

(Instructor: James Analytis)

# Physics 141B: Introduction to Solid State II Notes

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These are some notes taken from UC Berkeley's Physics 141B during the Fall '24 session, taught by James Analytis. This template is based heavily off of the one produced by [Kevin Zhou](#).

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## 1 January 22, 2025:

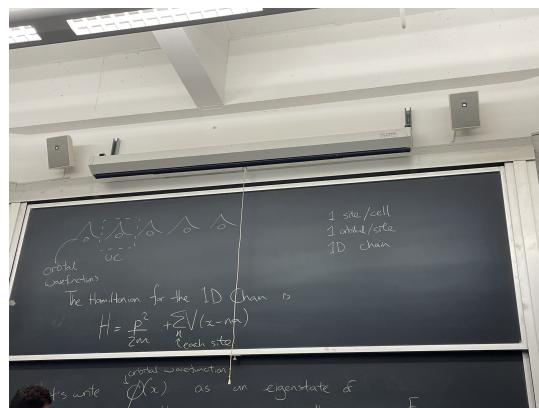
Office Hours Fri 1-2pm after Lecture.

Syllabus:

- Topology: (6-7 weeks)
  - Su-Shrieffer-Heeger Model
  - Berry's Phase and its application to Graphene
  - Haldane Model
  - Topological Insulators
- Superconductivity: (3-4 weeks)
  - Overview and Two-fluid Model
  - Cooper pairing
  - Bardeen, Cooper, Schrieffer (BCS) Model
  - Josephson Effect
- If we have time, Magnetism:
  - Phenomenology, Ferromagnets and Antiferromagnets
  - Direct-exchange and Super-exchange
  - Mean-field Model

### 1.1 Review: The Tight Binding model

Consider a 1D Chain of  $N$  sites with 1 orbital per site, and consider a unit cell with 1 site per cell defined as in the picture below:



The Hamiltonian for the 1D Chain is

$$H = \frac{\mathbf{p}^2}{2m} + \sum_n V(x - na)$$

Let  $\phi(x)$  be the eigenstate of

$$H_0 = \frac{\mathbf{p}^2}{2m} + V(x)$$

with energy  $E_0$  i.e.  $\phi(x)$  is the **Orbital Wavefunction**. The Hilbert Space for the chain consists of one orbital at each site  $\{\phi_n(x)\}_{n \in I}$  (the  $n$  subscript labels the different sites) and the wavefunction for the chain is then

$$\psi(x) = \sum_n c_n \phi_n(x - na)$$

(linear combination of atomic orbitals)

## 1.2 Review: Bloch's Theorem

Next, we recall Bloch's theorem for a system with Translational Symmetry. Bloch's Theorem tells us that

$$\psi_k(x + a) = e^{ika} \psi_k(x)$$

where  $a$  is the size of the Unit Cell, which in this case is the distance between atoms (**Add a proof**) .

From this, we can arrive at the conclusion that

$$c_n = c_0 e^{ikna}$$

and including the normalization, a chain of  $N$  atoms is described by wavefunctions

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \psi(x - na)$$

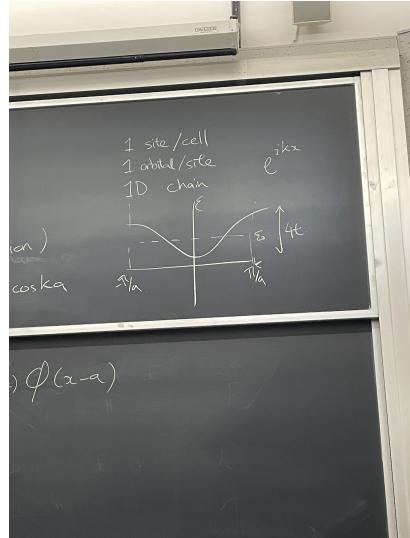
This can be interpreted as the single orbital wavefunction  $\phi(x)$  being modulated by the free-electron wavefunction  $e^{ikx}$ .

