Lecture 7/11

BERRY PHASES AND CURVATURES

The Berry phase is the most important concept in the study of symmetry-protected topological phases of matter. It refers to the phase angle that describes the global phase evolution of a complex vector as it is carried around a path in its vector space. It has its name after Michael Berry who, in a famous paper from 1984 [1], showed that its presence is a generic property of quantum mechanical systems. The phase had been discussed earlier, first by Pancharatnam in 1956 [2] when analyzing interference effects of polarized light. But the deeper understanding of its importance and generic role is due to Berry.

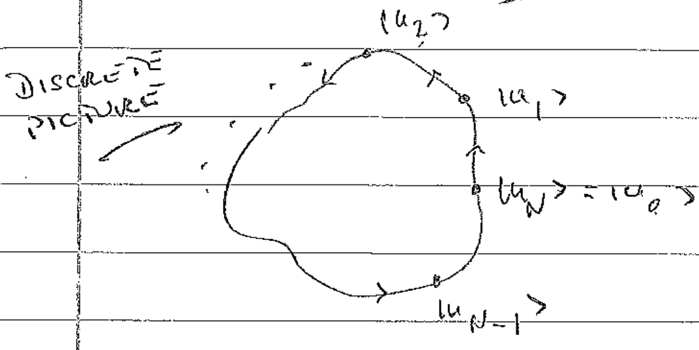
The concept entered into the study of topological phases, more specifically the IQHE and one year before Berry's paper was published*, in a work by Barry Simon [3] who showed that the "TKNN invariant"** is a Chern number with its origin in a Berry phase. More about that later. Here we will lay the groundwork and explore the basic math and physics of Berry phases.

1) M.V. Berry, Proc. Roy. Soc. London, Ser A 392, 45 (1984)
2) S. Pancharatnam, Proc. Indian Acad. Sci A44, 247 (1956)
3) B. Simon, Phys. Rev. Lett. 51, 2167 (1983)

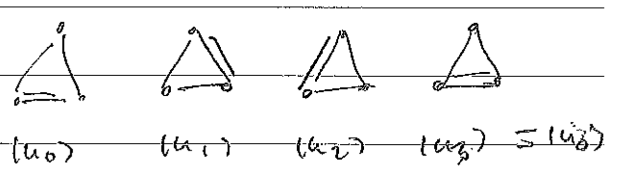
* Simon had received a private copy of Berry's paper one year before it was published!

** 1/4 of the 2016 Nobel prize in Physics!

The complex vectors that we'll be interested in will typically be identified with a ground state of some quantum system. When carrying them around a closed loop a global phase accumulates – the Berry phase.



EX. GROUNDSTATE OF A TRIATOMIC MOLECULE
$N = 4$



In the discrete picture we DEFINE the Berry phase by

sign convention

$$\Phi \equiv -\,\mathrm{Im}\ln\Big(\langle u_0|u_1\rangle\langle u_1|u_2\rangle\cdots\langle u_{N-1}|u_0\rangle\Big) \qquad (\mathrm{I}.1)$$

(Cf. a complex number $z = |z|e^{i\varphi} \Rightarrow \varphi = \mathrm{Im}\ln z$. Hence $\Phi = -\varphi$ when z = product of inner products of the state vectors at neighboring points around the loop)

The Berry phase as defined in (I.1) is obviously gauge invariant: Φ is the same before and after the gauge transformation

$$|u_j\rangle \to |\tilde{u}_j\rangle = e^{-i\beta_j}|u_j\rangle, \quad \beta_j \in \mathbb{R} \qquad (\mathrm{I}.2)$$

The gauge invariance of the Berry phase suggests that it has implications for observables!

However: An important subtlety

Important to note that Φ is defined only mod 2π (depending on choice of branch for the logarithm in (I.1)) GAUGE INVARIANCE MOD 2π !

