Topological Insulators and Topological Superconductors

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1 Introduction

I have decided to write up a set of notes following each chapter of the book *Topological Insulators and Topological Superconductors* by Andrei Bernevig. Topology in condensed matter physics is something that comes up quite frequently in current research papers, seminars, and in conversations among leading researchers in the field, but is a topic that I have not formally learned about before. A colleague and mentor of mine, Dr. Alfred Zong, once recommended this book to me, as a great read for the experimental physics graduate student wanting a comprehensive, yet rigorous introduction to the field. However, as I started reading the book, I realized it was very technical and filled with math. I have found that the best way to learn such complicated topics is to take detailed notes and then teach it to someone else. Writing up these sets of notes in a conversational manner is my attempt to do just that. I hope you (whomever you are) enjoy.

2 Berry Phase

We consider a general physical system characterized by a Hamiltonian H($\mathbf{R}$) that depends on several external parameters $\mathbf{R}$=$(R_1, R_2, R_3, ...)$ which could be, for example, magnetic field, electric field, or strain. We are interested in how the wavefunction of the system evolves as these external parameters are varied adiabatically. In other words, we would like to know what the states $|n(\mathbf{R})\rangle$ are at each value of $\mathbf{R}$ such that

$$H(\mathbf{R})\,|n(\mathbf{R})\rangle = E_n(\mathbf{R})\,|n(\mathbf{R})\rangle \tag{1}$$

We have the gauge degree of freedom such that the general state of the system will be $|\psi(t)\rangle = e^{-i\theta(t)}\,|n(\mathbf{R}(t))\rangle$. The time evolution of this state is given by

$$H(\mathbf{R}(t))\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle\,. \tag{2}$$

Translating this into the differential equation

$$E_n(\mathbf{R}(t))\,|n(\mathbf{R}(t))\rangle = \hbar\left(\frac{d}{dt}\theta(t)\right)|n(\mathbf{R}(t))\rangle + i\hbar\frac{d}{dt}\,|n(\mathbf{R}(t))\rangle \tag{3}$$

and taking the scalar product with $\langle n(\mathbf{R}(t))|$ gives

$$E_n(\mathbf{R}(t)) - i\hbar\,\langle n(\mathbf{R}(t))|\,\frac{d}{dt}\,|n(\mathbf{R}(t))\rangle = \hbar\left(\frac{d}{dt}\theta(t)\right) \tag{4}$$

with the phase

$$\theta(t) = \frac{1}{\hbar}\int_0^t E_n(\mathbf{R}(t'))dt' - i\int_0^t \langle n(\mathbf{R}(t'))|\,\frac{d}{dt'}\,|n(\mathbf{R}(t'))\rangle\,dt' \tag{5}$$

The first term of this expression is the conventional dynamical phase, whereas the second term is the negative of the *Berry phase*:

$$\gamma_n = i\int_0^t \langle n(\mathbf{R}(t'))|\,\frac{d}{dt'}\,|n(\mathbf{R}(t'))\rangle\,dt' \tag{6}$$

We can remove the time-dependence, since we only need to know how the eigenstates depend on the parameters R_i, which gives

$$\gamma_n = i\int_0^t \langle n(\mathbf{R}(t'))|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R}(t'))\rangle\,dt' = i\int_{\mathcal{C}} \langle n(\mathbf{R})|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R})\rangle\,d\mathbf{R} \tag{7}$$

We can define a vector function called the Berry vector potential such that

$$\mathbf{A}_n(\mathbf{R}) = i\,\langle n(\mathbf{R})|\,\frac{\partial}{\partial \mathbf{R}}\,|n(\mathbf{R})\rangle\,, \tag{8}$$

$$\gamma_n = \int_{\mathcal{C}} d\mathbf{R}\cdot\mathbf{A}_n(\mathbf{R}) \tag{9}$$

We should note the following things

- γ_n is real
- The Berry vector potential $\mathbf{A}_n(\mathbf{R})$ is gauge dependent.
- Under a closed path, application of Stokes theorem gives

$$\gamma_n = -\mathrm{Im}\int d\mathbf{S}\cdot(\nabla\times\langle n(\mathbf{R})|\,\nabla_{\mathbf{R}}\,|n(\mathbf{R})\rangle \tag{10}$$

  where we see that the Berry phase can be thought of as the integral over a surface of the Berry curvature $(\nabla\times\mathbf{A})$, which is some sort of magnetic field in parameter space. This Berry curvature is gauge-independent.

