Lecture 5

Berry's Phase

We have seen that under adiabatic evolution, the wavefunction evolves as

$$|\psi(t)\rangle = e^{-i\int^t \epsilon(t)dt/\hbar - i\int^t \langle\phi(t)|i\partial_t|\phi(t)\rangle}|\phi(t)\rangle. \tag{5.1}$$

where $|\phi(t)\rangle$ is the adiabatic wavefunction,

$$H|\phi(t)\rangle = \epsilon(t)|\phi(t)\rangle. \tag{5.2}$$

The second term

$$\Phi = \int^t \langle\phi(t)|i\partial_t|\phi(t)\rangle dt \tag{5.3}$$

is known as "Berry's Phase". By construction, it only depends on the path and not how fast the path is traversed. In general it depends on how we chose the phases of the $|\phi(t)\rangle$'s. That is it is gauge dependent.

However, if we go through a closed path $\phi(0) = \phi(t)$, then it should not depend on the gauge. The way to show this is to perform a general gauge transformation $|\phi(t)\rangle \to e^{i\lambda(t)}|\phi(t)$. [For a gauge transformation it suffices to make λ a function of ϕ, but this more general form is easier to work with.] The Berry phase then becomes

$$\Phi = \int^t dt\left[\langle\phi(t)|i\partial_t|\phi(t)\rangle - \lambda'(t)\langle\phi(t)|\rangle\right]. \tag{5.4}$$

The last term is zero as long as $\lambda(t) = \lambda(0)$, a condition which has to be true for any time independent gauge transformation on a cyclic path. Thus the Berry phase is "physical" in that it does not depend on the parameterization of our states.

One can get further insight into this term by being slightly more explicit about the parameterization of the Hamiltonian. Let $H(t) = H(r_1, r_2, \cdots r_n)$

be parameterized by an n-dimensional vector $\mathbf{R}$. This parameterization of H does not need to be one-to-one: that is there may be more than one $\mathbf{R}$ that correspond to the same H: but each $\mathbf{R}$ should uniquely define H – and hence ϕ. In this way we embed the control parameter space in $\mathcal{R}_N$. We can then eliminate time, to express the Berry phase as an integral in control space:

$$\Phi = \oint \langle\phi|i\nabla|\phi\rangle \cdot d\mathbf{R}. \tag{5.5}$$

Sometimes people define a "Berry Connection", via

$$\mathbf{A} = \langle\phi|i\nabla|\phi\rangle. \tag{5.6}$$

This is a vector which is analogous to the vector potential in electromagnetism. Unlike Φ, the vector A is gauge dependent.

An interesting way to write Eq. (5.5) is (by Gauss's theorem) as a surface integral of a curl

$$\begin{aligned} \Phi &= \iint \nabla \times \langle\phi|i\nabla|\phi\rangle && (5.7) \\ &= \iint i(\nabla\langle\phi|) \times (\nabla|\phi\rangle) d^2\mathbf{R}, && (5.8) \end{aligned}$$

where the integral is taken over the surface contained by the loop. One defines the "Berry Curvature via

$$\mathbf{\Omega} = i(\nabla\langle\phi|) \times (\nabla|\phi\rangle). \tag{5.9}$$

Of course the sophisticated reader realizes that these expressions are not quite right if $\mathbf{R}$ is not simply a three-vector. A reader sophisticated enough to realize this will also probably know how to solve the problem (replace the $\times$ with $\wedge$, and define $\mathbf{\Omega}$ as a 2-form).

Interestingly, $\mathbf{\Omega}$ is actually gauge independent. To see this, we once again transform $|\phi\rangle \to e^{i\Lambda}|\phi\rangle$. Under this transformation the connection transforms as

$$\mathbf{A} \to \mathbf{A} + i\nabla\Lambda. \tag{5.10}$$

When we take the curl of this quantity, the second term vanishes, so the curvature is independent of Λ.

Another interesting way to write things is to insert a resolution of the identity. Let $H(\mathbf{R})|n\rangle = E_n|n\rangle$. We can then write

$$\mathbf{\Omega} = i\sum_m (\nabla\langle\phi|m\rangle) \times (\langle n|\nabla|\phi\rangle). \tag{5.11}$$

First order perturbation theory then gives

$$\langle n(\mathbf{R})|\nabla|\phi(\mathbf{R})\rangle = \frac{\langle n|\nabla H|\phi\rangle}{E_n - E_\phi}, \tag{5.12}$$

which allows one to write

$$\mathbf{\Omega} \;=\; i\sum_n \frac{\langle \phi|\nabla H|n\rangle}{\times} \frac{\langle n|\nabla H|\phi\rangle}{(E_n - E_\phi)^2}. \tag{5.13}$$

What is particularly nice about Ω is that it is completely local, and is independent of the choice of gauge. Hence one does not even need to have a single valued representation of $|\phi\rangle$ in terms of $\mathbf{R}$. This will be extremely useful.

