Geometry in Quantum Mechanics:
Basic Training in Condensed Matter Physics

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Lecture Notes: Spring 2014

Preface

About Basic Training

Basic Training in Condensed Matter physics is a modular team taught course offered by the theorists in the Cornell Physics department. It is designed to expose our graduate students to a broad range of topics. Each module runs 2-4 weeks, and require a range of preparations. This module, "Geometry in Quantum Mechanics," is designed for students who have completed a standard one semester graduate quantum mechanics course.

Prior Topics

2006 Random Matrix Theory (Piet Brouwer)
Quantized Hall Effect (Chris Henley)
Disordered Systems, Computational Complexity, and Information Theory (James Sethna)
Asymptotic Methods (Veit Elser)

2007 Superfluidity in Bose and Fermi Systems (Erich Mueller)
Applications of Many-Body Theory (Tomas Arias)
Rigidity (James Sethna)
Asymptotic Analysis for Differential Equations (Veit Elser)

2008 Constrained Problems (Veit Elser)
Quantum Optics (Erich Mueller)
Quantum Antiferromagnets (Chris Henley)
Luttinger Liquids (Piet Brouwer)

2009 Continuum Theories of Crystal Defects (James Sethna)
Probes of Cold Atoms (Erich Mueller)
Competing Ferroic Orders: the Magnetoelectric Effect (Craig Fennie)
Quantum Criticality (Eun-Ah Kim)

2010 Equation of Motion Approach to Many-Body Physics (Erich Mueller)
Dynamics of Infectious Diseases (Chris Myers)
The Theory of Density Functional Theory: Electronic, Liquid, and Joint (Tomas Arias)
Nonlinear Fits to Data: Sloppiness, Differential Geometry and Algorithms (James Sethna)

2011 Practical Density Functional Theory (Tomas Arias)
Semiclassical Methods (Erich Mueller)
Ginzburg-Landau Theory of Superconductivity (Chris Henley)
Continuum Quantum Monte Carlo Methods in Chemistry and Physics (Cyrus Umrigar)

2012 Quantum 14-15 puzzle: mechanics of a single hole in a spin-1/2 lattice (Veit Elser)
The science of writing Science (Eun-Ah Kim)
Feynman diagrams and *ab-initio* computation of excited states in condensed matter (Tomas Arias)
Probes of Cuprate Superconductors (theorist's view) (Chris Henley)
Physics of Life (Jane Wang)

2013 Many Body Field Theory (Erich Mueller)
The Theory of Density Functional Theory: Electronic, Liquid, and Joint (Tomas Arias)
Conformal Symmetry (Andre Leclair)
Nonlinear Fits to Data: Sloppiness, Differential Geometry and Algorithms (James Sethna)

2014 Rigidity (James Sethna)
Practical Density Functional Theory (Tomas Arias)
Quantum Monte-Carlo (Cyrus Umrigar)
Geometry in Quantum Mechanics (Erich Mueller)

About these Notes

These are lecture notes. This is not a review article. This is not a textbook. I have stolen ideas, and borrowed arguments. I've used rigor where it appropriate, and flapped my arms where it isn't. The notes are designed to be self-contained, and I've tried to keep the number of citations down. The style is casual. I've included "group activities" which are done in class. I do this because most of my students are smarter than I am, and its good to hear what they say. I've also included "problems". Do them. They are fun.

Contents

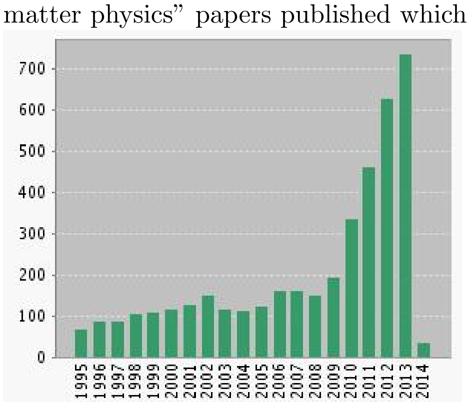
Chapter 1

Introduction

A. Excitement

> **Group Activity**: Find examples of the application of geometric ideas in quantum mechanics.

It is popular right now to find ways to apply concepts from geometry and topology to quantum systems. Here is a graph of the number of "condensed matter physics" papers published which topic "topological:"



The fact that this is rising is not the point (the number of scientists grows exponentially). The interesting thing is a sharp take-off around 2010.

Topology has been a niche area of interest in condensed matter physics for quite some time. In the 70's and 80's understanding "topological defects" was all the rage. David Mermin was a big player. In the mid 80's, Michael Berry realized that there was interesting geometric (and topological) physics associated with adiabatic transport. Starting in the 80's, there was also a great deal of progress in applying geometric and topological ideas to quantum Hall effects.

In general, physicists like math. They like finding new ways to apply math to physical systems. Topology and geometry are fun, and it is exciting to find ways of applying these ideas.

B. Geometry

The geometry I want to think about in this module is "differential geometry." This is the mathematics governing manifolds: think of a piece of paper in 3-dimensional space. The physics of topological insulators and topological superconductors is best described in this language. To make it more palatable, however, I am going to start with more concrete examples. We will first explore some simple properties of manifolds. Next we will look at electromagnetism, and see that it too has a geometric structure. This geometric structure of electromagnetism is behind most of the recent applications of topology and geometry in quantum mechanics. Next, we will explore the "geometry of parameter space," using geometric ideas to understand what happens when we vary the parameters in a Hamiltonian. Finally we will come to the geometry of momentum space, the idea which is at the heart of the modern discussion about topological insulators.

Where does topology come into this? Topology is the mathematical study of continuity. Is there a continuous path between two points? Generically I can continuously deform any Hamiltonian into any other. For example, $H = (1-\lambda)H_1 + \lambda H_2$ continuously interpolates between H_1 and H_2. If I add extra restrictions, such a continuous path may no longer be possible. For example, you might require a gap in the spectrum, and some symmetry – such as time reversal symmetry. Even if H_1 and H_2 have a gap and the symmetry, the linear combination may not. We will see many examples (mostly in the homework).

How do you tell if there is a continuous path between two points? One way is to try all paths. In many physical examples, such a direct approach works fine. In others, the space is too complicated to wrap your head around. In those cases one wants a more automated approach. For example, if you can calculate some number which cannot be changed by continuous deformations, then that "topological invariant" can distinguish the separate points.

As a concrete example, consider planar figures. Under typical rules of continuity, the figures with different numbers of holes in them cannot be deformed into one-another. The number of holes is a topological invarient. I won't give the expression here, but you can count the holes by integrating over the figure – one often extracts topological numbers from integrals of geometric quantities. This is the kernel at the center of De Rham Cohomology.

Chapter 2

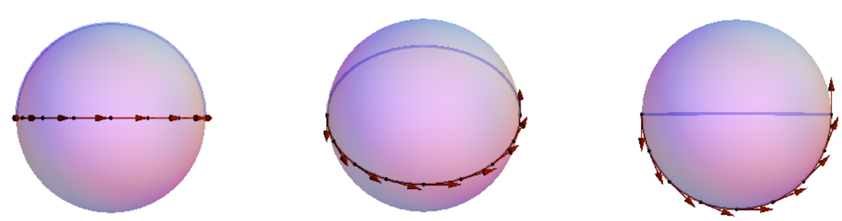
Geometry of Space

Parallel Transport and the Pancharatnam phase

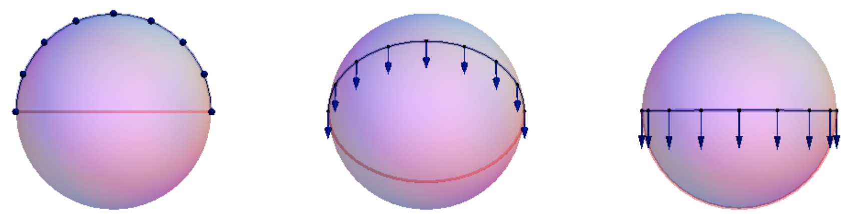
A. Parallel Transport

Imagine a sphere. Consider a vector of unit length $\mathbf{v}$ tangent to the sphere at one point $\mathbf{r}$. Move along the sphere, trying to rotate the vector as little as possible, but keeping the vector tangent. That is parallel transport. We are going to figure out how to do this. It turns out that we don't need to know much about 3D space to do this – we just need local information about the sphere.

Much of the physics we will be discussing is a generalization of this idea, so it will be important to understand it. The first thing to realize is that parallel transport depends on path. Consider two paths joining antipodal points on a sphere. Suppose we follow a path parallel to our vector $\mathbf{v}$. Then the vector "flips" during the transport:



On the other hand, if we follow a path perpendicular to the vector, it ends up pointing in its original direction:



Thus our end result will be an expression in terms of the path which the vector is transported along.

Our starting point is to consider parallel transport of the vector $\mathbf{v}$ between two nearby points $\mathbf{r}$ and $\mathbf{r}'$. We will denote the new vector as $\mathbf{v}'$. There the tangent space is spanned by two vectors $\mathbf{e_1'}, \mathbf{e_2'}$. As a 3D vector, $\mathbf{v}'$ is $\mathbf{v}$ when we "tilt" the plane. That is, let $\hat{n} = \mathbf{e_1} \times \mathbf{e_2}$ be the normal vector at $\mathbf{r}$, and lent $\hat{\mathbf{n}}' = \mathbf{e_1'} \times \mathbf{e_2'}$. We want the rotation that takes $\hat{n} \to \hat{n}'$ without introducing any extra "twist". Thus the vector $\mathbf{v}$ should be rotated into $\mathbf{v}' = v_1'\mathbf{e_1'} + v_2'\mathbf{e_2'}$. If we take a similar basis at $\mathbf{r}$, we can write $\mathbf{v} = \mathbf{v_1}\mathbf{e_1} + \mathbf{v_2}\mathbf{e_2}$. We then have

$$\begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = M \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}. \tag{2.1}$$

We want to know what the orthonormal matrix M is.

If the tangent planes had the same normal vector, one would have

$$M_0 = \begin{pmatrix} e_1 \cdot e_1' & e_2 \cdot e_1' \\ e_1 \cdot e_2' & e_2 \cdot e_2' \end{pmatrix}. \tag{2.2}$$

Unfortunately this does not in general preserve the norm. On the other hand, our normal vectors are typically almost parallel. In that case one finds to leading order in this deviation

$$M = \begin{pmatrix} e_2 \cdot e_2' + (1/2)(e_2 \cdot n')(e_2' \cdot n) & -e_1 \cdot e_2' - (1/2)(e_1 \cdot n')(e_2' \cdot n) \\ -e_2 \cdot e_1' - (1/2)(e_2 \cdot n')(e_1' \cdot n) & e_1 \cdot e_1' + (1/2)(e_1 \cdot n')(e_1' \cdot n) \end{pmatrix}. \tag{2.3}$$

There is probably a more elegant way to write this, but this was what I could come up with. For those who care about the derivation, I have a bonus problem on the homework which works you through this.

