Cyclic Evolution in quantal systems and the Adiabatic Approximation: The "Physics" versus the "Math" point of view

Suzanne Malitz
Math 189, Prof. Marsden
Dec. 14, 1990

Abstract

A comparison of papers by Berry (1984) and Aharonov and Anandan (1987) concerning geometric phases involved in quantum cyclic evolution. Berry considers adiabatic cyclic 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 Aharanov 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. Aharanov and Anandan derive this same geometric phase as a limiting case of the phase aquired 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 $|n(R)\rangle$ obeys the schrödinger equation:

$$H(R)\,|n(R)\rangle = E_n(R)\,|n(R)\rangle \quad . \qquad (1)$$

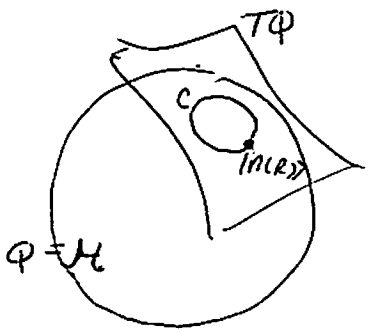
If we change $H(R)$ adiabatically by varying the parameters R, then $|n(R)\rangle$ will still ~~be~~ describe the state of the system when $R(t) \neq R(0)$. An adiabatic change in $H(R)$ means that

$\Delta t \gg \frac{\hbar}{\Delta E}$ where Δt is the time scale of the energy change $\frac{d}{dt}H(R)$ of the system. No restriction is placed on ΔE provided the change occurs slow enough. Berry considers a closed circuit C in what he calls the parameter space of $H(R)$;

and $\Delta E = E_n - E_m$

Δ the total change in the energy of an eigenstate

such that $R(T) = R(0)$. In a general sense, we can consider $|\psi(R)\rangle = |n(R)\rangle$ as a point in a manifold $\mathcal{Q}$ (= Hilbert space for the system at fixed parameters R). Then $T\mathcal{Q}$ at $|n(R)\rangle$, the tangent space at $|n(R)\rangle$ 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 $T\mathcal{Q}$ of $|n(R)\rangle$.



so at time $t = T$, $R(T) = R(0)$

and

$$|\psi(T)\rangle = \exp\left\{\frac{-i}{\hbar}\int_0^T dt\, E_n(R(t))\right\} \exp(i\gamma_n(T)) \,|n(R(T))\rangle \quad . \quad (2)$$

However, in writing $|\psi(T)\rangle$, we have assumed that ① $|n(R)\rangle$ is single valued in $T\mathcal{Q}$, and ② that $\gamma_n(t)$ is differentiable. The first phase factor in $|\psi(T)\rangle$

is just the dynamical phase, which expresses the passage of time for the system. It has no effect on the energy of $|\psi(t)\rangle$. The second phase factor, $\exp(i\gamma_n(T))$, as we will see, results from the geometry of the circuit in TQ. It has two important properties:

1.) It is coordinate independant, so it is a global rather than a local property of the circuit C in TQ

2.) It is not (generally) single valued.

$$\gamma_n(T) \neq \gamma_n(0) \qquad (3)$$

The second property implies that this phase is observable.

To find an explicit formula for $\gamma_n(t)$, Berry substitutes $|\psi(t)\rangle$ in (2) into

$$H|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle, \qquad (4)$$

the Schrödinger equation. Then

$$\gamma_n(C) = i\int_0^T dt \langle n(R(t))|\nabla_R n(R(t))\rangle \cdot \frac{dR}{dt}$$

$$= i\oint_C dR \cdot \langle n(R)|\nabla_R n(R)\rangle \quad . \qquad (5)$$

Clearly $\gamma_n(C)$ is real because $\nabla_R\langle n|n\rangle = \nabla_R 1 = 0$, and C is the circuit in TQ. In this form, $\gamma_n(C)$ is independant of the parametrization of the circuit C (as long as $H(R)$ still changes adiabatically).

