Lecture 11

Another form of Berry curvature we have previously obtained

\[ \Omega = \oint \mathbf{A} = \oint \mathbf{A}, \quad \Omega = \frac{q}{\hbar} \times \mathbf{A}. \]

We see that \( \Omega = \frac{q}{\hbar} \times (i \langle n | \psi_k \rangle) \) =

\[ = -\text{Im} \langle \hat{n} \hat{1} \times \hat{\psi} | \hat{n} \hat{1} \times \hat{\psi} \rangle (\text{E}\langle n | \psi_k \rangle = 0). \]

This form of \( \Omega \) suffers from the need to find a smooth gauge for \( |\psi_k\rangle \), in order to have decent-looking derivatives \( \partial |\psi_k\rangle \). It is generally hard to find such smooth wave functions, e.g. in numerical calculations.

We would like to find another form for \( \Omega \), which avoids differentiations of eigenvectors \( \sum_{m=1}^{\infty} \Omega = 1 \)

\[ \Omega_i = -\text{Im} \varepsilon_{ijk} \langle \hat{q} n | \hat{\psi}_k \rangle, \]

\[ = -\text{Im} \sum_m \varepsilon_{ijk} \langle \hat{q} n | m \rangle \langle m | \hat{\psi}_k \rangle. \]

We know that for \( m = n \), \( \langle \hat{q} n | n \rangle \) and \( \langle n | \hat{\psi}_k \rangle \) are imaginary, thus the product is real, and does not contribute to \( \Omega \). We therefore get
\[ Q_i = -\text{Im} \sum_{m \neq n} \langle \phi_n | m \rangle \langle m | \phi_k \rangle. \]

To find \( \langle m | \phi_k \rangle \), we use

\[ H | n \rangle = \varepsilon_n | n \rangle \Rightarrow \phi_k H | n \rangle + \varepsilon_k | n \rangle = \phi_k | \varepsilon_n | n \rangle + \varepsilon_k | n \rangle \]

which gives after projecting onto \( | n \rangle \):

\[ \langle m | \phi_k H | n \rangle + \varepsilon_k \langle m | \phi_k \rangle = \varepsilon_n \langle m | \phi_k \rangle \Rightarrow \]

\[ \Rightarrow \langle m | \phi_k \rangle = \frac{\langle m | \phi_k H | n \rangle}{\varepsilon_n - \varepsilon_k} \]

Analogously, \( \langle \phi_n | m \rangle = (\langle m | \phi_k \rangle)^* \). But let's do it explicitly to exercise on left-hand side:

\[ \langle n | H = \langle n | \varepsilon_n \Rightarrow \phi_k H | n \rangle + \langle n | \phi_k \rangle = \phi_k | \varepsilon_n | n \rangle + \varepsilon_k | n \rangle \]

\[ \Rightarrow \langle \phi_n | m \rangle (\varepsilon_n - \varepsilon_k) = -\langle n | \phi_k H | m \rangle \Rightarrow \]

\[ \Rightarrow \phi_n | m \rangle = -\frac{\langle n | \phi_k H | m \rangle}{\varepsilon_n - \varepsilon_k} \]

Check:

\[ \langle \phi_n | m \rangle = (\langle m | \phi_k \rangle)^* = \frac{\langle m | \phi_k H | n \rangle}{\varepsilon_n - \varepsilon_k} \]

\[ = \frac{\langle n | \phi_k H^+ | m \rangle}{\varepsilon_n - \varepsilon_k} + \frac{\langle n | \phi_k H^+ | m \rangle}{\varepsilon_n - \varepsilon_k} \]
The final result we get is

$$\Omega_c = -\text{Im} \sum_{m+n} \frac{\langle n |\partial_z H | m \rangle \langle m |\partial_z H | n \rangle}{(E_n - E_m)^2},$$

and

$$\Omega_n = -\text{Im} \sum_{m+n} \frac{\langle n |\partial_z H | m \rangle \times \langle m |\partial_z H | n \rangle}{(E_n - E_m)^2}.$$

This form has two advantages:
- it is gauge-independent. But $\vec{\Omega} = \text{curl} \vec{A}$ is also gauge-independent.
- more importantly, it does not require differentiability of eigenvectors, the latter is shifted to the Hamiltonian.