* $\Phi = -\sum_{j=0}^{N-1} \mathrm{Im}\ln\langle u_j|u_{j+1}\rangle$ can yield a result that differs by $2\pi m$

Choose a branch for $\mathrm{Im}\ln z$ in I.1 *

The Berry phase can also be described in terms of parallel transport:

Given $|u_0\rangle, |u_1\rangle, \dots |u_N\rangle$ (with no special relative phase relations), define a new set of "parallel transported" states $|\bar{u}_0\rangle, |\bar{u}_1\rangle, \dots |\bar{u}_N\rangle$ to be the same as the original set but with the phases adjusted so that $|\bar{u}_0\rangle = |u_0\rangle$, $\langle \bar{u}_0 | \bar{u}_1\rangle \in \mathbb{R}^+$, $\langle \bar{u}_1 | \bar{u}_2\rangle \in \mathbb{R}^+$, ...
(i.e. impose the condition $\operatorname{Im} \ln \langle \bar{u}_j | \bar{u}_{j+1}\rangle = 0$)
Conclude by choosing $|\bar{u}_N\rangle$ such that $\langle \bar{u}_{N-1} | \bar{u}_N\rangle \in \mathbb{R}^+$.
While $|u_N\rangle$ and $|u_0\rangle$ are identical, $|\bar{u}_N\rangle$ and $|\bar{u}_0\rangle$ typically differ by a phase = Berry phase!

Proof: $\phi = -\operatorname{Im} \ln \left(\langle \bar{u}_0 | \bar{u}_1 \rangle \dots \langle \bar{u}_{N-1} | \bar{u}_0 \rangle \right)$ replace *

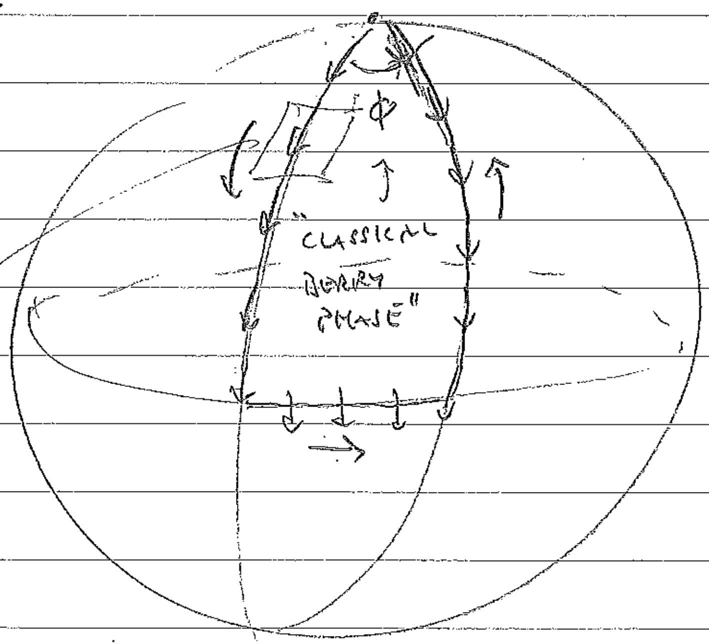
$$= -\operatorname{Im} \ln \left(\langle \bar{u}_0 | \bar{u}_1 \rangle \dots \langle \bar{u}_{N-1} | \bar{u}_N \rangle \langle \bar{u}_N | \bar{u}_0 \rangle \right)$$

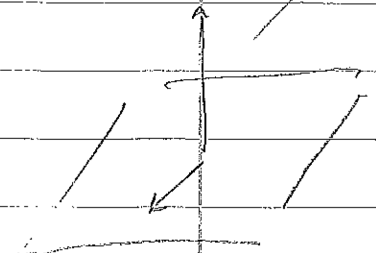
$$= -\operatorname{Im} \ln \langle \bar{u}_N | \bar{u}_0 \rangle$$

* ok since $|\bar{u}_0\rangle$ and $|\bar{u}_N\rangle$ differ only by a phase

The parallel transport generates a PARALLEL-TRANSPORT GAUGE.