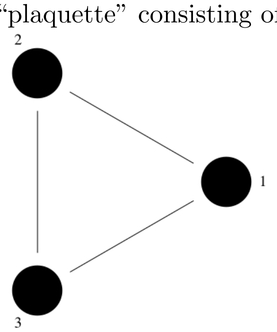
Regardless, this leads me to a mental model of a sphere (or any other surface) as a graph. The graph consists of a set of discrete points, representing my discretization of the sphere. Nearby points are connected by bonds. On each bond I record the distance and the matrix M. This representation is not unique:

it depends on by choice of local basis vectors $\mathbf{e_1}, \mathbf{e_2}$. The analog of this freedom in electromagnetism is Gauge freedom. Choosing the basis vectors is equivalent to choosing a Gauge in E&M. Note that this is a "directed graph," if M_{ij} is the basis transformation on going from i to j, then $M_{ji} = M_{ij}^{-1}$.

Note, most math textbooks take the continuum limit, but I find it clearer to think in this discrete picture. I know how to put this discrete system on a computer. One nice thing about this discrete version is that there is no need to choose your gauge to be smooth. The basis vectors on neighboring sites can be rotated arbitrarily. This is useful because there is no way to define the e_j's on a sphere such that they are smooth. We may prove this later. Regardless it makes the continuum version of things a bit complicated.

As a 2×2 orthonormal matrix, the M connecting site i and j is simply a rotation by some angle θ_{ij}. [Higher dimensional analogs will be more complicated, but lets start with this.] It is conventional to write $\theta_{ij} = \mathbf{r_{ij}} \cdot \mathbf{A}$, where $\mathbf{r_{ij}}$ is the vector connecting sites i and j. The logic for this definition comes from imagining we have a smooth gauge. Thus the θ's are small, and near-by θ's pointing in the same direction should be identical. Then the angle accumulated is just proportional to the distance hopped. The vector $\mathbf{A}$ is known as the *connection*. In our discrete model, it lives on bonds between neighboring sites. It tells you how to transform the basis vectors from one site to the next. The connection is gauge dependent.

One useful observation is that the angle accumulated when going around a closed path is independent of how one chooses the basis vectors. In other words, the product of the M's around a given closed path is "Gauge independent". You are comparing vectors on the same site. For example, lets look at an elementary "plaquette" consisting of three neighboring points, $i = 1, 2, 3$.



If I rotate the basis at site 2 by ϕ, without making any other changes, then $\theta_{12} \to \theta_{12} + \phi$ and $\theta_{23} \to \theta_{23} - \phi$ and the sum $\theta_{12} + \theta_{23} + \theta_{31}$ is unchanged.

It is also useful to note that if I consider the closed circuits $1 \to 2 \to 3$ or $2 \to 3 \to 1$ or $3 \to 1 \to 2$ I get the same angle. Thus I can introduce a dual representation, where for each plaquette I just specify the total angle rotated when I go around it. This angle, Ω is gauge independent.

I find it easier to understand Ω if I use a square plaquette. Then

$$\Omega = \theta_{12} + \theta_{23} + \theta_{34} + \theta_{41}. \tag{2.4}$$

This is conveniently regrouped as

$$\begin{aligned}
\Omega &= (\theta_{12} - \theta_{43}) - (\theta_{41} - \theta_{23}) && (2.5)\\
&= dy(A_y(x+dx) - A_y(x)) - dy(A_y(x+dx) - A_y(x)) && (2.6)\\
&= dxdy\nabla \times A. && (2.7)
\end{aligned}$$

Thus the phase accumulated is the area times the curl of A. The curl is gauge independent, as rotating one of the bases amounts to adding a gradient to $\mathbf{A}$.

It turns out that the curl of A is related to the curvature of the surface. To make that connection, however, we will need to figure out how to define curvature. Any sensible definition will give a sphere a constant curvature.

Lets begin by sitting at some point $\mathbf{r}$, where the normal vector is $\hat{n}$, which I will take to be the $\hat{z}$ direction. If I move some distance $d\mathbf{r}$ in the plane, the normal vector will tilt in the plane by an amount linear in $d\mathbf{r}$. Thus

$$d\hat{n} = \Lambda d\mathbf{r}, \tag{2.8}$$

where Λ is a 2×2 matrix. This matrix has two eigenvalues κ_1 and $\kappa 2$, with eigendirections corresponding to directions where the tilt is in the same direction as $\mathbf{dr}$. That is, if I move in those directions, I am simply following a circle of radius $R_j = 1/\kappa_j$. These are known as principle curvatures. You have probably heard of the Gaussian curvature, which is the product of these, ie $G = \det\Lambda$. You may also have heard of the Mean curvature, the algebraic mean of these two $H = \mathrm{Tr}\Lambda/2$.

There are elegant ways of calculating Ω, but I am always a big proponent of brute-force. Taking $\mathbf{r} = (0,0,0)$, and choosing our coordinate axes to be aligned with the principle curvature directions, our surface is defined by

$$z = 1 - \frac{\kappa_1 x^2}{2} - \frac{\kappa_2 y^2}{2}. \tag{2.9}$$

I will consider a grid with points $r_1 = (0,-\epsilon)$, $r_2 = (\epsilon, 0)$, $r_3 = (0,\epsilon)$, and $r_4 = (-\epsilon, 0)$. This gives a plaquette with area $2\epsilon^2$. To order ϵ, I can take the following local bases for the tangent spaces at these points

$$\begin{array}{lllllll}
e_1^{(1)} & = & \hat{x} & \qquad & e_2^{(1)} & = & \hat{y} + \kappa_2\epsilon\hat{z}\\
e_1^{(2)} & = & \hat{x} - \kappa_1\epsilon\hat{z} & & e_2^{(1)} & = & \hat{y}\\
e_1^{(3)} & = & \hat{x} & & e_2^{(1)} & = & \hat{y} - \kappa_2\epsilon\hat{z}\\
e_1^{(4)} & = & \hat{x} + \kappa_1\epsilon\hat{z} & & e_2^{(1)} & = & \hat{y}
\end{array} \tag{2.10}$$

The connection matrices are easily calculated

$$M_{12} = M_{23} = M_{34} = M_{41} = \begin{pmatrix} 1 & \kappa_1\kappa_2\epsilon^2/2 \\ -\kappa_1\kappa_2\epsilon^2/2 & 1 \end{pmatrix} \tag{2.11}$$

These correspond to $\theta_{12} = \theta_{23} = \theta_{34} = \theta_{41} = -\kappa_1\kappa_2\epsilon^2/2$. Thus $\Omega = 2\kappa_1\kappa_2\epsilon^2$. The curl of the connection is $\nabla \times A = \Omega/\text{area}{=}\kappa_1\kappa_2$. This is just the Gaussian curvature. [This is more-or-less the same as the relationship between the sum of the angles in a closed polygon and the curvature of a surface.

A final thing to do is think about the continuous limit. In the homework you will show that for a smooth gauge:

$$\begin{aligned} A &= e_1 \cdot \nabla e_2 - e_2 \cdot \nabla e_1 && (2.12) \\ \nabla \times A &= \partial_x A_y - \partial_y A_x = (\partial_x e_1) \cdot (\partial_y e_2) - (\partial_y e_1) \cdot (\partial_x e_2). && (2.13) \end{aligned}$$

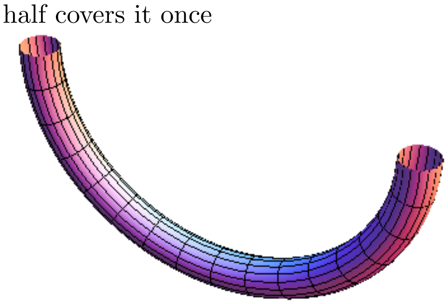
These latter two expressions are what you are most likely to find in the text-books.

A final, and equivalent, way to define the Gaussian curvature is that you imagine going around a small loop, and trace how the normal vector moves on the unit sphere. The ratio between the area traced out by the normal vector, and the area traced out on the surface, is the curvature.

B. Equivalence Classes of Surfaces

The normal vector can be thought of as a map from a surface to the surface of a sphere. We can distinguish two surfaces by asking how many times n, they cover the sphere (in a "handed" sense). This must be an integer for a closed surface. Clearly the normal vectors of a sphere cover the sphere once. Any surface which can be made by smoothly deforming a sphere will also have this property.

A torus, however, covers the sphere zero times (net). For example, the lower half covers it once



The upper half will cover the sphere in the exact opposite way. Because of this difference, we know we cannot continuously deform a sphere into a torus. A number which helps us break classes of objects into ones which cannot be mapped onto one-another is a "topological invarient."

It turns out that we do not need to know about the embedding to figure out this topological invarient. All we need is the curvature (or the connection):

$$n = \frac{1}{4\pi} \int ds \cdot \nabla \times A. \tag{2.14}$$

In a discretized version of our surface, this means you go around every plaquette, and calculate the phase accumulated when you go around it. The sum of all these accumulated phases is $4\pi n$.

It turns out that if one does not restrict ourselves to surfaces which can be embedded in three dimensional space, one can get n to also be a half integer. Regardless, here is a simple argument that it must be either an integer or half integer. The idea is that you imagine the phase accumulated when going around a small loop. For a small enough loop it must be roughly zero. But this must be the same as going around everything except the loop. Since rotations by multiples of 2π are identified with one-another, the sum of the phases accumulated must be a multiple of 2π. This makes n either an integer or half integer.

Chapter 3

Geometry of Electromagnetism

Space-time symmetries and quantum mechanics with gauge fields

A. Electromagnetic potentials as connections

In this lecture we will take the geometric reasoning developed last class, and apply it to thinking about electromagnetism. The standard formulation of electromagnetism is in terms of the scalar and vector potential $\phi, \tilde{\mathbf{A}}$. We are going to imagine discretizing space-time, and let the components of $\mathbf{A}$ live on the bonds between spatially separated sites, and the components of ϕ live on the bonds between temporally separated sites. These are supposed to play the role of the components of the "connection." Imagine we have a 2D unit vector (described by an angle θ) on the site at position $t, \mathbf{r}$. We will "parallel transport" this vector by using the connection. So when we move it a distance dx in the $\hat{x}$ direction, the angle rotates to $\theta + A_x dx$. In classical electricity and magnetism, there is no physical meaning to these vectors, but in quantum mechanics we will see that they are physical.