We should be concerned with this definition of the Berry phase though, because it requires us to derivatize the wavefunction as we traverse through parameter space, which is a highly nontrivial thing to do. We would like to find an expression for γ_n that is gauge-independent. With a few short steps, we can do this, giving

$$\gamma_n = -\int\int_{\mathcal{C}} d\mathbf{S}\cdot\mathbf{V}_n \tag{11}$$

$$= -\int\int_{\mathcal{C}} d\mathbf{S}\cdot\mathrm{Im}\sum_{m\neq m}\frac{\langle n(\mathbf{R})|\,(\nabla_{\mathbf{R}}H(\mathbf{R}))\,|m(\mathbf{R})\rangle\times\langle m(\mathbf{R})|\,(\nabla_{\mathbf{R}}H(\mathbf{R}))\,|n(\mathbf{R})\rangle}{(E_m(\mathbf{R})-E_n(\mathbf{R}))^2} \tag{12}$$

We can interpret this expression as the result of an interaction of the level $|n\rangle$ with all the other levels $|m\rangle$ that have been projected out by the adiabatic interaction. If we sum over the Berry phase of all energy levels, we get 0. This final expression should concern us a little bit, since we could ask what happens when two energy levels are degenerate? The denominator of this expression would blow up. In fact, the formalism outlined thus far only applies to singly-degenerate energy levels. We must treat the degenerate case separately.

Let us consider a two-level system with the generic Hamiltonian

$$H = \epsilon(\mathbf{R})I_{2\times 2} + \mathbf{d}(\mathbf{R})\cdot\sigma \tag{13}$$

where **d** is 3D vector that depends on the external coordinates **R**. If we use spherical coordinates, we can parameterize the vector **d** as $\mathbf{d}(\mathbf{R}) = |d|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. The corresponding eigenstates of the two-level system at energies $\pm\frac{1}{2}|d|$ would be

$$|-\mathbf{R}\rangle = \begin{pmatrix}\sin\left(\frac{\theta}{2}\right)e^{-i\phi}\\ -\cos\left(\frac{\theta}{2}\right)\end{pmatrix} \tag{14}$$

$$|+\mathbf{R}\rangle = \begin{pmatrix}\cos\left(\frac{\theta}{2}\right)e^{-i\phi}\\ \sin\left(\frac{\theta}{2}\right)\end{pmatrix} \tag{15}$$

Calculating the Berry vector potential of the state $|-\mathbf{R}\rangle$from these expressions, we get

$$A_\theta = i\,\langle -\mathbf{R}|\,\partial_\theta\,|-\mathbf{R}\rangle = 0,$$

$$A_\phi = i\,\langle -\mathbf{R}|\,\partial_\phi\,|-\mathbf{R}\rangle = \sin\left(\frac{\theta}{2}\right)^2$$

$$F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2}$$

We notice, though, that the eigenstates we have chosen are not well defined at $\theta = \pi$. We could perform a gauge transformation by letting $|-\mathbf{R}\rangle \to e^{i\phi}|-\mathbf{R}\rangle$ and we would find that

$$|-\mathbf{R}\rangle = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ -\cos\left(\frac{\theta}{2}e^{i\phi}\right) \end{pmatrix} \tag{16}$$

$$\tag{17}$$

with $|-\mathbf{R}\rangle$ undefined at $\theta = 0$. In this new gauge, we have

$$A_\theta = i\langle -\mathbf{R}|\,\partial_\theta\,|-\mathbf{R}\rangle = 0,$$
$$A_\phi = i\langle -\mathbf{R}|\,\partial_\phi\,|-\mathbf{R}\rangle = \cos\left(\frac{\theta}{2}\right)^2$$
$$F_{\theta\phi} = \partial_\theta A_\phi - \partial_\phi A_\theta = \frac{\sin\theta}{2}$$

where we see that the Berry vector potential has changed, but the Berry curvature has not, demonstrating the gauge-invariance of the latter. However, what we have shown is that there is no gauge we can choose for which the states are everywhere well-defined. We will later find that this means the system will have a nonzero Hall conductance. For now though, we can make some statement about this degenerate point in parameter space.

If we were to calculate the Berry curvature generated by the state $|-\mathbf{R}\rangle$, we would find that at the degeneracy point it is a monopole of field that exerts a field of a strength equal and opposite in sign from the field generated by the state $|+\mathbf{R}\rangle$ at the same point. In general then, **degeneracy points in parameter space act as sources and drains of the Berry curvature.** Integrating the Berry curvature over a sphere containing N number of monopoles gives a number equal to 2π times the number of monopoles within the sphere. This number is called the *Chern number*.