The Energy Spectrum (or dispersion relation) is given by

$$E(k) = E_0 - 2t \cos(ka)$$

where  $t$  is called the **Overlap integral**

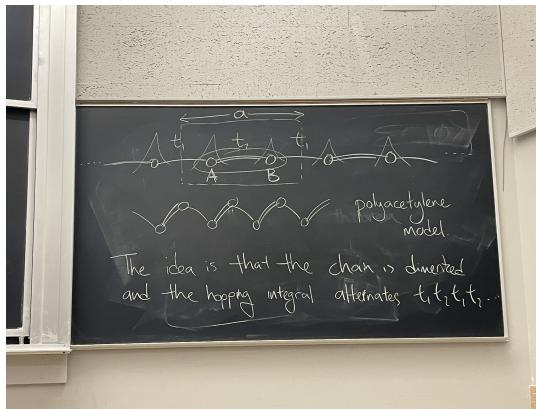
$$t \equiv \int dx \phi(x) V(x) \phi(x - a)$$



This model is too trivial to display any topological behavior. The physics we're interested in becomes apparent once we have **at least two bands and a bandgap**. As our first case, we study the SSH model (Phys. Rev. Lett. 42 1698 (1979)).

### 1.3 SSH Model

In the SSH model we, once again, have a 1D chain. However, this time, we have **two kinds of bonds** (alternating) with different overlap/hopping parameters  $t_1, t_2$ .



For example, Polyacetylene is described by an SSH model. The idea is that the chain is **dimerised** because the hopping integral alternates.

The wavefunctions for this system are

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} (\alpha_k \phi_{nA} + \beta_k \phi_{nB})$$

where  $a$  is the unit cell size and it is  $2 \times$  the distance between sites.  $\phi_{nA}, \phi_{nB}$  are the orbital waves on sites  $A$  and  $B$ .

What are  $\alpha_k, \beta_k$ ?  
Probability amplitudes.

- Now we need to solve the Schrödinger Equation to determine  $\alpha_k$  and  $\beta_k$ . We know that

$$|\alpha_k|^2 + |\beta_k|^2 = 1$$

- This is a 2D Hilbert Space
- We want to solve  $H\psi_k(x) = E(k)\psi_k(x)$ . To construct the matrix, take the product with  $\langle\phi_{nA}|$  and  $\langle\phi_{nB}|$ , giving us the two equations

$$\begin{aligned}\langle\phi_{nA}|H|\psi_k(x)\rangle &= E(k)\langle\phi_{nA}|\psi_k\rangle \\ \langle\phi_{nB}|H|\psi_k(x)\rangle &= E(k)\langle\phi_{nB}|\psi_k\rangle\end{aligned}$$

- Taking the first of these equations, the RHS is

$$\langle\phi_{nA}|\sum_{n'} e^{ikn'a} (\alpha_k \phi_{n'A} + \beta_k \phi_{n'B})\rangle$$

**(missed a bit here)** So, the RHS is  $E(k)\alpha_k e^{ikna}$

- Now, for the LHS,

$$\sum_{n'} \langle\phi_{nA}|H|e^{ikn'a} (\alpha_k \phi_{n'A} + \beta_k \phi_{n'B})\rangle$$

- Recall that  $H$  is described as

$$H = H_0 + \sum_{n'} V(x - n'a)$$

where  $H_0|\phi_{n'A}\rangle = E_0$ . When we take the inner product, only the  $n = n'$  inner product survives when we dot with  $H_0$ , giving

$$\langle\phi_{n'A}|H_0|(\alpha_k \phi_{n'A} + \beta_k \phi_{n'B})\rangle = E_0 \alpha_k e^{ikna}$$

- The Second Term (only nearest neighbor hopping) is equal to

$$\begin{aligned}&= e^{ikna} \langle\phi_{nA}|V_0(x - x_{n,B})|\beta_k \phi_{n,B}\rangle + e^{ik(n-1)a} \langle\phi_{nA}|V_0(x - x_{n-1,B})|\beta_k \phi_{n-1,B}\rangle \\&= \beta_k t_1 e^{ikna} + \beta_k t_2 e^{ik(n-1)a} \\&= \beta_k e^{ikna} (t_1 + t_2 e^{-ika})\end{aligned}$$

## 2 January 24, 2025:

Things get more interesting today. We won't reach the Topological aspects yet, but we'll cover them next Monday.