Now lets think about the curvature. If we go around a small loop in the $x-y$ plane: $(0,0) \rightarrow (dx, 0) \rightarrow (dx, dy) \rightarrow (0, dy) \rightarrow (0,0)$, the phase accumulated will be

$$\begin{aligned}
\Phi &= A_x(dx/2,0)dx + A_y(dx,dy/2)dy - A_x(dx/2,dy)dx - A_y(0,dy/2)dy && (3.1)\\
&= (\partial_x A_y - \partial_y A_x)dx\,dy && (3.2)\\
&= \mathbf{B}\cdot d\Omega, && (3.3)
\end{aligned}$$

which is just the magnetic flux enclosed in the loop. Thus if we interpret the vector potential as a connection, then the magnetic field can be interpreted as a curvature. Similarly we can think about the phase accumulated during a small loop in the $x-t$ plane:

$$\begin{aligned}
\Phi &= A_x(dx/2,0)dx + \phi(dx,dt/2)dt - A_x(dx/2,dt)dx - \phi(0,dt/2)dt && (3.4)\\
&= (\partial_x \phi - \partial_t A_x)dx\,dt && (3.5)\\
&= E_x dx\,dt. && (3.6)
\end{aligned}$$

Thus the electric field is also a curvature. The only difference is that an electric field is associated with loops involving time.

In this interpretation, gauge invariance is the ability to arbitrarily rotate the angles on each site,

Before quantum mechanics, this was just a convenient trick. In quantum mechanics, however, there is a physical meaning to the vectors: they are simply the real and imaginary parts of the wavefunction – or more simply, θ is the phase of the wavefunction.

The finite difference approximation to the Schrodinger equation on cubic grid is

$$i\frac{\psi(t+\delta t)-\psi(t)}{\delta t} = -\frac{\psi(\mathbf{r}+\delta\hat{\mathbf{z}})+\psi(\mathbf{r}-\delta\hat{\mathbf{z}})+\psi(\mathbf{r}+\delta\hat{\mathbf{y}})+\psi(\mathbf{r}-\delta\hat{\mathbf{y}})+\psi(\mathbf{r}+\delta\hat{\mathbf{x}})+\psi(\mathbf{r}-\delta\hat{\mathbf{x}})-6\psi(\mathbf{r})}{\delta^2}. \quad (3.7)$$

In the presence of a connection, we want to use parallel transport to compare two wavefunctions, so this should become

$$i\frac{e^{i\phi\delta t}\psi(t+\delta t)-\psi(t)}{\delta t} = -\frac{\hbar^2}{2m}\frac{e^{iA_z\delta}\psi(\mathbf{r}+\delta\hat{\mathbf{z}})+e^{-iA_z\delta}\psi(\mathbf{r}-\delta\hat{\mathbf{z}})+e^{iA_y\delta}\psi(\mathbf{r}+\delta\hat{\mathbf{y}})+e^{-iA_y\delta}\psi(\mathbf{r}-\delta\hat{\mathbf{y}})+e^{iA_x\delta}\psi}{\delta^2} \quad (3.8)$$

If we take the continuum limit we have

$$\left(i\partial_t - \phi\right)\psi = -\frac{\hbar^2}{2m}\left(\nabla + i\mathbf{A}\right)^2\psi, \quad (3.9)$$

which is the standard expression for the Schrodinger equation in a magnetic and electric field.

B. Gauge Invariance

Equation (3.9) is a Gauge theory, meaning that is is invariant under the following transformation

$$A \rightarrow A + \nabla\Lambda \tag{3.10}$$
$$\phi \rightarrow \phi + \partial_t\Lambda \tag{3.11}$$
$$\psi \rightarrow \psi e^{i\Lambda}. \tag{3.12}$$

All physically measurable quantities are invariant under this transformation. In our geometric interpretation, this freedom occurs because the phase of the wavefunction has no absolute meaning (just as there is no absolute meaning to the directions of the basis vectors for the tangent space on a sphere). Relative phases do matter, however. The electromagnetic potentials provide the *connection*, allowing us to compare wavefunctions on neighboring sites. Magnetic fields correspond to the situation where one picks up phases when one goes around closed loops in space, while electric fields correspond to phases coming from closed loops in space-time.

In physics, symmetries are typically associated with conservation laws. One usually ascribes gauge invariance to conservation of probability. That is, we define the current from the point $\mathbf{r}$ to the point $\mathbf{r} + \delta\hat{\mathbf{x}}$ to be

$$j_x = \frac{\hbar^2}{m}\frac{1}{i}\left[e^{iA_x\delta}\psi(\mathbf{r}+\delta\hat{\mathbf{x}})\psi^*(\mathbf{r}) - e^{-iA_x\delta}\psi(\mathbf{r}+\delta\hat{\mathbf{x}})^*\psi(\mathbf{r})\right], \tag{3.13}$$

then the rate of change of $|\psi(\mathbf{r})|^2$ will be given by the net current out of that node.

Often one thinks of superconductivity as a "spontaneous breaking of gauge invariance." That is, the order parameter is a pair wavefunction, and it has physical meaning – and particle number is no longer conserved (you have a reservoir of Cooper pairs). The London equations are, however, gauge invariant, as long as you also rotate the phase of the order parameter

It is also useful to comment that there is one difference between the vector space here, and the tangent space of a sphere. In the latter case the tangent space is itself geometric – it comes from the embedding of the sphere in 3-space – it is two dimensional because the manifold is two dimensional. The quantum mechanical wavefunction is something separate added on. It is two-dimensional, even though it lives in a four-dimensional world.

Chapter 4

Geometry of Parameter Space

Berry phase and the quantum mechanics of adiabatic processes

A. Adiabatic Theorem

Most of you have heard this story, but I want to repeat it with an eye to looking for the geometric aspects of the problem.

Imagine we have a time dependent Hamiltonian. For concreteness, think about a two-level system – a spin-1/2 in a time dependent magnetic field

$$H = \tilde{\mathbf{B}}(t) \cdot \vec{\sigma} \tag{4.1}$$

We can use spin up and spin down as a basis

$$\sigma_z | \uparrow\rangle = | \uparrow\rangle \qquad \sigma_x | \downarrow\rangle = -| \downarrow\rangle. \tag{4.2}$$

Suppose at time $t = 0$ the field is in the $\hat{z}$ direction, and our wavefunction is an eigenstate – say spin up. If we very slowly rotate the magnetic field, we expect the wavefunction to follow it. We have a classic problem of parallel transport. The key question is what happens to the phase of the wavefunction during this parallel transport.

To illustrate the conundrum, lets think about the eigenstates of H, when the magnetic field is pointing in an arbitrary direction with Euler Angles θ, ϕ:

$$\begin{aligned} |+\rangle &= e^{i\chi_+} \left[e^{i\phi/2} \cos(\theta/2) | \uparrow\rangle + e^{-i\phi/2} \sin(\theta/2) | \downarrow\rangle \right] & (4.3) \\ |-\rangle &= e^{i\chi_-} \left[e^{i\phi/2} \sin(\theta/2) | \uparrow\rangle - e^{-i\phi/2} \cos(\theta/2) | \downarrow\rangle \right]. & (4.4) \end{aligned}$$

The two angles χ_+ and χ_- are arbitary. These are still eigenstates no matter how we choose them. One natural choice is to set $\chi_+ = \chi_- = 0$. This seems sensible, but is clearly singular at the two poles. Another natural choice is $\chi_+ = -\phi/2, \chi_- = +\phi/2$, which is smooth at the North Pole, but singular at the South Pole. In fact, as with the tangent spaces on a sphere, there is no way to choose χ so that you have a globally smooth function. We will call a choice of χ as a choice of gauge.

In fact there is a correspondence between the quantum mechanical wavefunctions of a spin-1/2 particle, and the vectors on the surface of a sphere. [You were probably told that the correspondence was with the points on a sphere, but in fact it is with the vectors.] One such mapping is

$$\begin{aligned}
\mathbf{v} &= \cos(2\chi)\mathbf{v_1} + \sin(2\chi)\mathbf{v_2} && (4.5)\\
\mathbf{v_1} &= \cos\theta\cos\phi\hat{\mathbf{x}} + \cos\theta\sin\phi\hat{\mathbf{y}} - \sin\theta\hat{\mathbf{z}} && (4.6)\\
\mathbf{v_2} &= -\sin\phi\hat{\mathbf{x}} + \cos\phi\hat{\mathbf{y}}. && (4.7)
\end{aligned}$$

This is clearly not unique – but it indicates that the geometry of vectors on a sphere corresponds to the geometry of two-component wavefunctions. Note this mapping is two-to-one: two different quantum mechanical wavefunctions correpond to the same vector on the sphere. The 2 in 2χ appears so that the connections are the same in the two representations. This is a very famous mapping in geometry, known as the Hopf map. You can use it to define a homomorphism between the group $SU(2)$ and $SO(3)$.