A. Berry Phase of a Single Spin

The classic example, which many of you may have seen, of Berry's phase is to consider a single spin in a time dependent magnetic field

$$H = \mathbf{B}\cdot\mathbf{S}. \tag{5.14}$$

We will let the direction of $\mathbf{B}$ in space be the control parameter of the Hamiltonian.

Starting with a reference state with spin projection m in the $\hat{z}$ direction, one would like to write the adiabatic basis as

$$|\theta,\phi\rangle = R(\theta,\phi)|m,\hat{z}\rangle, \tag{5.15}$$

where θ, ϕ are Euler angles. The problem, of course, is that this definition does not give a single valued set of states. Thus we cannot directly calculate the Berry connection phase from this (at least using the definitions we have given). On the other hand, we can calculate the Berry Curvature – which should be isotropic. Moreover to do that we only need to deal with infinitesimal rotations.

Rotating about the $\hat{x}$ axis by angle δ_x is accomplished by

$$R_{\hat{x}}(\delta x) = e^{-iS_x\delta x} \approx 1 - iS_x\delta x. \tag{5.16}$$

Similarly the rotation about $\hat{y}$ is

$$R_{\hat{y}}(\delta y) = e^{-iS_y\delta y} \approx 1 - iS_y\delta y. \tag{5.17}$$

The Berry Curvature is

$$\Omega \;=\; i\left[(\partial_x\langle m,\hat{z}|)(\partial_y|m,\hat{z}\rangle) - (\partial_y\langle m,\hat{z}|)(\partial_x|m,\hat{z}\rangle)\right]. \tag{5.18}$$

Taking **R** to be a vector of length 1, and using Eqs. (5.16)-(A), one should have

$$\begin{aligned}\partial_x|m,\hat{z}\rangle &= -iS_x|m,\hat{z}\rangle && (5.19)\\ \partial_x\langle m,\hat{z}| &= i\langle m,\hat{z}|S_x && (5.20)\\ \partial_y|m,\hat{z}\rangle &= -iS_y|m,\hat{z}\rangle && (5.21)\\ \partial_y\langle m,\hat{z}| &= i\langle m,\hat{z}|S_y. && (5.22)\end{aligned}$$

Thus

$$\begin{aligned}\Omega &= i\langle m,\hat{z}|S_xS_y - S_yS_x\partial_y|m,\hat{z}\rangle) && (5.23)\\ &= \langle m,\hat{z}|S_z\partial_y|m,\hat{z}\rangle) && (5.24)\\ &= m. && (5.25)\end{aligned}$$

The Berry phase for any path is therefore m times the area subtended.

An interesting feature is that the area is only defined modulo 4π: there are two equivalent areas for any path. For these to give the same physics $4\pi m$ must be a multiple of 2π. Thus we must have that m is either an integer or half integer. [This same argument was more-or-less used by Dirac to argue for quantization of charge.]

Another interesting feature is that if you rotate a spin-1/2 particle by 2π, you get a phase of -1.

B. Berry Phase Definition of Polarization

The concept of Berry phase appears everywhere in modern physics. Here is an example from the early to mid 1990's: namely, how do you define polarization. It is worth considering this example for two reasons: (1) it is a many-body example, and (2) it is profound, and has profound impact.

The basic question is how do you define the electrical polarization of a crystal. [This is a particularly important question for ferroelectrics – materials with a spontaneous polarization; cf. Craig Fennie's multiferroic module.] The naive answer is that you look at a unit cell, and calculate its dipole moment. This works fine for an ionic crystal. The positive and negative charge are near eachother, and well separated from any other charge. In general, however, shows this procedure gives nonsense. There is no unique unit cell, and each choice will give a different value.

The next most obvious answer is that you look at surface charge. But polarization should be a bulk property. Moreover, you might be doing a DFT calculation, and it would be a big pain to need to model the boundary. Is there a way to determine the polarization from a bulk calculation?

Note, this difficulty keeps coming up in condensed matter physics. For example, one of the defining characteristics of quantum Hall effects and topological insulators are the nature of their edge states. How can you learn about these edges merely by studying the bulk?

One useful clue is to look at experiments. It turns out that most experiments that purport to measure polarization, actually measure *changes* in polarization. For example, a typical measurement would be investigating piezoelectricity. One begins by placing a (presumed unpolarized) sample between the plates of a shorted capacitor. One then applies pressure to the sample, and measures a current flowing between the plates. The total charge transfered tells you the polarization. [Or rather, it tells you the *change* in polarization.]