We left off looking at the LHS and RHS of the Schrödinger Equation for the SSH model, ending with the following equation:

$$\begin{aligned} \alpha_k E_0 e^{ikna} + \beta_k t_1 e^{ikna} + \beta_k t_2 e^{ik(n-1)a} &= \alpha_k E(k) e^{ikna} \\ \implies \alpha_k(E(k) - E_0) + \beta_k(t_1 + t_1 e^{-ika}) &= 0 \end{aligned}$$

Performing the same procedure, but taking the inner product with  $\langle \phi_{nB} |$  instead, we get a similar equation, giving us the following system of simultaneous equations:

$$\begin{aligned} \alpha_k(E(k) - E_0) + \beta_k(t_1 + t_1 e^{-ika}) &= 0 \\ \beta_k(E(k) - E_0) + \alpha_k(t_1 + t_1 e^{+ika}) &= 0 \end{aligned}$$

For a 2D Hilbert Space (in this case, spanned by  $|\phi_{nA}\rangle$  and  $|\phi_{nB}\rangle$ ) we can regard the wavefunctions as "S = 1/2" **spinors** or "Pseudospins".

Pseudospins or Spinors are objects of the form

$$\begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}$$

We can write these two simultaneous equations represented by this spinor as

$$\underbrace{\begin{pmatrix} E_0 & t_1 + t_2 e^{-ika} \\ t_1 + t_2 e^{+ika} & E_0 \end{pmatrix}}_{\text{"Bloch Hamiltonian"}} \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} = E(k) \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}$$

where it's called the "Bloch Hamiltonian" because everything is represented in  $k$ -space. The Bloch Hamiltonian has the form

$$H(k) \underbrace{\vec{\phi}_k}_{\text{Spinor}} = E(k) \vec{\phi}_k$$

Generally, a Bloch Hamiltonian is an  $N \times N$  matrix where

$$N = \left( \begin{array}{c} \# \text{ sites} \\ \text{per U.C.} \end{array} \right) \times \left( \begin{array}{c} \# \text{ orbitals} \\ \text{per site} \end{array} \right) \times \left( \begin{array}{c} \# \text{ of} \\ \text{dimensions} \end{array} \right)$$

So, in our case, we have  $N = 2 \times 1 \times 1 = 2$  We solve our  $2 \times 2$  matrix in the usual way.

### 2.1 What is the "Pseudospin" representation?

The Pseudospin is the 2-state system of each allowed value of momentum  $k$ .

### But what do $\alpha_k$ and $\beta_k$ represent?

Include figure of B and A sublattices (blue and yellow)

We visualize these as two interpenetrating sublattices. Basically,  $\alpha$  and  $\beta$  refer to the wavefunctions on the  $A$  and  $B$  sublattices respectively, but let's take this idea a little further.

Any  $2 \times 2$  matrix can be represented as a linear superposition of Pauli matrices and the identity.

$$\text{Pauli Matrices: } \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma_0 = \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Let us represent our Bloch Hamiltonian as

$$H(k) = \begin{pmatrix} E_0 & \Delta(k) \\ \Delta^*(k) & E_0 \end{pmatrix}, \Delta(k) = t_1 + t_2 e^{-ika}$$

Then, solving the Schrödinger Equation amounts to solving

$$\begin{aligned} \det \begin{bmatrix} E_0 - E(k) & \Delta(k) \\ \Delta^*(k) & E_0 - E(l) \end{bmatrix} &= 0 \\ \implies E_0 - E(k) &= \pm |\Delta(k)| \\ \implies |\Delta(k)| &= \left| t_1 + t_2 e^{ika} \right| = \sqrt{t_1^2 + t_2^2 + 2t_1 t_2 \cos(ka)} \end{aligned}$$

### The Band Structure

For the sake of convenience let's set  $E_0 = 0$ . Now, we have

$$\begin{aligned} k = 0 &\implies \Delta(0) = |t_1 + t_2| \\ k = \frac{\pi}{a} &\implies \Delta\left(\frac{\pi}{a}\right) = |t_1 - t_2| \end{aligned}$$

Include figure of the Band Structure.

Notice that the band structure just depends on  $|t_1 - t_2|$  and so doesn't actually care which one is bigger. (**Ask for clarification**)

Now that we have the Band Structure, let's get back to the pseudospin wavefunctions

$$\Delta(k) = \underbrace{\Delta_1(k)}_{\text{Re}(\Delta(k))} + i\underbrace{\Delta_2(k)}_{\text{Im}(\Delta(k))}$$

So

$$\begin{aligned} H(k) &= \begin{pmatrix} E_0 & \Delta_1 + i\Delta_2 \\ \Delta_1 - i\Delta_2 & E_0 \end{pmatrix} = E_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \Delta_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \Delta_2 \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \\ &= E_0 \mathbf{1} + \Delta_1 \sigma_x - \Delta_2 \sigma_y + 0 \sigma_z \end{aligned}$$