ANALOGY IN DIFFERENTIAL GEOMETRY





no twist around the normal to the local tangent plane

Choose local basis that is as "aligned as possible" with its neighbors.

(I.4

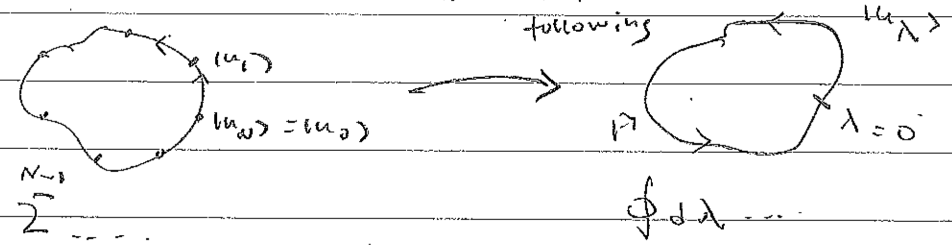
One may want to smooth out the phase discontinuity at the end of the loop in the parallel-transport gauge by applying phase twists

$$|\bar{u}_j\rangle \longrightarrow |\tilde{u}_j\rangle = e^{-ij\phi/N}\,|\bar{u}_j\rangle\ , \quad j = 0,1,\dots,N-1 \qquad (\text{I.3})$$

$-\operatorname{Im}\ln\langle\tilde{u}_j|\tilde{u}_{j+1}\rangle = \phi/N$ at every point in the loop.
This choice of gauge is called a TWISTED PARALLEL TRANSPORT GAUGE. We shall see examples where this gauge is particularly useful!

Now consider the continuum version of the Berry phase, with the states $|u_\lambda\rangle$ carried around a path Γ parameterized by $\lambda \in [\lambda_i, \lambda_f]$*, with $|u_{\lambda_i}\rangle = |u_{\lambda_f}\rangle$

* $= [0,1]$ in the following



$$\sum_{j=0}^{N-1} \dots \qquad \oint_\Gamma d\lambda \dots$$

Assume that $|u_\lambda\rangle$ is differentiable w.r.t. λ.
We can then write

$$\ln\langle u_\lambda|u_{\lambda+d\lambda}\rangle = \ln\Big[\langle u_\lambda|\Big(|u_\lambda\rangle + \underbrace{\frac{d|u_\lambda\rangle}{d\lambda}}_{\partial_\lambda|u_\lambda\rangle} d\lambda + \dots\Big)\Big]$$

$$= \ln\big[1 + \langle u_\lambda|\partial_\lambda u_\lambda\rangle d\lambda + \dots\big]$$

$$= \langle u_\lambda|\partial_\lambda u_\lambda\rangle d\lambda + \dots \qquad (\text{I.4})$$

* more general:
$\lambda \equiv (\lambda_1, \lambda_2, \dots)$
$\lambda_j \in [\lambda_i, \lambda_f],\ j = 1,2,\dots$

(I.5

Writing (I.1) as

$$\phi = -\sum_{j=0}^{N-1} \mathrm{Im}\,\ln \langle u_j | u_{j+1} \rangle \qquad (\text{I.5})$$

and taking the continuum limit, using (I.4) and $\sum_{j=0}^{N-1} \ldots \rightarrow \oint_{\Gamma} d\lambda \ldots$, one obtains:

$$\phi = -\mathrm{Im} \oint_{\Gamma} \langle u_\lambda | \partial_\lambda | u_\lambda \rangle \, d\lambda \qquad (\text{I.6})$$