Back to quantum mechanics. Let us imagine that we have a choice of χ which is smooth for the path that $\tilde{\mathbf{B}}$ takes. [We will describe dealing with the non-smooth version in a bit.] Then we can write

$$|\psi(t)\rangle = a(t)|+\rangle + b(t)|-\rangle. \tag{4.8}$$

The time dependent Schrodinger equation reads

$$ia'(t)|+\rangle + ia(t)\partial_t|+\rangle + ib'(t)|-\rangle + ib(t)\partial_t|-\rangle = a(t)B|+\rangle - b(t)B|-\rangle, \tag{4.9}$$

where B is the modulus of the magnetic field. Projecting this onto the basis states, we have

$$i\partial_t \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} B - i\langle+|\partial_t|+\rangle & -i\langle+|\partial_t|-\rangle \\ -i\langle-|\partial_t|+\rangle & -B - i\langle-|\partial_t|-\rangle \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}. \tag{4.10}$$

The pre-1984 wisdom was that as you go slower and slower, the derivative terms on the right become less and less important. This is in fact true, and to leading order

$$\begin{aligned} a(t) &= \exp(-i\int_0^t B(\tau)d\tau)a(0) && (4.11) \\ b(t) &= \exp(i\int_0^t B(\tau)d\tau)b(0). && (4.12) \end{aligned}$$

The wavefunction "adiabatically follows the field." Note that the dominant term gives a phase which is proportional to the time of the process. So in this adiabatic limit the phase is large. Note, however, the subdominant term does not vanish, as the process becomes infinitely slow – rather it stays constant. Thus it can still be important, even though it is subdominant. This is especially so if we know B – as we can readily subtract off the dominant part. If we let τ be the characteristic time over which $\mathbf{B}$ varies, then the off-diagonal terms make a contribution which is exponentially small in $|\mathbf{B}|\tau$ – thus we can throw it away, and get

$$\begin{aligned} a(t) &= \exp\left(-i\int^t B(\tau)d\tau - i\int_0^t \langle+|\frac{1}{i}\partial_t|+\rangle dt\right)a(0) && (4.13) \\ b(t) &= \exp\left(i\int^t B(\tau)d\tau - i\int_0^t \langle-|\frac{1}{i}\partial_t|-\rangle dt\right)b(0). && (4.14) \end{aligned}$$

A few comments are worth noting about the Berry Phase $\Phi = \int_0^t \langle+|\frac{1}{i}\partial_t|+\rangle dt$. First, this quantity is real, which follows from the fact that the normalization of our basis wavefunctions is preserved.

$$\begin{aligned} \partial_t\left[\langle+|+\rangle\right] &= 0 \\ (\partial_t\langle+|)|+\rangle + \langle+|(\partial_t|+\rangle) &= 0 \\ \left[\langle+|(\partial_t|+\rangle)\right]^* + \langle+|(\partial_t|+\rangle) &= 0 \end{aligned}$$

Second, this phase is independent of how fast the trajectory is traversed: the time derivative and the integration measure cancel.

It is natural to define a vector

$$\mathbf{A} = \langle+|\frac{1}{i}\nabla_B|+\rangle \tag{4.15}$$

To the extent that we do not choose our gauge to depend on the magnitude of $\mathbf{B}$, this vector always is tangent to $\mathbf{B}$, and depends on the gauge. This vector is a connection in the parameter space of the Hamiltonian. It tells you how to compare wavefunctions with different parameters. The Berry phase accumulated during the evolution

$$\Phi = \int_0^t \langle+|\frac{1}{i}\partial_t|+\rangle dt = \int dt\mathbf{B}\cdot\mathbf{A} = \int \mathbf{B}\cdot\mathbf{A}. \tag{4.16}$$

Now, how do you deal with the fact that there is no globally smooth gauge? One mental picture I like is to think of discretizing parameter space. At each point in parameter space I have a set of wavefunctions. On the bonds between them I have connections. It doesn't matter if things are smooth or not, because the connections will tell me how to rotate my wavefunctions. For example, consider two "nearby" points $\mathbf{B}$ and $\mathbf{B}'$. If I look at the overlap $\langle +B|+B'\rangle$, this should more-or-less be a phase factor $e^{i\phi_{BB'}}$. If I want to be precise, I define

$$e^{2i\phi_{BB'}} = \frac{\langle +B| + B'\rangle}{\langle +B'| + B\rangle}. \tag{4.17}$$

Then when I want to compare wavefunctions on these two sites, I just add this phase factor.

For example, the discretized time Schrodinger equation is

$$i\frac{e^{i\phi(t)}a(t+\delta t) - a(t)}{\delta t} = B(t)a(t), \tag{4.18}$$

where $\phi = \phi_{B(t)B(t')}$. The geometric phase accumulated is just the sum of all of these phases:

$$e^{2i\Phi} = \frac{\langle\psi(t_0)|\psi(t_1)\rangle\langle\psi(t_1)|\psi(t_2)\rangle\cdots < \psi(t_{N-1})|\psi(t_N)\rangle}{\langle\psi(t_N)|\psi(t_{N-1})\rangle\langle\psi(t_{N-1})|\psi(t_{N-2})\rangle\cdots < \psi(t_1)|\psi(t_0)\rangle} \tag{4.19}$$

This phase is gauge dependent – but all of the dependence just comes from the gauge of the initial and final wavefunction. This dependence is clear in the discrete formalism, as the intial and final states are the only ones which have only a *bra* or only a *ket*.

If you adiabatically traverse a closed path, then the phase becomes gauge independent: but it does depend on the exact path. A nice way to charactarize it is in terms of the curvature:

$$\oint \mathbf{B}\cdot\mathbf{A} = \iint d^2s\hat{s}\cdot\nabla\times\mathbf{A}. \tag{4.20}$$

The surface integral will be independent of the surface, as long as the boundaries are fixed to be the loop that B takes. Given the analogy with parallel transport on the sphere, you should not be surprised to find that the phase accumulated is simply half the area of the unit sphere which is subtended by the path. In the homework you will explicitly calculate the curvature, and verify this.

B. Generalization

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. 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:

$$\Phi = \oint \langle \phi | i\nabla | \phi \rangle \cdot d\mathbf{R}. \tag{4.21}$$

The "Berry Connection" is

$$\mathbf{A} = \langle \phi | i\nabla | \phi \rangle. \tag{4.22}$$

This is a vector which is analogous to the vector potential in electromagnetism. The vector A is gauge dependent.

Again we write Eq. (4.21) ias a surface integral of a curl

$$\Phi = \iint \nabla \times \langle \phi | i\nabla | \phi \rangle \tag{4.23}$$

$$= \iint i(\nabla \langle \phi |) \times (\nabla | \phi \rangle) d^2\mathbf{R}, \tag{4.24}$$

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

$$\mathbf{\Omega} = i(\nabla \langle \phi |) \times (\nabla | \phi \rangle). \tag{4.25}$$

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 transform $|\phi\rangle \to e^{i\Lambda}|\phi\rangle$. Under this transformation the connection transforms as

$$\mathbf{A} \to \mathbf{A} + i\nabla\Lambda. \tag{4.26}$$

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

$$\mathbf{\Omega} = i\sum_m (\nabla \langle \phi | m \rangle) \times (\langle n | \nabla | \phi \rangle). \tag{4.27}$$

First order perturbation theory then gives

$$\langle n(\mathbf{R}) | \nabla | \phi(\mathbf{R}) \rangle = \frac{\langle n | \nabla H | \phi \rangle}{E_n - E_\phi}, \tag{4.28}$$

which allows one to write

$$\mathbf{\Omega} \;=\; i\sum_n \frac{\langle\phi|\nabla H|n\rangle \times \langle n|\nabla H|\phi\rangle}{(E_n - E_\phi)^2}. \tag{4.29}$$

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.

C. Symmetries

If the Hamiltonian has certain symmetries, then that puts constrains on the order-parameter space. For example, suppose we have a constraint that the magnetic field is nonzero and always points in the x-z plane. Under those circumstances, the Berry phase for a closed path is restricted to be multiples of π – and it counts how many times the magnetic field winds around the sphere. Thus with symmetries the geometric phase can become *topological*: it labels equivalence classes of time dependent Hamiltonians which can be continuously mapped into one-another.

Note 1: A path with Berry phase π can be mapped into one with 0 if one breaks the symmetry.

Note 2: The curvature actually vanishes in this case. However, we have a manifold with a boundary (we excluded the point $B = 0$). The Berry phase came from this point. One can think about the curvature being a delta-function at that point.

D. Adiabaticity in Space

In addition to time dependent magnetic fields one can consider spatially varying magnetic fields. Suppose you have a spin-1/2 particle moving very slowly through an inhomogeneous field. The spin should then just adiabatically follow the field. In this transport the wavefunction will pick up phases which are completely analogous to the phases accumulated by a charged particle moving through a magnetic field. The non-trivial connection here comes from the curvature of the order-parameter space, rather than the magnetic field. Many of the "artificial magnetic fields" in cold atoms can be interpreted in this way.

Lets be concrete, Imagine a spin-1/2 Schrodinger equation of the form

$$i\partial_t \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} -\frac{\nabla^2}{2} - B_z(\mathbf{r},t) & -B_x(\mathbf{r},t) + iB_y(\mathbf{r},t) \\ -B_x(\mathbf{r},t) - iB_y(\mathbf{r},t) & -\frac{\nabla^2}{2} + B_z(\mathbf{r},t) \end{pmatrix} \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}. \tag{4.30}$$

If **B** is slowly varying, one can make the adiabatic ansatz:

$$\psi(\mathbf{r},t) = \phi(r,t)|\xi(r,t)\rangle \tag{4.31}$$

where

$$\begin{pmatrix} -B_z(\mathbf{r},t) & -B_x(\mathbf{r},t) + iB_y(\mathbf{r},t) \\ -B_x(\mathbf{r},t) - iB_y(\mathbf{r},t) & B_z(\mathbf{r},t) \end{pmatrix} |\xi(r,t)\rangle = -|B(r,t)||\xi(r,t)\rangle. \tag{4.32}$$

Of course, this does not uniquely define ξ: we have a gauge degree of freedom. Lets assume we have chosen some gauge, and that it is smooth. Note, we may be able to find a smooth gauge, even though there is no global way to define ξ in terms of **B**. The trick is that we do not attribute a unique ξ to each **B**. For example suppose

$$B_x = \cos(y)\sin(x) \tag{4.33}$$
$$B_y = \sin(y)\sin(x) \tag{4.34}$$
$$B_z = \cos(x) \tag{4.35}$$

Then a (non-unique) chose of ξ is

$$|\xi\rangle = \begin{pmatrix} e^{iy/2}\cos(x/2) \\ e^{-iy/2}\sin(x/2) \end{pmatrix}. \tag{4.36}$$

This is clearly continuous, but $\xi(x=0,y) = e^{iy/2}\xi(x=0,y=0)$ has a winding phase, even though **B** is constant when $x = 0$. The only time we will run into trouble with this approach is if we have periodic boundary conditions. Then we will need to use a singular gauge.