In closing, we should wonder *can the Berry phase be measured?*. The answer is, yes, it can be measured in an interference experiment if the experiment is designed to impart a relative phase into a wavefunction defined as a superposition state.

3 Hall Conductance and Chern Numbers

We will show that the Hall conductance of a band insulator when the Fermi level is in the gap equals the integral of the Berry curvature over the full Brillouin Zone.

$$\sigma_{xy} = \frac{e^2}{\hbar}\frac{1}{2\pi}\int\int d_{k_x}d_{k_y}F_{xy}(k) \tag{18}$$

To embark on this goal, we must first derive the current operator and then analyze the linear response of system to the application of an electromagnetic field. To get the Hall conductance, we seek the off-diagonal conductance. We will consider a generic system with Hamiltonian

$$H = \sum_k c^\dagger_{k\alpha} h^{\alpha\beta}_k c_{k\beta} \tag{19}$$

where α and β are orbital and/or spin quantum numbers. The current satisfies a continuity equation

$$\dot{\rho}(x) = \nabla\cdot\mathbf{J}(x) = 0 \tag{20}$$

that when Fourier transformed gives

$$r\dot{h}o_q - i\mathbf{q}\cdot\mathbf{J}_q = 0 \tag{21}$$

with the Fourier transformed density operator given by

$$\rho(\mathbf{q}) = \frac{1}{\sqrt{N}}\sum_k c^\dagger_{\mathbf{k}+\mathbf{q}}c_{\mathbf{k}} \tag{22}$$

With some algebra, we can show from equation 21 that

$$-\mathbf{q}\cdot\mathbf{J}_{\mathbf{q}} = -r\dot{h}o_q = i\left[\rho, H\right] = \frac{-1}{\sqrt{N}}\sum_{p,k}(h_{\mathbf{k}+\mathbf{q}} - h_{\mathbf{k}})c^{\dagger}_{\mathbf{k}+\mathbf{q}}c_{\mathbf{k}} \tag{23}$$

Making the small q, long wavelength approximation (i.e. $h_{k+q} - h_k \approx \partial h_k/\partial\mathbf{k}\cdot\mathbf{q}$), we get, to first order

$$\mathbf{q}\cdot\mathbf{J}_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{p,k}\left(\frac{\partial h_k}{\partial\mathbf{k}}\cdot\mathbf{q}\right)c^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}}c_{\mathbf{k}+\frac{\mathbf{q}}{2}} \tag{24}$$

From here, we can read off the current operator at small q as

$$\boxed{\mathbf{J}_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{p,k}c^{\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}}\frac{\partial h_k}{\partial\mathbf{k}}c_{\mathbf{k}+\frac{\mathbf{q}}{2}}} \tag{25}$$

Knowing the current operator, we can use linear response theory to determine the current produced in response to an applied electric field. A generic Hamiltonian for a quantum system in the presence of an electromagnetic field is

$$H = \sum_i \frac{1}{2}(p_i - eA(x_i,t))^2 + \sum_{i<j}V_{ij} \tag{26}$$

If we define the current operator as

$$J(x,t) = \frac{1}{2}\sum_i\left[(p_i - eA(x,t))\delta(x-x_i) + \delta(x-x_i)(p_i - eA(x,t))\right] \tag{27}$$

then we can rewrite the Hamiltonian as

$$H = H_0 - e\int d^3x\int(\delta\mathbf{A}(x,t))\cdot\mathbf{J} \tag{28}$$

where H_0 is the Hamiltonian without the perturbing electromagnetic field. To first order, this becomes

$$H = H_0 - e\int d^3x\mathbf{A}(x,t)\cdot\mathbf{j}(x) = H_0 + H_{\text{ext}} \tag{29}$$

We now imagine that we begin in some eigenstate of the Hamiltonian H_0 which we will call $|E_N\rangle$. Shroedinger's equation tells us that this state will evolve according to

$$i\frac{\partial\left|E_N(t)\right\rangle}{\partial t} = H\left|E_N(t)\right\rangle \tag{30}$$

where

$$\left|E_N(t)\right\rangle = e^{-iH_0t}U_{\text{ext}}\left|E_N\right\rangle \tag{31}$$

