi} |\psi(0)\rangle \]

\[ H \in |\psi(t)\rangle \]

\[ |\psi(t)\rangle = |\psi(0)\rangle \]

In particular, consider

\[ \pi : X \to P \]

\[ |\tilde{\psi}(t)\rangle = e^{-i\tilde{f}(t)} |\psi(t)\rangle \quad (21) \]

For \( |\psi(t)\rangle \) satisfying \( \langle \psi(t) | \psi(t) \rangle = 1 \), such that

\[ f(t) - f(0) = \phi \quad (22) \]

Thus \( |\tilde{\psi}(t)\rangle \) defines a closed circuit in \( P \).

Then plug \( |\psi(t)\rangle = e^{if(t)} |\tilde{\psi}(t)\rangle \) into the Schrödinger equation and subtract out the
dynamical phase \[ \frac{t}{\pi} \int_0^t \langle 4(t) \hat{1} 1 4(t) \rangle \mathrm{d}t. \]

This leaves

\[ \beta = \phi - \text{dynamical phase} \]

\[ = \int_0^t \mathrm{d}t \langle \hat{\Phi}(t) \mid \frac{i}{\hbar} \frac{\mathrm{d}}{\mathrm{d}t} \mid \hat{\Phi}(t) \rangle \]

as the geometric phase. Here, "geometric" refers to the geometry of the circuit in \( \mathcal{P} \). The phase \( \beta \) is independent of the particular \( H(t) \) chosen and of the total phase \( \phi \). For any \( H(t) \), we can find \( \hat{f}(t) \) such that \( \hat{1} 4(t) = e^{i \hat{f}(t) \hat{1} 4(t)} \)

satisfies the Schrödinger equation. Proper choice for any curve \( \gamma \) in \( \mathcal{H} \)

\( \hat{f}(t) \) also enables us to use the same \( \hat{1} 4(t) \) for all curves \( \gamma \) in \( \mathcal{H} \) for which \( \pi(\gamma) = \hat{C} \). Thus \( \beta \) is also independent of the time parametrization of \( \hat{C} \) in \( \mathcal{P} \).

How does this relate to Berry's phase?
A closer look at the adiabatic approximation

Let's examine \[ |\psi(t)\rangle = \sum_n a_n(t) \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t \sum_n E_n(t') dt' \right\} |\psi_{t_0}\rangle \] (24)

which is a solution of \[ H_0 |\psi\rangle = \hbar \frac{d}{dt} |\psi\rangle \],

and where \[ H_0 |\psi\rangle = E_n |\psi\rangle \] . (25)

Differentiating (25) we get

\[ \hbar \frac{d}{dt} \sum_n a_n(t) |\psi_{t_0}\rangle \equiv \hbar \sum_n \frac{d}{dt} a_n(t) |\psi_{t_0}\rangle + \sum_n E_n a_n(t) |\psi_{t_0}\rangle \] (26)

Substituting \[ |\psi(t)\rangle \] into the above equation, we find:

\[ \dot{a}_m = -a_m \langle m | H_1 | n \rangle - \sum_{n \neq m} \frac{\langle m | H_1 | n \rangle}{E_n - E_m} \exp \left\{ \frac{-i}{\hbar} \int_{t_0}^t (E_m - E_n) dt' \right\} \] (27)

and for \[ n \neq m \]

\[ a_n(t) \approx \frac{\langle m | H_1 | n \rangle}{(E_n - E_m)^2} \left( \exp \left\{ \frac{-i}{\hbar} \int_{t_0}^t (E_m - E_n) dt' \right\} - 1 \right) \] (28)

So, for an adiabatically changing \[ H(t) \]

\[ \left| \sum_{n \neq m} \frac{\langle m | H_1 | n \rangle}{(E_n - E_m)^2} \right| \ll 1 \] (29)

and if \[ a_n(t_0) = \delta_{mn} \].
Then: (1) the probability amplitude \( \|a_m(t)\|^2 \) stays constant in time.

(2) the state \( |\psi(t)\rangle \rightarrow |m(t)\rangle \), so the corresponding geometric phase \( \beta \) is given by:

\[
\beta = \int_0^T -i \langle m(t) | \dot{m}(t) \rangle dt
\]

\[
\approx \int_0^T -i \langle m(t) | \hat{m}(t) \rangle \cdot \delta R \cdot dt
\]

\[
= -i \oint \langle m | \nabla_R m \rangle \cdot \delta R = \text{Berry's result.}
\]

Since \( \beta \) is \( \text{H} \)-independent, as we have previously seen, then we can always find an \( \text{H}(t) \) such that the adiabatic approximation will be valid for a given curve \( C \) in \( \mathcal{P} \). This makes the computation of the geometric phase much simpler. It also shows that there is a connection between a cyclic evolution in state space and a cyclic evolution in "parameter" space.
(Theoretical) Advantages of the Aharonov–Anandan Formulation:

The Aharonov–Anandan formulation uses the symplectic structure of Hilbert space (and projective Hilbert space) in order to define the geometric phase $\beta$. The geometric phase is equivalent to the symplectic area of any 2-dimensional surface (submanifold) in $\mathcal{H}$ which is bounded by $\hat{\mathcal{O}}$. Namely, for $\Omega: \mathcal{H} \times \mathcal{H} \to \mathbb{C}$

$$\beta = \frac{i}{\hbar} \int_{t_0}^{t} \Omega(\hat{\psi}, \dot{\hat{\psi}}) \, dt,$$  

(33)

where

$$\Omega(\psi_1, \psi_2) = -2\hbar \text{Im} \langle \psi_1, \psi_2 \rangle$$  

(34)

Thus $\beta$ is invariant under canonical transformations of $\{ \psi \}$'. These transformations are the projection maps $\Pi: \mathcal{H} \to \mathcal{P}$ for which $\Pi(\mathcal{O}) = \hat{\mathcal{O}}$ for some $\hat{\mathcal{O}} \in \mathcal{P}$. 
Conclusion:

Berry's phase is examined as a limiting case of the more general geometric phase derived by Aharonov and Anandan. Aharonov and Anandan's paper also gives a clearer mathematical foundation for the origin reduction techniques of these phases using n. Berry gives a more intuitive physically yet less mathematically viable explanation of these phases.

References:


Schiff, Quantum Mechanics, 1955, McGraw-Hill