To formally derive the equations of motion of $\phi(r,t)$, we take the derivative

$$i\partial_t|\psi\rangle = (i\partial_t\phi)|\xi\rangle + i\phi\partial_t|\xi\rangle \tag{4.37}$$
$$\langle\xi|ipartial_t|\psi\rangle = i\left[\partial_t - iA_t\right]\phi \tag{4.38}$$

where

$$A_t = \langle\xi|i\partial_t|\xi\rangle. \tag{4.39}$$

Similarly

$$\langle\xi| - \partial_x^2|\psi\rangle = i\left[\partial_t - iA_x\right]^2\phi \tag{4.40}$$

where

$$A_x = \langle\xi|i\partial_x|\xi\rangle. \tag{4.41}$$

Thus we have something which looks exactly like a Schrodinger equation in an electric and magnetic field.

$$i\left[\partial_t - iA_t\right]\phi = -\frac{1}{2}\left[\nabla - i\mathbf{A}\right]^2\phi + |B|\phi. \tag{4.42}$$

These equations are invariant under the gauge transformation

$$|\xi\rangle \rightarrow e^{i\chi}|\xi\rangle \tag{4.43}$$

$$\phi \rightarrow e^{-i\chi}\phi \tag{4.44}$$

$$A_\nu \rightarrow A - \partial_\nu A. \tag{4.45}$$

My students should be familiar with the following important example. Suppose the $\uparrow$ and $\downarrow$ are two hyperfine states of a Rb atom in a magnetic field gradient. A real magnetic field plays the role of the $\hat{z}$ component of $\mathbf{B}$. A pair of Raman lasers drive a transition for $\uparrow$ to $\downarrow$. If these are counterpropegating, than t he phase of the matrix element winds in space. This yields a Schrodinger equation

$$i\partial_t\left(\begin{array}{c}\psi_\uparrow\\ \psi_\downarrow\end{array}\right) = \left(\begin{array}{cc}-\frac{\nabla^2}{2} - \mu Bx & \Omega(x)e^{iky}\\ \Omega(x)e^{-iky} & -\frac{\nabla^2}{2} + \mu Bx\end{array}\right)\left(\begin{array}{c}\psi_\uparrow\\ \psi_\downarrow\end{array}\right). \tag{4.46}$$

The intensity of the beams $\Omega(x)$ are generically a Gaussian. Within the adiabatic approximation there is a vector potential corresponding to a nontrivial magnetic field. Ian Spielman has created vortices with this trick.

E. Breakdown of Adiabaticity

Here I will give the classic argument for the breakdown of adiabaticity. Imagine we have a spin-1/2 particle in a time dependent magnetic field

$$H(t) = \left(\begin{array}{cc}\alpha t & \Delta\\ \Delta & -\alpha t\end{array}\right). \tag{4.47}$$

The time dependent Schrodinger equation is

$$i\hbar\partial_t\psi = H\psi. \tag{4.48}$$

In the limit $\hbar\alpha/\Delta^2 \ll 1$ the time dependence of H is slow. Once again we transform to the "adiabatic basis". That is, we diagonalize $H(t)$ to find $H(t)|+(t)\rangle = \epsilon(t)|+(t)\rangle$ and $H(t)|-(t)\rangle = -\epsilon(t)|-(t)\rangle$. Explicitly,

$$\epsilon(t)^2 = \Delta^2 + \alpha^2 t^2 \tag{4.49}$$

$$|+(t)\rangle = \left(\begin{array}{c}\cos(\xi/2)\\ \sin(\xi/2)\end{array}\right) \tag{4.50}$$

$$|-(t)\rangle = \left(\begin{array}{c}-\sin(\xi/2)\\ \cos(\xi/2)\end{array}\right) \tag{4.51}$$

where $\tan\xi = \alpha t/\Delta$. As before$|e\rangle$ and $|g\rangle$ are ambiguous. We could always add an arbitrary phase to them. In the present case the ambiguity is trivial, and it has no effect.

We want to know if you start at time $-\infty$ in state $|-\rangle$, what is the probability that you end up in the state $|+\rangle$. To lowest order the probability is zero, and

$$|\psi(t)\rangle = e^{i\int^t \epsilon(t)dt/\hbar}|-(t)\rangle. \tag{4.52}$$

One gets this result by looking at the equations of motion for $|\psi\rangle = a|+\rangle + b|-\rangle$. Schrodinger's equation reads

$$\begin{aligned} \langle -|i\hbar\partial_t|\psi\rangle &= i\hbar\partial_t b + a\langle -|i\hbar\partial_t|+\rangle + b\langle -|i\hbar\partial_t|-\rangle & (4.53)\\ &= \langle -|H|\psi\rangle = -b\epsilon, & (4.54)\end{aligned}$$

and a similar expression of a. Rewriting, this becomes

$$(i\hbar\partial_t + \epsilon)b = -a\langle -|i\hbar\partial_t|+\rangle - b\langle -|i\hbar\partial_t|-\rangle. \tag{4.55}$$

The right hand side is small in the semiclassical limit, leading to Eq. (4.56). The first term on the right hand side is responsible for the tunneling between branches, while the second term is a phase factor. If we neglect the first term, but include the second, we can improve Eq. (4.56) to become

$$|\psi(t)\rangle = e^{i\int^t \epsilon(t)dt/\hbar - i\int^t \langle -|i\partial_t|-\rangle}|-(t)\rangle. \tag{4.56}$$

For the gauge we have chosen, $\langle -|i\partial_t|-\rangle = 0$, so we can ignore this Berry Phase.

E.1. Classic Approach to the Landau-Zener problem

Explictly, the equations of motion for a and b are

$$\begin{aligned} (i\hbar\partial_t - \epsilon)a &= \frac{i}{2}\partial_t\xi b & (4.57)\\ (i\hbar\partial_t + \epsilon)b &= -\frac{i}{2}\partial_t\xi a & (4.58)\end{aligned}$$

with

$$\partial_t\xi = \frac{\alpha/\Delta}{1+\alpha^2t^2/\Delta^2}. \tag{4.59}$$

Solving these is a real pain. The classic approach is to avoid this adiabatic basis altogether, and instead work in the original basis:

$$|\psi\rangle = \begin{pmatrix} C_1 e^{-\frac{i}{\hbar}\int^t \epsilon_1 dt} \\ C_2 e^{-\frac{i}{\hbar}\int^t \epsilon_2 dt}\end{pmatrix} \tag{4.60}$$

where $\epsilon_1 = \alpha t$, and $\epsilon_2 = -\alpha t$ are the energies of the two basis states in the absence of coupling between the levels. This leads to equations of motion

$$\begin{aligned} i\hbar\partial_t C_1 &= \Delta e^{\frac{i}{\hbar}\int(\epsilon_1-\epsilon_2)dt} C_2 &(4.61)\\ i\hbar\partial_t C_2 &= \Delta e^{\frac{i}{\hbar}\int(\epsilon_2-\epsilon_1)dt} C_1 &(4.62)\end{aligned}$$

with boundary conditions that at large negative time $C_1 = 0$ and $C_2 = 1$. The two equations can be recast into a single second order differential equation, for

$$U_1 = e^{-\frac{i}{2\hbar}\int(\epsilon_1-\epsilon_2)dt} C_1, \tag{4.63}$$

that reads

$$\partial_z^2 U_1 + (n + 1/2 - z^2/4)U_1 = 0 \tag{4.64}$$

where $z = \alpha^{1/2} e^{-i\pi/4} t$, $n = i\Delta^2/\alpha$, and I lost my hbar's somewhere. Regardless, equation (4.64) is nothing but the equation of motion for a quantum mechanical harmonic oscillator – except that we have a funny boundary condition. The solution is a "parabolic cylinder function" whose asymptotics can be used to calculate the probability of a transition:

$$P = \exp\left(-\frac{\pi}{2}\frac{\Delta^2}{\alpha}\right). \tag{4.65}$$

Ugh – I would hardly wish this on my worst enemy.

E.2. Analytic Continuation approach to the Landau-Zener Problem

There is a trick, similar to the one we used to find our connection formulas, which spares us much of that 18th century mathematics. Again it is not rigorous, but is a heck of a lot easier. What we do is assume that adiabaticity holds, and write

$$|\psi(t)\rangle = |\xi(t)\rangle_- e^{\frac{i}{\hbar}\int^t \epsilon(t)}, \tag{4.66}$$

where we have written $|\xi(t)\rangle_-$ as a slightly more explicit notation for $|-\rangle$.

Now we do a bit of profound "out of the box" thinking. Equation (4.66) defines $|\psi(t)\rangle$ on the entire complex t plane. There are two branch points in the complex plane at $t = \pm i\Delta/\alpha$. If one moves around one of them, $|-\rangle$ turns into $|+\rangle$. Lets be adventurous and follow this path around the upper branch point

$$\begin{aligned} |\psi(t)\rangle &= e^{i\Phi} e^{2i\int_0^{i\Delta/\alpha}\epsilon(t)dt/\hbar} |\xi(t)\rangle_+ &(4.67)\\ &= e^{i\Phi} e^{-2\int_0^{\Delta/\alpha}\sqrt{\Delta^2-\alpha^2\tau^2}d\tau/\hbar} |\xi(t)\rangle_+, &(4.68)\end{aligned}$$

where Φ is an unimportant phase factor.

Thus the probability of tunneling is

$$P = e^{-\frac{\pi}{2}\Delta^2}\hbar\alpha, \tag{4.69}$$

and the adiabatic approximation works when $\Delta^2/\hbar\alpha \gg 1$.

Chapter 5

The Geometry of Momentum Space I

Bloch States, Wannier States, and Zac's Phase

In this chapter I will present a story from the 1990's, when it was realized that one needs to include Berry Phase concepts in order to understand the polarization of solids. To tell this story, I will begin by a discussion of Bloch states. We will find a geometric phase there which relates to the center of mass of Wannier States.

A. Band Structure

Consider the quantum mechanics of a particle in a one dimensional periodic potential

$$E\psi(x) = -\frac{1}{2}\partial_x^2\psi(x) + V(x)\psi(x), \tag{5.1}$$

where $V(x+L) = V(x)$. Bloch's theorem states that we can write the solutions as

$$\psi_k(x) = e^{ikx}u_k(x), \tag{5.2}$$

where $u_k(x+L) = u_k(x)$, and

$$E_k u_k(x) = -\frac{1}{2}(\partial_x - ik)^2 u_k(x) + V(x)u_k(x). \tag{5.3}$$

Clearly $E_{k+2\pi/L} = E_k$ and $u_{k+2\pi/L}(x) = u_k e^{2\pi x/L}$. From the perspective of this course, this defines a mapping from a ring (the points $0 < k < 2\pi$) to the space of square integrable functions on the interval $[0, L]$. This is a manifold, and its geometry will have implications. In higher dimensions it is related to the map of a torus into this large space.