We can use this same trick. Formally we recognize that the gradient of the polarization is the charge density

$$\nabla \cdot \mathbf{P} = -\rho. \tag{5.26}$$

Next we use the continuity equation

$$\partial_t \rho + \nabla \cdot \mathbf{j} =, \tag{5.27}$$

to get

$$\nabla \cdot (\partial_t \mathbf{P} - \mathbf{j}) = 0. \tag{5.28}$$

Thus, up to a divergence free term

$$\partial_t \mathbf{P} = \mathbf{j}. \tag{5.29}$$

This issue of the divergence free term can be solved by looking at the surface, and in most cases it suffices to take that term to be zero. Thus we will explore

$$\Delta \mathbf{P} = \int_0^t \mathbf{j} dt. \tag{5.30}$$

The remarkable thing is that from Eq. (5.30), we will be able to relate $\mathbf{P}$ to a Berry phase.

Let us first start from an independent electron picture, and imagine that we are dealing with an insulator. The result is actually more general, but this is a clear way to see it. Let λ be the control parameter which represents our perturbation, with $\lambda = 0$ being the original Hamiltonian, and $\lambda = 1$ be the final Hamiltonian. According to our previous semiclassical arguments (ie. the adiabatic theorem) we can get the particle current by summing up the velocity of the particles in all the occupied bands:

$$\mathbf{j} = \sum_n \int_{\mathrm{BZ}} \mathbf{dq} v_n(q) \tag{5.31}$$

$$= \sum_n \int_{\mathrm{BZ}} \mathbf{dq} \frac{1}{\hbar} \partial_q \epsilon_n(q). \tag{5.32}$$

By symmetry this sum is zero. For simplicity we will define our measure so that

$$\int_{\mathrm{BZ}} \mathbf{dq} = 1. \tag{5.33}$$

It turns out that when the Hamiltonian is time dependent there is a Berry Phase correction to the expression for the group velocity of a wave packet, and this correction modifies Eq. (5.31). Consider a wave packet,

$$|\psi\rangle = \sum_q f_q(t)|q\rangle, \tag{5.34}$$

where f_q is a function which is sharply peaked about q_0, and

$$\begin{aligned} f_q(t) &= f_q e^{-i\Phi_q(t)} && (5.35)\\ &= f_q e^{-i\int^t \epsilon_q t - i\gamma_q}, && (5.36)\end{aligned}$$

where $\gamma_q = \int^t \langle q|i\partial_t|q\rangle$ is a Berry Phase. The position of this packet is

$$\begin{aligned} r(t) &= \sum_q f_q^*(t) i\partial_q f_q(t) && (5.37)\\ &= \sum_q |f_q|^2 \partial_q \Phi_q && (5.38)\\ &\approx \left(\partial_q \Phi_q\right)_{q=q_0}. && (5.39)\end{aligned}$$

Taking a time derivative yields

$$\begin{aligned} v_q &= \partial_q \epsilon_q + \partial_q \gamma_q && (5.40)\\ &= \partial_q \epsilon_q - i\left[\partial_q \langle q|\partial_t|q\rangle - \partial_t \langle q|\partial_q|q\rangle\right] && (5.41)\\ &= \partial_q \epsilon_q - i(\partial_t \lambda)\left[\partial_q \langle q|\partial_\lambda|q\rangle - \partial_\lambda \langle q|\partial_q|q\rangle\right] && (5.42)\end{aligned}$$

The latter correction term has the form of a Berry Curvature in $q - \lambda$ space, and we will define

$$\Omega_{q\lambda} = i\left[\partial_q \langle q|\partial_\lambda|q\rangle - \partial_\lambda \langle q|\partial_q|q\rangle\right] \tag{5.43}$$

Substituting into Eq. (5.31) gives

$$\mathbf{j} = -\partial_t \lambda \sum_n \int_{\mathrm{BZ}} \mathbf{dq} \Omega_{q\lambda}^{(n)}. \tag{5.44}$$

The change in the polarization is the time integral, so

$$\Delta P = -\int_0^1 d\lambda \sum_n \int_{\mathrm{BZ}} \mathbf{dq} \Omega_{q\lambda}^{(n)}, \tag{5.45}$$

is expressible in terms of an integral of the Berry Curvature over the Brillioun zone.

One can further simplify things by using Stokes theorem to express ΔP as an integral over the boundaries. Given that the Brillioun Zone is periodic, the only boundaries are at $\lambda = 0, 1$ yielding

$$\Delta P = -i \sum_n \int_{\mathrm{BZ}} \mathbf{dq} \left[\langle q, 1 | \partial_q | q, 1 \rangle - \langle q, 0 | \partial_q | q, 0 \rangle \right]. \tag{5.46}$$

Thus the change in the polarization is simply the difference of a Berry Connection integrated over the Brillioun zone.