$\langle u_\lambda | \partial_\lambda | u_\lambda \rangle$ is purely imaginary since
$\langle u_\lambda | \partial_\lambda u_\lambda \rangle^* = \langle \partial_\lambda u_\lambda | u_\lambda \rangle$ implies that
$\langle u_\lambda | \partial_\lambda u_\lambda \rangle + \langle u_\lambda | \partial_\lambda u_\lambda \rangle^* = \partial_\lambda \langle u_\lambda | u_\lambda \rangle = 0$
$\Rightarrow 2\,\mathrm{Re} \langle u_\lambda | \partial_\lambda | u_\lambda \rangle = 0$. We can then write

$z^* = \cancel{x} - iy$
$y = -\mathrm{Im}\, z^*$
$\Rightarrow iy = iz^*$

$$\phi = \oint_{\Gamma} \langle u_\lambda | i\partial_\lambda | u_\lambda \rangle \, d\lambda \qquad (\text{I.7})$$ *

One usually writes this as (dropping "Γ" from now).

$$\phi = \oint A(\lambda) \, d\lambda \qquad (\text{I.8})$$

where

$$A(\lambda) = \langle u_\lambda | i\partial_\lambda | u_\lambda \rangle \qquad (\text{I.9})$$

is the BERRY CONNECTION ("BERRY POTENTIAL").

* $-\mathrm{Im} \underbrace{\langle u_\lambda | \partial_\lambda | u_\lambda \rangle}_{= i\alpha} = -\mathrm{Im}(i\alpha) = -\alpha = i(i\alpha)$
$\uparrow$

Let's again consider a gauge transformation

$$|u_\lambda\rangle \to |\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}|u_\lambda\rangle \qquad (\mathrm{I}.10)$$

It follows that

$$A(\lambda) \to \tilde{A}(\lambda) = \langle \tilde{u}_\lambda | i\partial_\lambda | \tilde{u}_\lambda\rangle$$

$$= \langle u_\lambda | e^{i\beta(\lambda)} i\partial_\lambda e^{-i\beta(\lambda)} | u_\lambda\rangle$$

$$= \langle u_\lambda | i\partial_\lambda | u_\lambda\rangle + \partial_\lambda \beta(\lambda)$$

$$= A(\lambda) + \partial_\lambda \beta(\lambda) \qquad (\mathrm{I}.11)$$

$\Rightarrow$ BERRY CONNECTION NOT GAUGE INVARIANT

$\tilde{A}(\lambda) = \langle \tilde{u}_\lambda | i\partial_\lambda \tilde{u}_\lambda\rangle = C$

HW rewrite! If $\tilde{A}(\lambda) \neq$ CONST (excluding parallel-transport and twisted parallel-transport gauge) then $|\tilde{u}_{\lambda=1}\rangle = |\tilde{u}_{\lambda=0}\rangle$, and it follows that

$$\beta(1) = \beta(0) + 2\pi m \qquad (\mathrm{I}.12)$$

winding number specifying how many times $e^{-i\beta}$ circulates around the unit circle in the complex plane as the state moves around Γ, i.e. by carrying $\lambda = 0 \to 1$

and hence, from (I.11)

$$\tilde{\phi} = \phi + 2\pi m \qquad (\mathrm{I}.13)$$

$m = 0 \Rightarrow$ "small" gauge transformation

$m \neq 0 \Rightarrow$ "large" — " —

Thus, the Berry phase is only gauge invariant mod 2π.

(Expected, from the discrete case!)

Note: (I.13) applies generally, also for $\tilde{A}(\lambda) =$ CONST.

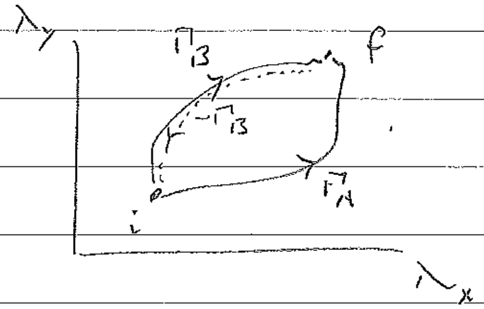
Importantly: The Berry phase is not quantized. Instead, the space of gauge transformation matrices on the loop Γ does admit a topological classification, with the winding number serving as topological index.