Final expr. for the Berry phase:

$$\gamma_n = -\oint \vec{A} \cdot \text{Im} \sum_{m+n} \frac{\langle n |\partial_z H | m \rangle \times \langle m |\partial_z H | n \rangle}{(E_n - E_m)^2}$$

A few observations:
- $\sum_n \gamma_n = 0$ — the sum of all B. pl. over all states is zero.
- $\vec{\Omega}$ blows up near degeneracies $E_n \to E_m$. These are eventually the sources of Berry phases.
Berry phases in two-level systems.

Generally we deal with a two level system when either the system generally has two levels (e.g. $\alpha \beta$), or a pair of levels is well-separated from all others in energy space:

$$R$$

The general $2 \times 2$ Hamiltonian (in the truncated $2 \times 2$ space, as for the $8 \times 8$ case) is

$$H = \begin{pmatrix} \varepsilon_1 & V^* \\ V & \varepsilon_2 \end{pmatrix}$$

- we have seen this many times by now.

It has 4 real parameters: $\varepsilon_1, \varepsilon_2$, keV, Im V.

We can write this Hamiltonian using 3 Pauli matrices and the unit matrix:

$$\boldsymbol{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

This is how they look in the basis where $\sigma_2/\sigma_3$ is diagonal but unitarily-equivalent representations are equally valid.

Properties of $\boldsymbol{\sigma}_i$:

$$\sigma_i = \sigma_i^+ \quad - \text{Hermitian - good for Hamiltonians}.$$  

$$\sigma^2 = \sigma_0 (= 1)$$

For $\alpha \beta \neq 0$, $\{ \sigma_i, \sigma_j \} = 2 \delta_{ij}$.
\[ \sigma_i \sigma_j = \delta_{ij} + i \epsilon_{ijk} \sigma_k \]

\[ [\sigma_i, \sigma_j] = \epsilon_{ijk} \sigma_k \]

The last property ensures that for \( \sigma_i \rightarrow \frac{1}{2} \sigma_i \), we have

\[ [\sigma_i, \sigma_j] = i \epsilon_{ij k} \sigma_k \]

which are the commutation relations for the angular momentum. Indeed, \( \sigma^2 = \frac{1}{2} \sigma_i \sigma_i \) is the operator for spin-\( \frac{1}{2} \).

Using these, we can express it as

\[ H = \frac{E_0 + \varepsilon_0}{2} \sigma_0 + \frac{E_0 - \varepsilon_0}{2} \sigma_2 + i [\sigma_0, \sigma_2] + 2\mu V \left( e^{i \theta} \right) \]

\[ = E_0 \sigma_0 + \vec{h} \cdot \vec{\sigma} \]

where \( \vec{h} \) is a real vector.

To ensure the hermiticity of the Hamiltonian, it is clear that \( E_0 \sigma_0 \) is absolutely essential; it only shifts the origin of energy, so we will discard it from now on. Thus, our Hamiltonian is

\[ H_{\text{final}} = \vec{h} \cdot \vec{\sigma} \]

where \( \vec{h} \) is just a set of \( 3 \) real numbers.

Note that up to a sign and some redefinitions, this is just a Hamiltonian of spin (or \( j \)) on a magnetic ("magnetic") field \( \vec{h} \).
Eigen system of a TLS:

\[ H = \hat{H} \otimes \sigma = \hbar \omega \sigma_z. \]

To find eigen energies, consider

\[ H^2 = \hbar^2 \sigma_z, \quad H \otimes \sigma_\delta = \hbar^2 \omega \sigma_z \sigma_\delta (\Sigma \eta \mp \Sigma \xi \kappa \delta), \]

since \( \hbar \omega \sigma_z = \hbar \omega \sigma_z \) (just numbers), we set

\[ H^2 = \hbar^2 (x \Pi), \quad \text{and since} \quad H = U^\dagger (\lambda_1 \lambda_2) U, \quad \text{we conclude that} \quad \hbar^2 = \lambda_2 = \hbar^2 \mu \quad \text{in order to have} \quad H^2 \otimes \sigma_\delta. \]

Thus, the eigen energies are \( \pm \hbar \omega \).