To gain some physical intuition into the expression for $\gamma_n(C)$, Berry considers the case where TQ is 3-dimensional. Then Stokes theorem says:

$$\gamma_n(C) = -\mathrm{Im}\iint_C dS \cdot \nabla_R \times \langle n(R)|\nabla_R n(R)\rangle \qquad (6)$$

$$= -\iint_C dS \cdot V_n(R) \quad , \qquad (7)$$

where $$V_n(R) \equiv \mathrm{Im}\sum_{m\neq n} \frac{\langle n(R)|\nabla_R H(R)|m(R)\rangle \times \langle m(R)|\nabla_R H(R)|n(R)\rangle}{\left(E_m(R) - E_n(R)\right)^2} \qquad (8)$$

If TQ is 4-dimensional, $V_n(R)$ becomes a 2-form

and $\gamma_n(C)$ is the integral of this two form over a surface in TQ bounded by C. This two form, however, may not be symplectic, if the manifold TQ does not have a symplectic structure.

Moreover, $V_n(R)$ is independent of the phase relationship between different vectors $|n(R(t))\rangle$ in TQ of $|n(R(0))\rangle$, thus, any basis $\{|n(R)\rangle\}$ which satisfy

$$H(R)|n(R)\rangle = E_n(R)|n(R)\rangle \qquad (9)$$

may be used to compute $\gamma_n(C)$. Nor is single-valuedness of $|n(R)\rangle$ required since $\gamma_n(C)$ does not depend on $|n(R)\rangle$ being differentiable. Instead, only $H(R)$ must be differentiable. In 3-dimensions (ie. TQ is 3-dimensional) $\gamma_n(C)$ can be interpreted as the "flux" through a surface in TQ bounded by C where $V_n(R)$ is analagous to a magnetic field. This description is valid

in higher dimensions except for the analogy of $V_n(R)$ 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 point of degeneracy in TQ. 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 $TQ = \mathbb{R}^3$, then for

$$H(R) = \frac{1}{2}\begin{bmatrix} Z & X-iY \\ X+iY & -Z \end{bmatrix}, \tag{10}$$

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

$$\nabla H(R) = \frac{1}{2}\hat{\sigma}, \tag{11}$$

where $\hat{\sigma}$ = Pauli spin matrices, and $\{|n\rangle\} = \{|+\rangle, |-\rangle\}$

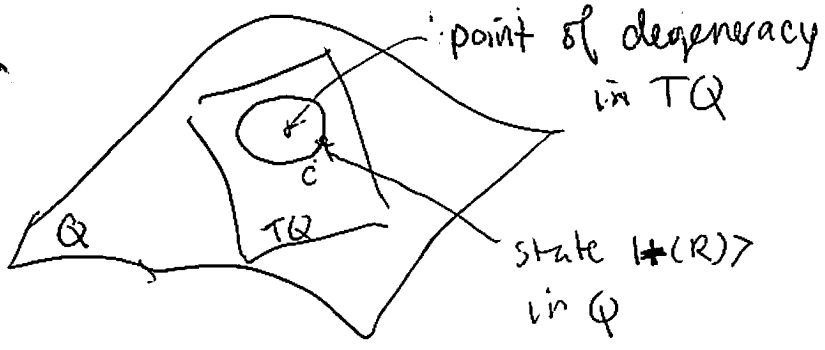
is a natural choice of eigenstates.

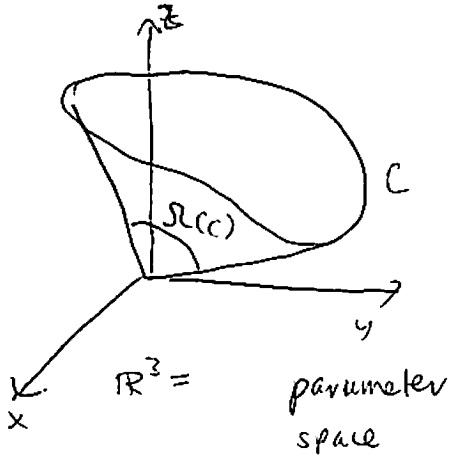
Calculating $V_+(R) = \frac{1}{2R^2}$ for $\hat{k}$ along R