Open paths Berry phases are NOT gauge invariant. (I.7

$\phi = \int_{\lambda_i}^{\lambda_f} A(\lambda) d\lambda$

However, the relative Berry phase $\Delta\phi = \phi_B - \phi_A$ for two open paths, both of which start (end) at λ_i (λ_f) <u>is</u> gauge invariant mod 2π.

<u>Ex</u>



$\Gamma = \Gamma_A - \Gamma_B$ closed

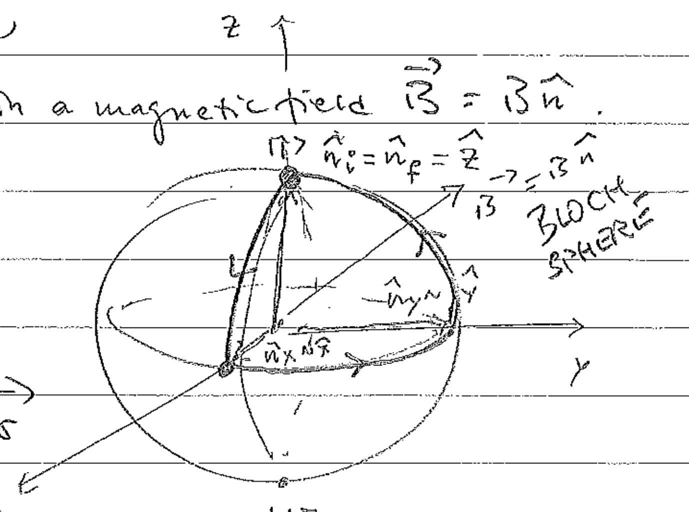
(Cf. the Aharonov - Bohm effect when Γ encloses an e.m. potential ... can be described via a Berry phase analysis ...)

$\sim$

In physics applications $|u_\lambda\rangle$ is usually the <u>ground state</u> of some quantum mechanical Hamiltonian H_λ, with λ being varied slowly so that both H_λ and $|u_\lambda\rangle$ evolve smoothly in time. In particular, the variation of λ is so slow so that $|u_\lambda\rangle$ is (approximately)* equal to the instantaneous (static) ground state at the current value of λ. * ADIABATIC APPROXIMATION (lifted in later work by Y. Aharonov & J.S. Anandan, Phys. Rev. Lett. <u>58</u>, 1593 (1987))

$\sim$

<u>Example</u> : Spin - $\frac{1}{2}$ particle in a magnetic field $\vec{B} = B\hat{n}$.



$$H_{\hat{n}} = -\gamma \vec{B}\cdot\vec{S}$$

$\nearrow$ parameter λ

$$= -\left(\frac{\gamma\hbar B}{2}\right)\hat{n}\cdot\vec{\sigma}$$

$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$

$= |\uparrow_{\hat{n}}\rangle$

Ground state $|u_{\vec{B}}\rangle$ is an eigenstate of $\hat{n}\cdot\vec{\sigma}$ with spin directed along $\hat{n}$ (and independent of the strength B) (I.8

Recall: representation of a spinor on the Bloch sphere:

$$|\uparrow_{\hat{n}}\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + e^{i\varphi}\sin\frac{\theta}{2}|\downarrow\rangle \; \Rightarrow$$

$\Rightarrow |\uparrow_{\hat{n}}\rangle = \begin{pmatrix}\cos\frac{\theta}{2}\\ e^{i\varphi}\sin\frac{\theta}{2}\end{pmatrix}$ where $|\uparrow_{\hat{n}}\rangle$ is the spinor with "spin up along $\hat{n}$", with (θ,φ) the polar and azimuthal angles of $\hat{n}$. It follows that

$$|\uparrow_{\hat{x}}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad |\uparrow_{\hat{y}}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \quad |\uparrow_{\hat{z}}\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad \text{(I.14)}$$