Group Activity: Is this expression Gauge invariant?

It turns out that this expression is only Gauge invariant up to an integer. To see this, we once again perform a gauge transformation, $|q\rangle \to e^{i\Lambda}|q\rangle$, and calculate

$$P \quad \to \quad \int_{\mathrm{BZ}} \mathbf{dq} i \langle q | \partial_q | q \rangle - \partial_q \Lambda. \tag{5.47}$$

In order for the Gauge transformation to be single-valued, we need $e^{i\Lambda}$ to be the same on antipodal sides of the Brillioun zone. Thus we can write the second term as

$$\int_{\mathrm{BZ}} \partial_q \Lambda = \sum_{\mathrm{faces}_j} \int dq 2\pi n_j \tag{5.48}$$

where n_j is an integer associated with each face. If we take $\mathbf{P}$ along one of the lattice directions, we end up with the uncertainty in $\mathbf{P}$ quantized in units of the lattice constant in that direction. This simply reflects the periodicity of the lattice. The original expression, Eq. (5.45) does not suffer this problem.

As an aside, we see that if the Hamiltonian at $\lambda = 0$ is the same as the one at $\lambda = 1$, then the integrated charge moved must be an integer. This then connects to "quantum turnstiles" and "adiabatic pumping" which were hot topics in mesoscopics just a few years ago.

Finally, one can generalize this result to a generic Many-body system [Niu and Thouless].

Problem 5.1. We will consider a classic 1D model for an insulator with nontrivial polarization/charge transport. We start with a typical tight binding model:

$$H_0 = t \sum_i \left[a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} \right]. \tag{5.49}$$

We will do two things to move charge around. First, we will dimerize the lattice, changing the strength of the hopping between subsequent sites

$$H_d = \delta \sum_i (-1)^i \left[a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} \right]. \tag{5.50}$$

You can think of this as moving sites closer/farther apart. Positive δ means that sites 1 and 2 are far apart, while 2 and 3 are close. Negative δ is the opposite dimerization. Second we will imagine adding a superlattice, moving the energy of alternative sites up and down

$$H_s = \Delta \sum_i (-1)^i a_i^\dagger a_i. \tag{5.51}$$

One can imagine pumping charge by sequentially changing δ and Δ. In the following questions feel free to use whatever mix of analytic and numerical arguments that you feel most comfortable with.

5.1.1. Find the band structure ϵ_q. [There should be 2 bands.] Plot this for a couple different values of the parameters. Be sure to include the cases: $\delta = \Delta = 0$, and the four cases where each of δ and Δ are positive and negative.

5.1.2. Imagine the lowest band is completely filled. Make a density plot of $\langle n_{\text{even}} - n_{\text{odd}} \rangle$ in the $\delta - \Delta$ plane. Explain in words what is happening.

5.1.3. Calculate the Berry Connection

$$i \langle q | \partial_q | q \rangle. \tag{5.52}$$

Note there should be an arbitrary phase hanging around. How can you choose this phase so that the connection is single valued as one periodically moves from one Brillioun zone to the next. This is the "periodic gauge" and is the most convenient to work in. Plot the connection as a function of q for a few parameters – again, play with how the signs of δ and Δ matter.

5.1.4. In the periodic gauge, calculate the integral of the Berry Connection over the Brillioun zone. [This is one of the cases where you might want to use numerics – it turns out the result can be expressed in terms of the complete elliptic integrals of first kind – but there is not much point in writing it as such. Its a 1D integral, and trivial to do numerically.] Using this result, plot polarization as a function of δ and Δ.

Problem 5.1.

5.1.5. Calculate the Berry Curvatures:

$$\Omega_{q\delta} = i(\partial_\delta \langle q|)(\partial_q |q\rangle) - \partial_q \langle q|)(\partial_\delta |q\rangle) \tag{5.53}$$

$$\Omega_{q\Delta} = i(\partial_\Delta \langle q|)(\partial_q |q\rangle) - \partial_q \langle q|)(\partial_\delta |q\rangle). \tag{5.54}$$

One can define a vector field in the $\delta - \Delta$ plane which is

$$\int dq \, (\Omega_{q\delta}, \Omega_{q,\Delta}) \, . \tag{5.55}$$

Plot this vector field.

5.1.6. Using the intuition you have gained from these calculations, consider a generic cyclic adiabatic deformation $\delta(0) = \delta(t)$ and $\Delta(0) = \Delta(t)$. Under what circumstances is charge transported during such a cyclic path. Can you give a simple picture of why?