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

So $$\gamma_+(C) = -\iint_C dS \cdot \frac{\hat{R}}{2R^2} = -\frac{1}{2}\Omega(C) \quad , \qquad (12)$$

where $\Omega(C)$ is the solid angle subtended by the circuit in TQ





General Case : Spin Rotation by a B-field

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

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

where $$\hat{H}(B)|n,s\rangle = k\hbar n |n,s\rangle \qquad (14)$$

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

$$\nabla_B H(B) = K\hbar\hat{S}, \tag{15}$$

with $\hat{s} = (S_+, S_-, S_z) = (S_x+iS_y, S_x-iS_y, S_z)$

gives the analagous results

$$V_n(B) = n\frac{\hat{B}}{B^2} \quad \text{for } \vec{B} \text{ along a general direction}, \tag{16}$$

and

$$\gamma_n(C) = -n\Omega(C), \tag{17}$$

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 $\gamma_n(C)$ is independant of the amount of degeneracy in the system, i.e. $\gamma_n(C)$ is independant

of s. The point of degeneracy can perhaps be seen as a "point" of intersection of the tangent spaces of the degenerate states for a particular value of R. That is, the amount of degeneracy does not contribute to the phase $\gamma_n(C)$ must correspond to these tangent spaces being somehow distinct.

The last example Berry discusses is the Aharanov-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 questions:

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, Aharanov and Anandan published a paper which attempts to answer these questions. Rather than consider a cyclic evolution as occurring in the parameter space of $H(R)$, 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 $H(R)$ 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 $$H(t)|\psi(t)\rangle = i\hbar \frac{d}{dt}|\psi(t)\rangle, \qquad (18)$$

the Schrödinger equation, determines the evolution

of the state $|\psi(t)\rangle$. After some time τ

$$|\psi(\tau)\rangle = e^{i\phi}\,|\psi(0)\rangle\,, \tag{19}$$

where ϕ = total phase

= dynamical + geometric phases,

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

$$\pi : \mathcal{H} \longrightarrow \mathcal{P}$$

$$|\psi\rangle \longmapsto \{|\psi'\rangle : |\psi'\rangle = c|\psi\rangle\,,\ c \text{ complex}\}\,. \tag{20}$$

That is, quotient $\mathbb{C}$ out of $\{|\psi\rangle\}$ ($\mathbb{C} \subset \mathcal{H}$), so

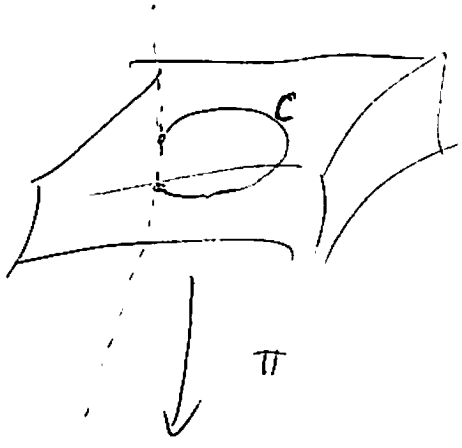
$\{|\psi'\rangle\} \cong \{|\psi\rangle\}/\mathbb{C}$. (This is an example of reduction.) Then $\pi(C) = \hat{C}$

where $\hat{C}$ is a closed curve in $\mathcal{P}$ = projective Hilbert space (the quotient space)

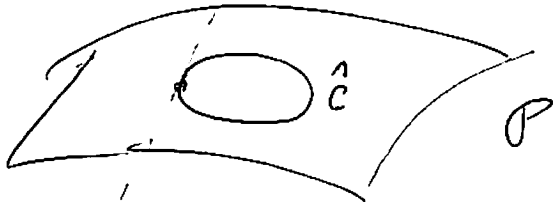
Pictorially:

$|\psi(\tau)\rangle = e^{i\phi}|\psi(0)\rangle$

$\neq |\psi(0)\rangle$



$|\psi'(\tau)\rangle = |\psi'(0)\rangle$



In particular, consider

$$\pi : \mathcal{H} \longrightarrow \mathcal{P}$$

$$|\tilde{\psi}(t)\rangle = e^{-if(t)}|\psi(t)\rangle \,, \tag{21}$$

for $|\psi(t)\rangle$ satisfying $\langle\psi(t)|\psi(t)\rangle = 1$,

such that

$$f(\tau) - f(0) = \phi \,. \tag{22}$$

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

Then plug $|\psi(t)\rangle = e^{if(t)}|\tilde{\psi}(t)\rangle$ into the Schrödinger equation and subtract out the

dynamical phase $\frac{1}{\hbar}\int_0^\tau \langle\psi(t)|H|\psi(t)\rangle dt$.