Using a discrete formulation to calculate the Berry phase resulting from changing $\vec{B}$ around the blue closed loop in the figure on the previous page, using only the states in (I.14), we have (dropping the irrelevant normalization factors in (I.14))

$$\Phi = -\mathrm{Im}\ln\left[\langle\uparrow_{\hat{z}}|\uparrow_{\hat{x}}\rangle\langle\uparrow_{\hat{x}}|\uparrow_{\hat{y}}\rangle\langle\uparrow_{\hat{y}}|\uparrow_{\hat{z}}\rangle\right]$$

$$= -\mathrm{Im}\ln\left[(1)(1+i)(1)\right] = -\mathrm{Im}\ln\left(\sqrt{2}\,e^{i\pi/4}\right) \quad \text{(I.15)}$$
$$= -\pi/4.$$

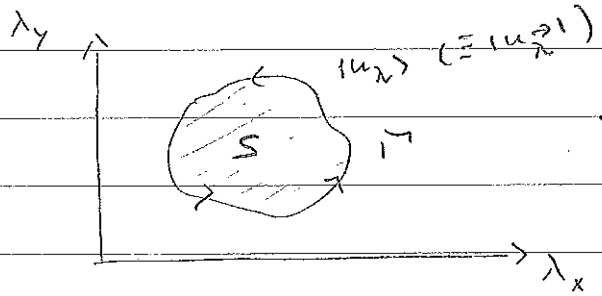
This result is actually exact! (We shall prove this after having introduced the notion of Berry curvature and Berry flux.)

From now on, let's restrict attention to a 2D parameter space, $\vec{\lambda} \equiv (\lambda_x, \lambda_y)$. (In the Bloch sphere example above, "λ_x" $= \theta$, "λ_y" $= \varphi$ ... "x" and "y" here only label two orthogonal directions in the parameter space.) We can then construct a 2-component Berry connection

$$A_\mu = \langle u_\lambda | i \partial_\mu u_\lambda \rangle \qquad (\text{I}.16)$$

and the Berry phase around a closed loop in the space of states $|u_\lambda\rangle$

$$\phi = \oint_{\Gamma = \partial S} \vec{A} \cdot d\vec{\lambda} \qquad (\text{I}.17)$$



By Stokes' theorem

$$\phi = \int_S \vec{F}(\vec{\lambda}) \cdot d\vec{S} \qquad (\text{I}.18)$$

where

Cartesian coordinates $\vec{\nabla} \times \vec{A} = (\partial_x A_y - \partial_y A_x)\hat{z}$

$$\vec{F}(\vec{\lambda}) = \vec{\nabla}_\lambda \times \vec{A}(\vec{\lambda}) \quad \text{BERRY CURVATURE} \qquad (\text{I}.19)$$

and where $d\vec{S} = dS\,\hat{n}$, with $\hat{n}$ a unit vector normal to the surface element dS (after having embedded the 2D parameter space into a 3D parameter space).

Rewriting (I.11) in vector notation (making explicit that we now work in a 2D parameter space with $\vec{\lambda} = (\lambda_x, \lambda_y)$):

$$\vec{A}(\vec{\lambda}) \xrightarrow[\text{TRANSFORMATION}]{\text{GAUGE}} \vec{A}'(\vec{\lambda}) = \vec{A}(\vec{\lambda}) + \nabla_{\vec{\lambda}}\beta(\vec{\lambda}) \qquad (\text{I}.20)$$

it follows immediately that $\vec{F}(\vec{\lambda})$ is gauge invariant. (Cf. the gauge invariance of a magnetic field $\vec{B} = \nabla \times \vec{A}$, with $\vec{A}$ not gauge invariant.)
Thus, while ϕ calculated by (I.17) is only well-defined mod 2π while ϕ calculated by (I.18) is uniquely defined! To keep this in mind, we shall sometimes refer to ϕ calculated by (I,18) as a BERRY FLUX through the surface S