These are energies for \( \sigma_z \) along a magnetic field \( \mp \hbar \lambda_1 \) and opposite to it \( \mp \hbar \lambda_1 \). Again,

\[ H |\pm\rangle = \pm \hbar \omega |\pm\rangle, \quad \pm = \pm \hbar \lambda_1. \]

What are \( |\pm\rangle \) - the eigen states?

It is customary to go to spherical coordinates for \( \hat{H} \):

\[ \hat{H} = \hbar \omega \cos \theta \sin \phi \sigma_z. \]

\( \theta, \phi \) angles do not correspond to any direction in real space unless we are talking about the real spin in magnetic field, but it is nice to think in terms of angles on the "Bloch sphere" when thinking about the "linear" of eigenstates (same Bloch, different context).
Let us just check that \( |+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} e^{i \phi} \end{pmatrix} \) is another possible choice of "gauge" for this \( \mathbf{H} \). Another one could be \( |+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i \phi} \\ i \sin \frac{\theta}{2} \end{pmatrix} \), etc.

\[
\mathbf{H} = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i \phi} \\ \sin \theta e^{i \phi} & -\cos \theta \end{pmatrix}. \quad \hbar
\]

\[
\mathbf{H} |+\rangle = \begin{pmatrix} \cos \theta \cos \frac{\theta}{2} + \sin \theta \sin \frac{\theta}{2} \\ \sin \theta \cos \frac{\theta}{2} - \cos \theta \sin \frac{\theta}{2} e^{i \phi} \end{pmatrix} \hbar = \hbar \begin{pmatrix} \cos \frac{\theta}{2} \\ i \sin \frac{\theta}{2} e^{i \phi} \end{pmatrix} = \hbar |+\rangle,
\]

thus \( |+\rangle \) is indeed the eigenstate corresponding to \( E_+ = \frac{\hbar}{2} \). We can check that \( |-\rangle = \begin{pmatrix} -i \sin \frac{\theta}{2} e^{i \phi} \\ \cos \frac{\theta}{2} \end{pmatrix} \). It is easily seen that

\[
<+|+\rangle = <-|-\rangle = 1, \quad <+|-\rangle = 0.
\]
The angles $\theta, \phi$ can be viewed as parameters that the Hamiltonian depends upon. The $|\pm\rangle$ states are the corresponding eigenstates at each value of the parameters which are followed in the adiabatic evolution.

Let us calculate the corresponding $\hat{A}$ and $\hat{D}$.

Consider the "excited" state $|+\rangle$. We have 3 parameters, $x$, $\theta$, $\phi$ but $|+\rangle$ does not depend on $x$, thus we have:

$$A_\theta = i (<+| \hat{D}|+>) = (\cos \frac{\theta}{2} \sin \frac{\theta}{2} e^{-i\phi}) \left( \frac{1}{2} \sin \frac{\theta}{2} e^{-i\phi} \right) = 0.

$$

$$A_\phi = i \left( \cos \frac{\theta}{2} - \sin \frac{\theta}{2} e^{i\phi} \right) \left( \begin{array}{c} 0 \\ \sin \frac{\theta}{2} e^{i\phi} \end{array} \right) =

= - \sin^2 \frac{\theta}{2}

$$

The corresponding Berry curvature (the only component) is

$$\Omega_{\theta\phi} = \partial_\phi A_\theta - \partial_\theta A_\phi = - \sin \frac{\theta}{2} \cos \frac{\theta}{2} - \frac{1}{2} \sin \theta

$$

We can calculate the Berry phase accumulated on adiabatic evolution. Consider the trajectory shown in the Fig.
the field goes around $z$ axis (ccw if $t$ points at the eye), at
the given value of $\theta = \theta_0$.

\[
\chi = \oint \int d\Omega d\xi \cdot \left( -\frac{1}{2} \sin \theta \right) =
\frac{2\pi}{2\pi} \left( \frac{1}{2} \sin \theta \right) = \frac{\pi}{2} - \frac{1}{2} \left( 1 - \cos \theta_0 \right)
\]

\[
= - \frac{1}{2} \left[ 2\pi \left( 1 - \cos \theta_0 \right) \right] = - \frac{1}{2} \left[ \text{solid angle subtended by the trajectory} \right].
\]

In general, $\pm \frac{1}{2} \left[ \text{solid angle} \right]$ depending on the sense of trajectory and whether we choose $\leftrightarrow$ state.