Now, since we have  $E_0 = 0$  we can write

$$H(k) = \vec{\sigma} \cdot \vec{b}(k)$$

where

$$\vec{b}_x = \begin{pmatrix} \Delta_1(k) \\ 0 \\ 0 \end{pmatrix}, \quad \vec{b}_y = \begin{pmatrix} 0 \\ \Delta_2(k) \\ 0 \end{pmatrix}, \quad \vec{b}_z = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

and  $\vec{b}(k) = b_x \hat{x} + b_y \hat{y} + b_z \hat{z}$

This looks a lot like a spin in a magnetic field, and so we identify  $\vec{\sigma}$  as being our pseudospin or spinor and  $\vec{b}(k)$  as being our "Zeeman" field.

Note that there is no  $\vec{\sigma}_z$  component. This follows from the fact that the orbitals on site  $A$  and  $B$  are the same, and we have only allowed nearest neighbor hopping. If we did not restrict to nearest neighbors, we'd need to have a third parameter, but we would also lose all topological properties of the model (we'll show this later).

Now, in our case, the Hamiltonian only consists of  $\sigma_x, \sigma_y$  and we know the Pauli matrices anti-commute with each other. As a result,  $\sigma_z$  anticommutes with the Hamiltonian  $\{\sigma_z, H\} = 0$ .

This is actually a special case of when some unitary operator  $\Theta$  acts on  $H$  as

$$\Theta H \Theta^\dagger = -H$$

The existence of such a relationship implies for  $H|\psi\rangle = E|\psi\rangle$ . that there exists another eigenstate with energy  $-E$ .

This is a kind of **Chiral** symmetry, and such symmetries have very special consequences for the eigenvalues and are intimately related to the Topology in such systems.

We'll see later how this is a chiral symmetry in the sense of breaking all mirror symmetries.

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### 3 January 27, 2025:

Last time, we left off by expressing the SSH Hamiltonian in the form

$$H = \alpha \vec{\sigma} \cdot \vec{b}$$

where  $\vec{b}(k) = (t_1 + t_2 \cos(ka))\hat{x} + t_2 \sin(ka)\hat{y}$ .

- The point of  $\vec{b}(k)$  helps us visualize the spinor wavefunctions, and the topological aspects of the SSH model will become apparent through the visualization.
- For each wavenumber  $k$ , the two eigenstates are "Pseudospin" states that are parallel and anti-parallel to the "Spinor field"  $\vec{b}(k)$ . These are separated in energy by  $2|\vec{b}(k)|$ .
- This is where things get a bit more geometrical... We can trace the trajectory of  $\vec{b}(k)$  as  $k$  varies across the 1D Brillouin zone from  $-\pi/a$  to  $\pi/a$ .
- In general, for 1D, this is a map from a circle (obtained by connecting the ends of the 1D BZ) to a surface in 3D (since  $\vec{b}(k)$  has three components).

Include figure

- For the SSH model with chiral symmetry (as discussed last lecture),  $b_z(k) = 0$  (no  $\hat{z}$  component) of  $\vec{b}(k)$ .
- So,  $\vec{b}(k)$  vectors actually lie on the  $xy$ -plane and the surface becomes a contour in the  $xy$ -plane.

Include figure

Let's calculate some important values of  $\vec{b}(k)$  as we move across the BZ from  $-\pi/a$  to  $\pi/a$  and we'll consider  $t_1 > t_2$

- $\vec{b}(-\pi/a) = (t_1 - t_2)\hat{x} + 0\hat{y}$
- $\vec{b}(-\pi/2a) = t_1\hat{x} - t_2\hat{y}$
- $\vec{b}(0) = (t_1 + t_1)\hat{x} + 0\hat{y}$
- $\vec{b}(\pi/2a) = t_1\hat{x} + t_2\hat{y}$
- $\vec{b}(\pi/a) = (t_1 - t_2)\hat{x} + 0\hat{y}$

Include figure

- The interesting bit is that this conclusion for the trajectory of  $\vec{b}(k)$  depends on the relative magnitudes of  $t_1$  and  $t_2$ .
- Above, we assumed  $t_1 > t_2$ . What about the opposite case where  $t_2 > t_1$ ? We might imagine that our solutions would be exactly the same since
  - energy states are the same (bandstructure only depended on  $|t_1 - t_2|$ ), and
  - the physical situation looks the same.