This leaves

$$\beta \equiv \phi - \text{dynamical phase}$$
$$= \int_0^\tau dt \langle \tilde{\psi}(t)| i\frac{d}{dt}|\tilde{\psi}(t)\rangle \qquad (23)$$

as the geometric phase. Here, "geometric" refers to the geometry of the circuit in $\mathcal{P}$. The phase β is independent of the particular $H(t)$ chosen and of the total phase ϕ. For any $H(t)$, we can find $f(t)$ such that $|\psi(t)\rangle = e^{if(t)}|\tilde{\psi}(t)\rangle$ satisfies the Schrödinger equation. Proper choice of $f(t)$ (for any curve C in $\mathcal{H}$) also enables us to use the same $|\tilde{\psi}(t)\rangle$ for all curves C in $\mathcal{H}$ for which $\pi(C) \equiv \hat{C}$. Thus β 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 $$|\psi(t)\rangle = \sum_n a_n(t) \exp\left\{\frac{-i}{\hbar}\int E_n(t')dt'\right\}|n(t)\rangle \qquad (24)$$

which is a solution of $H|\psi\rangle = i\hbar \frac{d}{dt}|\psi\rangle$,

and where $$H|n\rangle = E_n|n\rangle \,. \qquad (25)$$

Differentiating (25) we get

$$\frac{\partial H}{\partial t}|n\rangle + H\frac{\partial}{\partial t}|n\rangle = \frac{\partial E_n}{\partial t}|n\rangle + E_n\frac{\partial|n\rangle}{\partial t} \,. \qquad (26)$$

Sustituting $|\psi(t)\rangle$ into the above equation.

we found:

$$\dot{a}_m = -a_m\langle m|\dot{m}\rangle - \sum_{n\neq m}\frac{\langle m|\dot{H}|n\rangle}{(E_n-E_m)}\exp\left\{\frac{i}{\hbar}\int(E_m-E_n)\,dt\right\} \qquad (27)$$

and for $n \neq m$

$$a_n(t) \cong \frac{\hbar\langle m|\dot{H}|n\rangle}{(i(E_m-E_n))^2}\left(\exp\left\{\frac{i}{\hbar}\int(E_m-E_n)dt\right\} - 1\right) \,. \qquad (28)$$

So, for an adiabatically changing $H(t)$

$$\left|\sum_{n\neq m}\frac{\hbar\langle m|\dot{H}|n\rangle}{(E_n-E_m)^2}\right| \ll 1 \,, \qquad (29)$$

and if $a_n(0) = \delta_{mn}$,

then: (1) the probability amplitude $|a_m(t)|^2$ stays $\approx$ constant in time

(2) the state $|\psi(t)\rangle \longrightarrow |m(t)\rangle$, so

The corresponding geometric phase β is given by:

$$\beta = \int_0^T -i \langle m(t) | \dot{m}(t) \rangle dt \tag{30}$$

$$\approx \int_0^\tau -i \langle m(t) | \nabla_R m(t) \rangle \cdot \frac{dR}{dt} dt \tag{31}$$

$$= -i \oint_C \langle m | \nabla_R m \rangle \cdot dR \quad = \text{Berry's result.} \tag{32}$$

Since β is ### independant, as we have previously seen, then we can always find an $H(t)$ such that the adiabatic approximation will be valid for a given curve $\hat{C}$ 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 β. The geometric phase is equivalent to the symplectic area of any 2-dimensional surface (submanifold) in $\mathcal{P}$ which is bounded by $\hat{C}$. Namely, for $\Omega : \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C}$

$$\beta = \frac{i}{\hbar}\int_0^\tau -\Omega(\tilde{\Psi}, \dot{\tilde{\Psi}})\,dt \quad , \tag{33}$$

where $$\Omega(\Psi_1, \Psi_2) = -2\hbar\, \mathrm{Im}\langle \Psi_1, \Psi_2 \rangle \tag{34}$$

Thus β is invariant under canonical transformations of $|\Psi(H)|$. These transformations are the projection maps $\pi : \mathcal{H} \to \mathcal{P}$ for which $\pi(C) = \hat{C}$ for some $\hat{C} \subset \mathcal{P}$.

Conclusion:

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

References:

Y. Aharanov & J. Anandan, "Phase Change during a Cyclic Quantum Evolution". Phys. Rev. Lett. 58, 1593 (1987)

M. Berry, "Qrantal Phase factors accompanying adiabatic changes", Proc. R. Soc. Lond. A 392, 45-57 (1984

M. Berry "The Geometric Phase" Scientific American, p.46-57, Dec. 1988

Schiff. Quantum Mechanics, 1955, McGraw-Hill