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

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

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

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 $\mathbf{d}$ is 3D vector that depends on the external coordinates $\mathbf{R}$. If we use spherical coordinates, we can parameterize the vector $\mathbf{d}$ 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.