Include figure

- However, when we look at the trajectory of  $\vec{b}(k)$  in the  $t_2 > t_1$  case, it's actually **different** than the  $t_1 > t_2$  case.
- More precisely, they are **Topologically Distinct** (we'll elaborate on what this means).

The expressions remain the same,

- $\vec{b}(-\pi/a) = (t_1 - t_2)\hat{x} + 0\hat{y}$
- $\vec{b}(-\pi/2a) = t_1\hat{x} - t_2\hat{y}$
- $\vec{b}(0) = (t_1 + t_2)\hat{x} + 0\hat{y}$
- $\vec{b}(\pi/2a) = t_1\hat{x} + t_2\hat{y}$
- $\vec{b}(\pi/a) = (t_1 - t_2)\hat{x} + 0\hat{y}$

it's just that we now have  $t_2 > t_1$ . But because of this, the first point is to the **left of the origin**. The rest of the points are also correspondingly offset, so the contour looks like the same circle but shifted over.

Include figure

- $t_1 > t_2$ :  $\vec{b}(k)$  only points East.
- $t_2 > t_1$ :  $\vec{b}(k)$  points in all directions (N, S, E, W, etc.) and the trajectory encloses the origin.
- Sometimes it's easier to visualize using unit vectors

$$\hat{b}(k) = \frac{\vec{b}(k)}{|\vec{b}(k)|}$$

In this case,  $\hat{b}(k)$  for  $t_1 > t_2$  only traces out an arc on the Unit sphere wherease for  $t_2 > t_1$  it traces out the full circle.

Include two figures

These two states correspond to different **Solid Angles**  $\Omega = 0$  for  $t_1 > t_2$  and  $\Omega = 2\pi$  for  $t_2 > t_1$ . The solid angle is directly proportional to the **Berry Phase** (we'll derive this result later) which is itself related to the **Chern Number** - a topological invariant. Thus, the  $\Omega = 0$  case is **Topologically Trivial**, whereas the  $\Omega = 2\pi$  case is **topologically non-trivial**.

Now, there is some critical point between the  $t_1 > t_2$  and  $t_2 > t_1$  cases where the circle just touches the origin.

Include figure

We define a "winding number"  $W$  which is 0 or 1 and measures how many times the mapping encloses the Origin i.e. how many times  $\vec{b}(k)$  covers the entire circle.

- In order to go from  $W = 0$  to  $W = 1$ , we must go through the origin. This means  $\vec{b}(k) = 0$  for some  $k$ .
- Recall that the energy gap between the negative and positive eigenstates was  $2|\vec{b}(k)|$ .
- This means that in order to go from  $W = 0$  to  $W = 1$ , we must close the energy gap!
- So, in order to Adiabatically go through the topological transition from  $W = 0$  to  $W = 1$  we must close the gap and there are zero-energy states.

This is an important property of topological systems! In order to go between topologically distinct states, the energy gap must close.

What do we mean by **Adiabatic**?

Roughly, we mean changing things slowly enough that none of the quantum numbers for the system change. See the **Adiabatic Theorem**.

Next time, we'll see what happens to the Winding number exactly when the energy gap closes and how that relates to Edge States.

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## 4 January 29, 2025:

- Last time, we left off discussing Winding Numbers, which characterized the cases  $t_1 > t_2$  and  $t_2 > t_1$ , making them distinct topological phases.
- Note that in general 1D systems, we don't have distinct topological phases. The SSH model is special because of the restriction that the Hamiltonian only contains  $\sigma_x$  and  $\sigma_y$ .
- If we allow the  $\sigma_z$  term to be finite so that the Hamiltonian is of the form

$$H = \beta_x(k)\sigma_x + \beta_y(k)\sigma_y + \beta_z(k)\sigma_z$$

we cannot generally define a winding number.

- The reason has to do with the bandgap. For the SSH model, in order to go from the  $W = 0$  to  $W = 1$  case, we need to close the bandgap. However, if the  $\sigma_z$  term is non-zero, we can transform between them adiabatically without needing to close the gap because we allow  $b_z$  to help us evolve continuously. (**Find more detailed discussion in Asboth 1.5**)

Include figure

WE need to go to higher dimensions to see examples of "generic" insulating states with topological invariants that cannot be changed without closing a gap.

### 4.1 Are there observable consequences?

- In the bulk, there's no physical difference.
- The relevant observables are seen at the boundaries between the two situations i.e. the  $W = 0$  chain and the  $W = 1$  chain.
- To see this, we consider the fully dimerised limit (meaning make  $t_1$  finite and make  $t_2 = 0$  or vice-versa), whose solutions are essentially the same for a bunch of diatomic molecules.