Note on gauges:

$\ket{ \leftrightarrow } = (\cos \frac{\theta}{2}, e^{i\phi})$ is poorly defined at $\theta = \pi$, where

$\cos \frac{\theta}{2} = 0$ (south pole). There is no well defined, so
we do not know what to assign to $e^{i\phi}$.

We could have chosen $\ket{ \leftrightarrow } = (\cos \frac{\theta}{2}, \bar{e}^{i\phi})$, which
is well behaved at the south pole but it has a problem at the north pole now! In general
when there is a net Berry phase through a manifold
(here $\frac{1}{2}\int d\Omega d\xi = -1$, Chern number = -1), it
is impossible to find a gauge "good" on the
entire manifold.
Let us calculate the Berry flux through the entire parameter manifold (it is a sphere - closed manifold) in three different ways: 1) using the Berry curvature; 2) using a single gauge choice on the manifold - having to deal with multi-valued funtions; 3) using single valued functions, defined on overlapping patches on the manifold.

1) To integrate \( \oint \) over the sphere, we just need to put \( \Theta = \pi \) in the formula for \( f \), obtained before, to get \( \oint S = -2\pi \).

11') If we stick with \( \Theta = \pi \), we see that it is bad at \( \Theta = \pi \):

\[
\Theta = \pi = (0, i\pi) = e^{i\pi}(0)
\]

When we do \( \oint d\Omega \), we observe that \( \hat{A} = (0, 0) = \hat{A}(0, \pi) \), thus the integrals over IV and II will cancel each other. The I is a point, the II is well behaved, so \( \oint d\Omega = 0 \) too. 

II is region where it is troublesome. Even though it is physically a single point, we "stretched" it into a line and assigned different phases to along that line. Thus we are dealing with a multivalued.
Function in that region. We can do the integral nevertheless:

\[ \int d\Omega \vec{F} = -2\pi i \cdot \vec{A} \cdot \vec{B} = -2\pi \Rightarrow \int d\Omega \vec{F} = -2\pi, \text{ as in i).} \]

iii) The procedure in ii) is very fishy. Let us do a well-behaved calculation by assigning different gauges on different patches of the manifold.

Since \( \vec{A} \) is well-behaved at the North pole, and \( \vec{A} \) is well-behaved at the South pole, we have covered the entire manifold with single-valued functions defined on overlapping patches.

Let us call the corresponding Berry connections \( \vec{A}_1 \) and \( \vec{A}_2 \).

Then \( \int d^2\Omega \vec{F} = \int d\Omega \vec{A} + \int d\Omega \vec{B} \). Let \( \text{Left} \) and \( \text{Right} \).

Since \( \vec{A} \) is well-behaved in \( L \), integrals

\[ \int_1 \vec{A} \cdot \vec{F} = 0 \quad \text{vanish, and} \quad \int_1 \vec{B} d\vec{F} = \int_1 \delta \cdot \vec{A}_2 \cdot \vec{B} (\delta). \]

Analogously, since \( \vec{A} \) is well-behaved in \( R \), we have

\[ \int_2 \vec{A} \cdot \vec{F} = 0, \quad \text{and} \quad \int_2 \vec{A} \cdot \vec{B} = \int_2 \delta \cdot \vec{A}_1 (\delta), \text{ or} \]

\[ \int_2 \vec{A} \cdot \vec{B} = \int_2 \delta \left[ \vec{A} (\delta) - \vec{A} (\epsilon) \right]. \]
In the overlap region, \( |+\rangle \) and \( |+\rangle' \) are related by a gauge trans formation, which allows us to connect \( \mathcal{A} \) and \( \mathcal{A}' \):

\[
|+\rangle = e^{i\theta} |+\rangle' \Rightarrow
\]

\[
A\phi = i \langle + | \partial \phi | + \rangle = -1 + i \langle + | \partial \phi | + \rangle' = -1 + A\phi' \Rightarrow
\]

\[
\Rightarrow A\phi - A\phi' = -1, \text{ and } \oint d\vec{r} \cdot \mathbf{A} = -2\pi, \text{ as in the previous two ways of doing things.}
\]