Since the space of square integrable functions is hard to grasp, it might be better to think about a tight binding model with a superlattice. Say

$$E\psi_j = -\left[t+(-1)^j\epsilon\right]\psi_{j+1} - \left[t-(-1)^j\epsilon\right]\psi_{j-1} + (-1)^j\Delta\psi_j. \tag{5.4}$$

Here Δ represents an energy difference between even and odd sites, while ϵ represents a difference between the strength of alternate bonds. Bloch's theorem states $\psi_j = e^{ikj}u_k$ on even sites and $\psi_j = e^{ikj}v_k$ on odd sites, and since the unit cell has length two, $-\pi/2 < k < \pi/2$. Taking j even, we find

$$E_k e^{ikj}u_k = \left[-(t+\epsilon)e^{ik(j+1)} - (t-\epsilon)e^{ik(j-1)}\right]v_k + \Delta e^{ikj}u_k \tag{5.5}$$

Taking j odd, we instead find

$$E_k e^{ikj}v_k = \left[-(t-\epsilon)e^{ik(j+1)} - (t+\epsilon)e^{ik(j-1)}\right]u_k - \Delta e^{ikj}u_k \tag{5.6}$$

These are conveniently combined to a matrix equation

$$\begin{pmatrix} \Delta & -2t\cos(k)+2i\epsilon\sin(k) \\ -2t\cos(k)+2i\epsilon\sin(k) & -\Delta \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix} = E_k\begin{pmatrix} u_k \\ v_k \end{pmatrix} \tag{5.7}$$

Thus at each k we just have the Hamiltonian for a spin-1/2 in a magnetic field

$$B_k = \Delta\hat{z} - 2t\cos(k)\hat{x} - 2\epsilon\sin(k)\hat{y}, \tag{5.8}$$

and we can read off the band structure

$$E_k^2 = \Delta^2 + 4t^2\cos^2(k) + 4\epsilon^2\sin^2(k), \tag{5.9}$$

which as expected has period π (since $L = 2$). One can easily imagine similar dynamics in 2 or higher dimension.

The Bloch wavefunction is formally a two-component spinor:

$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = e^{i\chi_k}\begin{pmatrix} \cos(\theta_k/2)e^{i\phi_k/2} \\ \sin(\theta_k/2)e^{-i\phi/2} \end{pmatrix}, \tag{5.10}$$

with $\tan(\theta_k) = \sqrt{4t^2\cos^2(k)+4\epsilon^2\sin^2(k)}/\Delta$, and $\tan(\phi_k) = (\epsilon/t)\tan(k)$. As before, the phases χ_k are arbitrary – and there is no Canonical choice for them. In this one dimensional case we can always choose χ_k so that the wavefunctions vary smoothly with k – but even so they are not unique. In two or higher dimension we might come up against the "hairy ball" problem.

Although the dispersion was periodic with period π, the u's and v's will not. We require instead $u_{k+\pi}(0) = u_k(0)$ and $v_{k+\pi}(1) = -v_k(1)$. [In general, for any reciprocal lattice vector G, $u_{k+G}(x) = e^{iGx}u_k(x)$] Thinking of (u, v) as a point on the Bloch sphere, this corresponds to a rotation by π about the $\hat{z}$ axis.

As a concrete example, lets take $t = \epsilon$, then we could take

$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \begin{pmatrix} \cos(\theta/2)e^{ik} \\ \sin(\theta/2) \end{pmatrix}, \tag{5.11}$$

where $\tan\theta = 2t/\delta$. The connection is

$$A_k = \begin{pmatrix} u_k & v_k \end{pmatrix} \frac{1}{i}\partial_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \cos^2(\theta/2) \tag{5.12}$$

This connection depends on the choice of χ_k, but as long as $u_{k+\pi} = u_k$ and $v_{k+\pi} = -v_k$, the total phase accumulated when k increases by π will be independent of χ. In this case

$$\Phi = \int_{-\pi/2}^{\pi} /2 A_k \, dk = \pi\cos^2(\theta/2) = \frac{\pi}{2}\left[1 + \frac{\Delta}{\sqrt{4t^2 + \Delta^2}}\right]. \tag{5.13}$$

This phase is known as "Zac's phase," and it is geometric, but not topological: it clearly can take on any value between 0 and 2π.

An important caution is in order. Although Zac's phase is independent of gauge, it depends on the origin of space. If I shift the origin by δ, I need to shift my boundary conditions:

$$u_{k+\pi} = e^{i\pi\delta}u_k \tag{5.14}$$
$$v_{k+\pi} = e^{i\pi(1+\delta)}v_k. \tag{5.15}$$

This can be accomplished by taking

$$u_k \rightarrow u_k e^{ik\delta} \tag{5.16}$$
$$v_k \rightarrow v_k e^{ik\delta}, \tag{5.17}$$

This transform takes $A_k \rightarrow A_k + \delta$, and $\Phi \rightarrow \Phi + \delta\pi$.

As we will shortly see, this behavior emerges because Φ physically corresponds to the displacement of the center of mass of the Wannier state from the origin. To prove that, we will need to understand how to define Wannier states.

B. Wannier States

Consider the projection of the position operator into the lowest band:

$$\begin{aligned}\hat{X}_p &= \hat{P}\hat{X}\hat{P} && (5.18)\\ &= \sum_{kk'} |k\rangle\langle k|X|k'\rangle\langle k'| && (5.19)\\ &= \sum_{k,k'x} |k\rangle\langle k|x\rangle x\langle x|k'\rangle\langle k'|. && (5.20)\end{aligned}$$

You may have seen other definitions in your solid state class, but here we will take the eigenstates of $\hat{X}_p$ to be the "Wannier states". They are the position eigenstates projected into the lowest band.

As a particularly simple case, consider what happens when $\Delta > 0$, but $t = \epsilon = 0$. Then $u_k = 1$ and $v_k = 0$ so

$$\langle x|k\rangle = \begin{cases} e^{ikx} & x \text{ odd} \\ 0 & x \text{ even} \end{cases} \tag{5.21}$$

The projected position operator is then

$$\begin{aligned}\hat{X}_p &= \sum_{x \text{ even}} x \sum_{k,k'} |k\rangle e^{ikx} e^{-ik'x}\langle k'| && (5.22)\\ &= \sum_{x \text{ even}} x|x\rangle\langle x|, && (5.23)\end{aligned}$$

where we uses $|x\rangle = \sum_k e^{ikx}|k\rangle$. Thus the Wannier states are just the even sites.

Suppose we have one Wannier state $|x_0\rangle = \sum_x \phi(x)|x\rangle$, which satisfies $\hat{X}_p|x_0\rangle = x_0|x_0\rangle$. We can construct a new state

$$|x_N\rangle = \sum_x \phi(x)|x_0 - NL\rangle \tag{5.24}$$

which obeys $\hat{X}_p|x_N\rangle = (x_0 + NL)|x_N\rangle$. That is, we have one Wannier state per unit cell. The eigenvalue is the location of the center of the packet. The position of the packet in the unit cell is shifted $\Phi L/2\pi$ from the origin.

First to prove that the eigenvalue is the location of the packet, we note that by construction $P|x_0\rangle = |x_0\rangle$ Thus

$$\langle x_0|PXP|x_0\rangle = \langle x_0|X|x_0\rangle = x_0. \tag{5.25}$$

Since translations by a multiple of a lattice constant do not take us out of the band, we have

$$\langle x_N|X|x_N\rangle = \langle x_0|T_{NL}^{-1}XT_{NL}|x_0\rangle = \langle x_0|X + NL|x_0\rangle. \tag{5.26}$$

To understand the shift, it is convenient to introduce the position operator modulo L, defined by

$$R_p = e^{iX_p/L} = Pe^{iX/L}P. \tag{5.27}$$

We should have that $R_p = e^{\imath\alpha}P$, where $\alpha = (2\pi/L)(x_0 \mod L)$. I claim $\alpha = \Phi$.

To prove this, I consider the operator

$$R_p(\epsilon) = e^{i\epsilon X_p/L}, \tag{5.28}$$

such that $R_p = R_p(\epsilon)^{1/\epsilon}$.

$$\begin{aligned} R_{kk'}(\epsilon) &= \langle k|R_p(\epsilon)|k'\rangle & (5.29)\\ &= \sum_x \langle k|x\rangle e^{i2\pi\epsilon x/L}\langle x|k'\rangle & (5.30)\\ &= \sum_x e^{i(k'-k+2\pi\epsilon/L)x}u_{k'}(x)u_k^*(x). & (5.31)\end{aligned}$$

Since the u's are periodic, this is zero unless $k' = k + 2\pi\epsilon/L$, whence

$$\begin{aligned} R_{kk'}(\epsilon) &= \delta_{k'-k-2\pi\epsilon/L}\int_0^L dx u_k^*(x)u_{k+2\pi\epsilon/L}(x) & (5.32)\\ &\approx \delta_{k'-k-2\pi\epsilon/L}e^{(2\pi\epsilon/L)A_k}, & (5.33)\end{aligned}$$

where we assum ϵ is small. Raised to the $1/\epsilon$ power, this yields

$$R_{kk'} = \delta_{kk'}e^{i\Phi}. \tag{5.34}$$

C. Beyond 1D

This Wannier state construction does not work in 2D (or higher). The problem is that the projected position operators X_p and Y_p do not necessarily commute.

To understand the structure, lets consider a square lattice and imagine we have some Hamiltonian which we diagonalize to get for each k in the 2D Brillioun zone a periodic function $u_{k_x,k_y}(r)$. We require

$$\begin{aligned} u_{k_x+2\pi/L,k_y} &= e^{i2\pi/Lx}u_{k_x,k_y} & (5.35)\\ u_{k_x,k_y+2\pi/L} &= e^{i2\pi/Ly}u_{k_x,k_y+2\pi/L}. & (5.36)\end{aligned}$$

Unlike the 1D case, there may not be any smooth way to define u_{k_x,k_y}

We now construct $X_p(k_y)$, the x operator projected into the part of the Brillioun zone with fixed k_y. This gives us the location of a Wannier state $x_0(k_y)$. If we do things right, $X_p(k_y + 2\pi/a) = X_p(k_y)$. Thus $x_0(k_y + 2\pi/a) = x_0(k_y) + na$. The integer n is independent of the choice of origin. It is a topological invariant. In fact, we can relate it to the Chern number.

To this this relation we note that up to a multiple of the lattice period

$$x_0(k_y) = \frac{L}{2\pi}\int_0^{2\pi/L} dk_x\, A_x(k_x,k_y). \tag{5.37}$$

What I would like to do is count the number of periods we move as

$$\Delta x_0 = \int_0^{2\pi/L} dk_y\, \partial_y x_0(k_y). \tag{5.38}$$

This almost works – we just have the issue of those discontinuities. The solution is to parallel transport: If I have the x-Wannier state at k_y I should be able to construct the x-Wannier state at $k_y+\delta$ by parallel transport

$$\begin{aligned} x_0(k_y+\delta) &= \frac{L}{2\pi}\int_0^{2\pi/L} \left[e^{iA_y\delta}\langle k_x,k_y+\delta|\right]\frac{1}{i}\partial_x\left[|kx,ky+\delta\rangle e^{-iA_y\delta}\right] && (5.39)\\ &= x_0(k_y)+\delta\,\frac{L}{2\pi}\int_0^{2\pi/L}\partial_y A_x-\partial_x A_y. && (5.40)\end{aligned}$$

Adding up these small displacements gives the result

$$\Delta x_0 = \frac{L}{2\pi}\int dk_x dk_y \Omega. \tag{5.41}$$

This is in fact the most physical way to think about a Chern insulator. It is a system where as you move through momentum space your Wannier states move. We will see this a different way when we discuss wavepackets.