Plugging this in, we get

$$i\frac{\partial U_{\text{ext}}}{\partial t}\left|E_N\right\rangle = e^{iH_0t}H_{\text{ext}}e^{-iH_0t}U_{\text{ext}}\left|E_N\right\rangle = H_{\text{ext}}(t)U_{\text{ext}}\left|E_N\right\rangle \tag{32}$$

which, when solved for U_{ext} gives to first order

$$U_{\text{ext}}(t) = 1 - i\int_0^t H_{\text{ext}}(t')dt' \tag{33}$$

with $H_{\text{ext}}(t) = e^{iH_0t}H_{\text{ext}}e^{-iH_0t}$ What we want is to solve for

$$\left\langle E_N(t)\right|\mathbf{J}(x,t)\left|E_N(t)\right\rangle = \left\langle E_N(t)\right|\mathbf{j}(x,t)\left|E_N(t)\right\rangle - ne\mathbf{A}(x,t) \tag{34}$$

which is the expectation value of the current, which is the sum of paramagnetic and diamagnetic components. Given that $|E_N(t)\rangle = e^{-iH_0 t}U_{\text{ext}}|E_N\rangle$ and we just solved for $U_{\text{ext}}(t)$, we can evaluate this expectation value as

$$\langle E_N(t)|\,\mathbf{J}(x,t)\,|E_N(t)\rangle = \langle E_N|\,\mathbf{j}(x)\,|E_N\rangle + i\int_0^t dt'\,\langle E_N|\,[H_{\text{ext}}(t'),\mathbf{j}(x,t)]\,|E_N\rangle - ne\mathbf{A}(x,t) \tag{35}$$

where $j(x,t) = e^{iH_0 t}j(x)e^{-iH_0 t}$. Using H_{ext} defined in equation 29 and measuring only deviations in the current from the case without the electric field present, we get

$$\langle E_N(t)|\,\mathbf{J}_i(x,t)\,|E_N(t)\rangle = \langle E_N(t)|\,\mathbf{j}_i(x)\,|E_N(t)\rangle + \int dt'\int d^3x\sum_j R_{ij}(x-x',t-t')A_j(x',t') \tag{36}$$

where the response function $R_{ij}(x-x',t-t')$ is defined as

$$R_{ij}(x-x',t-t') = -i\theta(t-t')\,\langle E_N|\,[j_i(x,t),j_j(x',t')]\,|E_N\rangle - ne\delta_{ij}\delta(x-x')\delta(t-t') \tag{37}$$

where $\theta(t)$ is a switch-on term. The remainder of the chapter is devoted towards determining this response function explicitly so that the off-diagonal current response to the applied electric field can be calculated precisely. I will just provide the end result and interpretation here and leave all the details of determining R_{ij} from Green's functions to the interested reader.

If we look at equations 36 and 37 we see that computing the Hall conductance depends on the eigenstates of the system, but doesn't depend explicitly on the energies of the occupied bands. This is a hint to us that the Hall conductance is a topological invariant. As such, we can perform a trick called "band flattening" which is a trick that will come in handy for us throughout the course of this book. The idea goes as follows: assuming the Fermi energy lies at $\epsilon = 0$, we will rescale all the bands in the valence band to lie at an energy $\epsilon_G < 0$ and all the bands the conduction band to lie at energy $epsilon_E > 0$. This is a reasonable thing to do, since the Hall conductance is a topological quantity and the band flattening procedure preserves the insulating gap. After performing the band-flattening procedure, one can more easily (still with several pages of math) compute the off-diagonal Hall conductivity, which turns out to be

$$\boxed{\sigma_{\text{i,j Hall}} = \int \frac{dk_x dk_y}{(2\pi^2}\sum_{\alpha=1}^{m} -i(\langle\partial_i(\alpha,k)|\,\partial_j\,|\alpha,k\rangle - \langle\partial_j(\alpha,k)|\,\partial_i\,|\alpha,k\rangle)} \tag{38}$$

in units of $e^2/\hbar$. What we see from this expression is that the Hall conductivity is an integral over the filled bands of the Berry curvature.

Let us make a few final comments about the Hall conductivity. For one, the Hall conductivity of a filled band must be an integer. This integer is called the **Chern number**. It is also often mentioned that the Chern number is understood to be "an obstruction to Stokes' theorem. What does this mean?

The Brillouin zone of a lattice with periodic boundary conditions is a torus and hence, it has no boundary. We just showed above that the Hall conductance of a filled band is equal to the integral of the Berry curvature over the Brillouin zone (which is a surface). By Stokes' theorem, we can relate an integral over a surface to an integral over a curve. But, the a torus has no boundary. This would imply that the Hall conductance (σ_{xy}) would be zero as long as the Berry vector potential, $\mathbf{A}(k)$, is well-defined over the whole BZ. If there is a nonzero Hall conductance, it must be true then that $\mathbf{A}(k)$ is NOT well-defined over the whole BZ.