The homework has a concrete example.

D. symmetries

An interesting observation is that if we have inversion symmetry about a site, then $\epsilon = 0$. If we have inversion symmetry about a bond, then $\Delta = 0$. In both those cases, Zac's phase is quantized. This is sensible, the Wannier state is then either symmetric or antisymmetric about the inversion point. Thus there is a Z_2 classification of 1D inversion symmetric insulators: Inversion centers always occur in pairs, and this classification is just saying about which of the two centers you have inversion symmetry.

Chapter 6

The Geometry of Momentum Space II

The anomalous Hall effect, and the quantum mechanics of Chern insulators

In this chapter we will explore what happens when you apply a force to a Bloch wave packet. We will think of this as a problem in "parallel transport." The punch line is that a force will generically produce a transverse velocity. We show how this Anomalous Hall effect can be used to understand the Integer quantum Hall effect. Finally we discuss some topological invariants related to the geometry of momentum space.

A. Wavepackets

One thing we would like to do in a lattice is build wavepackets – the analog of gaussian wavepackets that we deal with in free space. These should looks something like:

$$|\psi\rangle = \sum_p \phi(p)|p\rangle, \tag{6.1}$$

where $\phi(p)$ is some peaked function – like a gaussian. The hitch, of course, is that $|p\rangle$ has an arbitrary phase on it. We need a connection.

Let $\phi(p)$ be peaked about p_0. We can always assume that our gauge is smooth near p_0:

$$A_\mu(p) = A_\mu^{(0)} + B_{\mu\nu}(p - p_0)_\nu \tag{6.2}$$

where

$$\begin{aligned} A^{(0)} &= A(p = p_0) && (6.3) \\ B_{\mu\nu} &= \left.\frac{\partial A_\mu}{\partial p_\nu}\right|_{p=p_0}. && (6.4) \end{aligned}$$

Given that the gauge is smooth, a Gaussian with a linear phase on it should be a good choice for $\phi(p)$,

$$\phi(p) = e^{-\alpha(p-p_0)^2 + i\lambda_\nu (p-p_0)_\nu}. \tag{6.5}$$

We now want to ask where this wave-packet is in real space,

$$\langle r \rangle = \int dp \int dq \, \phi_p \phi_q^* \int dr \, r \, \langle q|r\rangle \langle r|p\rangle. \tag{6.6}$$

By definition

$$\langle r|p\rangle = e^{ipr} u_p(r), \tag{6.7}$$

where $u_p(r)$ is periodic. If the packet is sufficiently tight in momentum space we can expand this about $p = p_0$,

$$u_p(r) \approx u_{p_0}(r) e^{iA(p-p_0)} \tag{6.8}$$

and hence

$$\begin{aligned} \langle r \rangle &= \int dp \int dq \, \phi_p \phi_q^* \int dr \, r \, e^{i(p-q)\cdot r + iA(p-q)} |u_{p_0}(r)|^2 && (6.9) \\ &\approx \int dp \int dq \, \phi_p \phi_q^* \int dr \, r \, e^{i(p-q)\cdot r + iA(p-q)} && (6.10) \end{aligned}$$

where we replaced the rapidly oscillating $|u_{p_0}(r)|^2$ with its average. The r integral gives the derivative of a delta function

$$\begin{aligned} \langle r_\mu \rangle &= \int dp \int dq \, \phi_p e^{iA(p-p_0)} \phi_q^* e^{-iA(q-p_0)} \frac{1}{i} \partial_{p_\mu} \delta(p-q) && (6.11) \\ &= \int dp \left[\phi_p e^{iA(p-p_0)} \right]^* \frac{1}{i} \partial_{p_\mu} \left[\phi_p e^{iA_\nu (p-p_0)_\nu} \right] && (6.12) \\ &= \lambda_\nu + A_\nu^0. && (6.13) \end{aligned}$$

Where the connection is evaluated at $p = p_0$. This makes sense. In the absence of a connection, λ is the center of the packet. If we put arbitrary phases in momentum space, we need to concel them out.

Now we will ask what happens when we apply an impulse δ to the packet. A small impulse should just parallel transport us in k-space, so

$$\begin{aligned} \phi_p &\to e^{-iA_\nu(p)\delta_\nu} \phi_{p-\delta} && (6.14) \\ &= e^{-iA_\nu^0 \delta} \exp(-\alpha(p-p_0-\delta)^2 + i(\lambda_\nu - B_{\mu\nu}\delta_\mu)(p-p_0-\delta)_\nu) \end{aligned}$$

Thus

$$\begin{aligned} \langle r_\mu \rangle \quad to \quad & (\lambda_\nu - B_{\mu\nu}\delta_\mu) + (A_\nu^0 + B_{\nu\mu}\delta_\mu && (6.15) \\ = \quad & \langle r_\mu \rangle + (B_{\nu\mu} - B_{\mu\nu})\delta_\mu. && (6.16) \end{aligned}$$

That is, an impulse translates the wave packet. The displacement is related to the curvature of momentum space:

$$(B_{\nu\mu} - B_{\mu\nu}) \quad = \quad \partial_\nu A_\mu - \partial_\mu A_\nu = \Omega_{\mu\nu}. \tag{6.17}$$

When momentum space is "curved", an impulse generates a displacement. This should be somewhat familiar from fluid dynamics: it is the principle of the "Magnus force" – which generates lift on an airplane wing.

One consequence is that even in the absence of a magnetic field you can get a Hall effect: ie. you place a voltage across the $\hat{x}$ axis, and get a current flowing along the $\hat{y}$ axis. This is known as the "Anomalous Hall effect". Note that the classical Hall effect relies on the finite conductivity of a metal, and the Schrodinger equation alone is insufficient to describe it: one really needs to solve a Boltzmann equation. This "Anomalous" term gets added to the Boltzmann equation.

In particular the displacement u_k of the particles of momentum k induced by an impulse $F\Delta t$ is

$$u_\mu = F_\nu \Delta t \Omega_{\mu\nu}(k) \tag{6.18}$$

The current is then

$$j_\mu = F_\nu \sum_k \Omega_{\mu\nu}(k). \tag{6.19}$$

If one just worries about the contribution coming from the Berry curvature, and puts in the right dimensional constants, the Anomalous Hall conductivity will come from summing up all the velocities from all the occupied states:

$$\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{d^d k}{(2\pi)^d} f(\epsilon_k) \Omega_{k_x,k_y}, \tag{6.20}$$

where f is a step function at the Fermi surface. Using Stoke's theorem (and specializing to 2d), we can write this as

$$\sigma_{xy} = \frac{e^2}{\hbar} \oint dk \cdot A_k. \tag{6.21}$$

Thus the Anomalous-Hall conductivity can be viewed as the Berry phase accumulated in moving around the Fermi surface.

This effect is particularly simple in the case of a band insulator, where there is normally no transport. Then only conductivity comes only from the Anomalous Hall effect

$$\sigma_{xy} = \frac{e^2}{\hbar} \int_{\mathrm{BZ}} \frac{d^2 k}{2\pi}^2 \Omega_{kx,ky}. \tag{6.22}$$

This conductivity is quantized as the phase winding around an infinitesmal Fermi surface must be a multiple of 2π. It only remains to show that Landau levels can be thought of as Bloch states with a finite curvature.

The natural question is what materials have non-zero $\mathbf{\Omega}$ and hence a significant Anomalous Hall effect?

First of all $\mathbf{\Omega} = \mathbf{0}$ if the system has both time reversal and inversion symmetry. Time reversal takes $v \to -v$, $E \to E$ and $k \to -k$. Consequently, if the system has time reversal symmetry then $\Omega(-k) = -\Omega(k)$. Inversion symmetry takes $v \to -v$, $E \to -E$ and $k \to -k$. Consequently if the system has inversion symmetry then $\Omega(-k) = \Omega(k)$. The only consistent way to have both symmetry is to have $\Omega = 0$.

Time reversal symmetry is broken in ferromagnets and antiferromagnets. In fact, it is often the Hall effect in ferromagnets which is referred to as the "Anomalous Hall Effect". A simple example would be a two-dimensional tight binding model with a Rashba spin-orbit term $\hat{z} \cdot (S \times p))$ and an exchange splitting

$$\begin{aligned} H &= \sum_{i,\sigma,\tau} \left[a^\dagger_{i,\sigma} a_{i-\hat{x},\tau}(-t\delta_{\sigma\tau} + i\alpha(S_y)_{\sigma\tau}) + a^\dagger_{i,\sigma} a_{i-\hat{y},\tau}(-t\delta_{\sigma\tau} - i\alpha(S_x)_{\sigma\tau}) \right] + \mathrm{HC} \\ &\quad + \epsilon \sum_i (a^\dagger_{i\uparrow} a_{i\uparrow} - a^\dagger_{i\downarrow} a_{i\downarrow}). \end{aligned} \tag{6.23}$$

The fact that spin-orbit coupling is important is somehow natural. The idea is that as you adiabatically move through k-space, your spin rotates. This rotation in spin space yields a Berry phase. You will play with this model in your homework.

A.1. Integer Quantum Hall Effect as a Chern Number

We wish to understand the single particle problem defined by the Hamiltonian

$$H = \frac{(p - eA/c)^2}{2m} \tag{6.24}$$

where

$$B = \nabla \times A \tag{6.25}$$

is constant. This is a standard textbook problem, and if you have never done it before, do homework 2. Here we will approach it from a slightly more formal direction, which will make contact with Berry's phase.

The punch line is that Eq. (6.24) has a spectrum consisting of a set of bands. When you have a full band you have an insulator. However, it has a non-zero Chern number, so it manifests a quantized Hall effect. The classic picture is in terms of edge modes, but remarkably this purely bulk argument gives the same structure.

To understand the structure, we introduce magnetic translation operators

$$T_\delta = e^{i\mathbf{p}\cdot\delta - i(e/c)(\mathbf{\Delta}_\delta \mathbf{A})\cdot\mathbf{r}} \tag{6.26}$$

$$(\mathbf{\Delta}_\delta \mathbf{A}) = A(r+\delta) - A(r). \tag{6.27}$$

The quantity $\mathbf{\Delta}_\delta \mathbf{A}$ is a constant, independent of $\mathbf{r}$.

These magnetic translations commute with the Hamiltonian. Hence if I have one eigenfunction of the Hamiltonian $H\psi = E\psi$, I can generate a new one $T_\delta\psi$ with the same eigenvalue. Thus the eigenstates will be degenerate.

Typically what we would next do is try to find the mutual eigenstates of the T's and H. In the magnetic field-free case these are plane waves. The magnetic translations do not, however, commute with one-another. In fact

$$T_{\delta_1} T_{\delta_2} = e^{i2\pi\phi/\phi_0} T_{\delta_2} T_{\delta_1}, \tag{6.28}$$

where $\phi = \mathbf{B}\cdot\delta_1 \times \delta_2$ in the flux through the closed path formed by moving along the path $\delta_1, \delta_2, -\delta_1, -\delta_2$, and $\phi_0 = hc/e$ is the quantum of flux. Thus we cannot be simultaneously an eigenstate of all of the T's. Hence no plane waves.

On the other hand, if ϕ is an integer multiple of ϕ_0 they do commute. Thus we can find a subset of the T's which commute with one-another and with H. This is the same structure as Bloch waves. The connection is more than just formal. Lets take our commuting set of T's to be

$$T_{nm} = T_{n\ell\hat{\mathbf{x}}} T_{m\ell\hat{\mathbf{y}}} \tag{6.29}$$

where $\ell^2 = (hc)/(eB)$ is the "magnetic length". These operators are unitary, so their eigenvalues must have modulus 1. Thus we define the state $|q_x, q_y\rangle$ with $-\pi < q < \pi$ and satisfying

$$T_{nm}|q_x, q_y\rangle = e^{2\pi i(q_x n + q_y m)}|q_x, q_y\rangle. \tag{6.30}$$

As you can see, there is an arbitrary phase hanging around – which once again will lead us to a geometric phase. An equivalent definition is

$$[p_x - (e/c)(\partial_x A_y)y]|q_x, q_y\rangle = \frac{2\pi}{\ell} q_x |q_x, q_y\rangle, \tag{6.31}$$

$$[p_y + (e/c)(\partial_y A_x)x]|q_x, q_y\rangle = \frac{2\pi}{\ell} q_y |q_x, q_y\rangle, \tag{6.32}$$

up to a possible integer multiple of 2π.

In Homework 2, you found exactly these functions: they are Jacobi Theta functions. [Actually you just did the case $q_x = q_y = 0$, but the generalization is obvious.] We do not however need to explicitly write them down. All we need to note is that given one state $|q_x, q_y\rangle$, we can construct others by applying magnetic translations:

$$\begin{aligned} T_{nm} T_\delta |q_x, q_y\rangle &= e^{iB(n\ell\delta_y - m\ell\delta_x)} T_\delta T_{nm} |q_x, q_y\rangle & (6.33) \\ &= \exp\left[2\pi i \left(q_x + \frac{B\ell\delta_y}{2\pi}\right) n + 2\pi i \left(q_y - \frac{B\ell\delta_x}{2\pi}\right) n\right] T_\delta |q_x, q_y\rangle & (6.34) \end{aligned}$$

and the magnetic translation operator moves us around in q-space. We can calculate the curvature by looking at the phase we accumulate when we go around a small loop in q-space. This is clearly a constant. A little algebra shows that it corresponds to a Chern number of 1.

Chapter 7

Spin-Orbit Coupling

A. time reversal invariance

In this chapter we see what happens when we have lattice models where spin is important. Recently, interest has largely focussed on "time reversal invarient" systems. Time reversal invariance is most simply illustrated by an example: Let ψ_i be the quantum mechanical amplitude to have a spin-up particle on site i and ϕ_i the same quantity for spin-down. Suppose the energy of a particle is lower when it is moving in the direction of its spin? This then gives

$$E\begin{pmatrix}\psi_j\\ \phi_j\end{pmatrix}=\begin{pmatrix}-t & -i\epsilon\\ -i\epsilon & -t\end{pmatrix}\begin{pmatrix}\psi_{j+1}\\ \phi_{j+1}\end{pmatrix}+\begin{pmatrix}-t & i\epsilon\\ i\epsilon & -t\end{pmatrix}\begin{pmatrix}\psi_{j-1}\\ \phi_{j-1}\end{pmatrix}. \tag{7.1}$$

One way to understand this is that we rotate our basis by $\pi/2$:

$$a_i = (\phi_i+\psi_i)/\sqrt{2} \tag{7.2}$$

$$b_i = (\phi_i-\psi_i)/\sqrt{2} \tag{7.3}$$

This yields

$$E\begin{pmatrix}a_j\\ b_j\end{pmatrix}=\begin{pmatrix}-t-i\epsilon & 0\\ 0 & -t+i\epsilon\end{pmatrix}\begin{pmatrix}a_{j+1}\\ b_{j+1}\end{pmatrix}+\begin{pmatrix}-t+i\epsilon & 0\\ 0 & -t-i\epsilon\end{pmatrix}\begin{pmatrix}a_{j-1}\\ b_{j-1}\end{pmatrix}. \tag{7.4}$$

In momentum space, these two different representations yield

$$E\begin{pmatrix}\psi_k\\ \phi_k\end{pmatrix} = \begin{pmatrix}-2t\cos(k) & -2\epsilon\sin(k)\\ -2\epsilon\sin(k) & -2t\cos(k)\end{pmatrix}\begin{pmatrix}a_k\\ b_k\end{pmatrix} \tag{7.5}$$

$$E\begin{pmatrix}\psi_k\\ \phi_k\end{pmatrix} = \begin{pmatrix}-2t\cos(k)-2\epsilon\sin(k) & 0\\ 0 & -2t\cos(k)+2\epsilon\sin(k)\end{pmatrix}\begin{pmatrix}a_k\\ b_k\end{pmatrix} \tag{7.6}$$

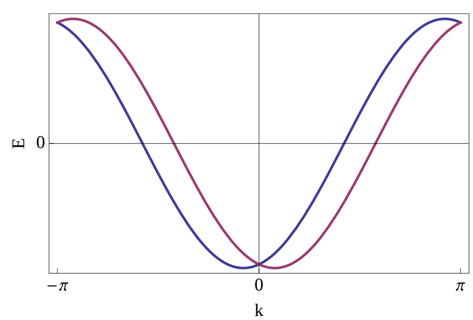
This represents a typical form of spin-orbit coupling. We will discuss microscopic origins later, but for now we will think about the symmetries. Equation (7.5) looks like the Hamiltonian for a spin-1/2 particle. The "magnetic field" has the form

$$\mathbf{B} = \hat{\mathbf{n}} 2\epsilon \sin(k). \tag{7.7}$$

This has the property that it is invariant under the mapping $k \to -k$ and $\hat{n} \to -\hat{n}$. This is time reversal invariance: One reverses all momenta and all magnetic fields. The energy is

$$E = -2t\cos(k) \pm 2\epsilon \sin(k). \tag{7.8}$$

This looks like



This has the property that the spectrum at momentum k is the same as that at momentum $-k$. Furthermore, the spectrum is degenerate at $k = 0, \pi$. The fact that each energy appears twice is referred to as "Kramers degneracy."

Although we will not work too much with it, it is useful for your education to consider the operator which generates this symmetry. We want

$$\begin{aligned} T^{-1} p T &= -p \quad (7.9) \\ T^{-1} \vec{\sigma} T &= -\vec{\sigma} \quad (7.10) \\ T^{-1} x T &= x. \quad (7.11) \end{aligned}$$

Its properties acting on a wavefunction are clearly

$$T\left[e^{ikx}e^{i\chi}\begin{pmatrix} \cos(\theta/2)e^{i\phi/2} \\ \sin(\theta/2)e^{-i\phi/2} \end{pmatrix}\right] = e^{-ikx}e^{i\chi'}\begin{pmatrix} -\sin(\theta/2)e^{i\phi/2} \\ \cos(\theta/2)e^{-i\phi/2} \end{pmatrix}. \tag{7.12}$$

The only question is what χ' is. We can deduce this by noting that $T(A+B) = TA + TB$ and that T does not change x. Thus we can consider $\bar{\chi} = \chi + kx$ as one phase. Since kx gets multiplied by -1, so does χ, and the answer is $\chi' = -\chi + \delta$, for some δ. It is pretty clear that the requirements in Eq. (7.9) do not pin down δ. Gauge symmetry leaves this as arbitrary, but it seems like a pretty good convention to take $\delta = 0$. Thinking of this as a "time reversal" operator, I believe the phase δ can be associated with the origin of time.

One usually writes this as

$$T \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -v^* \\ u^* \end{pmatrix}. \tag{7.13}$$

This is a pretty weird operator. It is not actually a linear operator, as $Te^{i\phi}|\psi\rangle = e^{-i\phi}T|\psi\rangle \neq e^{i\phi}T|\psi\rangle$. It is however well defined. A norm-preserving transitive operator with this property is known as "antiunitary".

If $|\psi\rangle$ is an eigenstate of a time-reversal-invarient Hamiltonian, than so is $T|\psi\rangle$ with the same eigenvalue. Kramer's degeneracy arises from the fact that the state $T|\psi\rangle$ is orthgonal to $|\psi\rangle$. This is obvious from Eq. (7.13), as $|\psi\rangle = (u, v)$ and $T|\psi\rangle = (-v^*, u^*)$. The inner product is $-uv + uv = 0$.

B. Wannier States

Lets now explore the Wannier states of Hamiltonians like Eq. (7.1), or more general spin dependent Hamiltonians. Equation (7.1) is actually a marginal example, as it only has two bands, which touch. If we consider these two bands together as one, our entire Hilbert space is made up of them, and the Wannier states are just our lattice points. We can either break the time-reversal symmetry, splitting the bands, or we can consider a four-band model. Lets first go with the split bands as a warm-up. The punch line will be that the Wannier state have a spin-up component and a spin-down component. These can be separate from one-another. In the two-dimensional model, as one moves through the Brillioun zone, these two components can move in opposite direction. The tricky thing of course is that up and down might not be the right labels.

Chapter 8

Edge Modes

Edge modes are actually pretty common in solid state physics. For example, Copper has a nice surface mode. The thing of current interest is when symmetries/topology guarantees that an insulator has a conducting edge mode.