Include Figure

- Consider the boundaries of a finite chain. (**An infinite chain is not useful to us because in that case, the  $W = 0$  and  $W = 1$  cases only differ by a translation of  $a$  and cannot be different.**)
- Imagine the system is 1/2 filled.

Include figure of the dispersion for 1/2 filled

There is one electron per dimer.

- In the first situation, the electron sits happily on each dimer.

Include fig

- In the second situation, we have just as many sites and therefore just as many electrons, but now one electron sits at a single site rather than being shared. As a result, one site has  $+\frac{1}{2}e$  more than expected from the bulk and the other has  $-\frac{1}{2}e$  less than expected.

Include figure

- The boundary states in each situation look different! The topological system  $W = 1$  has  $\pm\frac{1}{2}e$  more (less) than expected at its ends!

### **What happens if we have an odd number of sites instead?**

We can make a similar argument, but we'd have to tile the system differently. (**Exercise: Analyse the SSH model with 7 sites.**)

### **Band Structure for Fully Dimersized System**

Include fig

#### **4.2 Boundary states from another perspective**

- Consider a domain wall between a  $W = 0$  and  $W = 1$  system.

Include fig

- At the boundary, there is a non-bonded atom at energy  $E_0$  (the atomic energy) or  $E - E_0 = 0$ .
- This is a zero energy state! So, in order to cross between topologically distinct states, we have to close the gap (move through the zero energy state). This is consistent with the idea that the gap must close in order to go from one topological phase to another.

### **What happens if we relax the dimerization condition?**

The boundary state remains pinned to  $E - E_0 = 0$  and gap remains in order for the system to maintain its Chiral Symmetry.

Next time, Berry Phases in Higher Dimensional Systems.

**15** 5. January 31, 2025:

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**5 January 31, 2025:**

Missed lecture. Fill in later.

## 6 February 3, 2025:

Picking up where we left off last time, we'll move from the finite to continuous case of the Berry phase.

Recall that we considered the following triangle lattice situation,

Include figure

with a tight-binding Hamiltonian

$$H = \begin{pmatrix} 0 & -t & -t \\ -t & 0 & -t \\ -t & -t & 0 \end{pmatrix}$$

We Diagonalized it and found the energies and corresponding eigenstates.

Include figure of energy

- Eigenvectors have to be complex for the Berry's Phase to make any sense (**write why exactly this is the case**) .
- In our case, the "loop" corresponds to rotations of a "distorted triangle".

Include fig of distorted triangle being rotated and corresponding hamiltonians

- Recall that the entries of the tight-binding hamiltonian are exactly the hopping parameters between the different lattice sites (since we're taking  $E_0 = 0$ ) and so we just need to modify the hopping parameters in whatever row corresponds to the double-bond.
- The original equilateral triangle has two degenerate states  $|\alpha\rangle$  and  $|\beta\rangle$  that we will now use as a basis to describe a distored triangles energy levels.
- Consider the lower of the two degenerate undistorted energies after they are split by the distortion. Call this state  $|u_i\rangle$  where  $i \in \{a, b, c\}$

Include figure of energy splitting.

Now we're going to do something that might seem a bit ad-hoc. We're going to assume that the following expressions hold true:

**(Fill in the expressions above from picture)**

Now, the expression for the Berry Phase we'll use is

$$\phi = -\text{Im}(\ln\langle u_a | u_b \rangle \langle u_b | u_c \rangle \langle u_c | u_a \rangle)$$

where the negative sign is just there by convention (**Read about why this is up to convention**)

Anyway, this comes out to

$$\begin{aligned} \phi &= -\text{Im}\left(\ln\left(e^{i\pi/3}\right)^3\right) \\ &= -\pi \end{aligned}$$

(It's important to use a complex space, otherwise you will have only  $\phi = 0$  or  $\phi = \pi$  for purely real eigenvectors).

- The point of this is that if I multiply by a phase this product ( $\phi$ ) will be invariant i.e. if we multiplied each eigenvector by a (possibly different) phase

$$|\tilde{u}_j\rangle = e^{i\beta_j} |u_j\rangle$$

it would not affect  $\phi$  because the inner product comes with partnets of bras and kets  $|u_j\rangle\langle u_j|$  and so the extra phases cancel

$$e^{-i\beta_j} e^{i\beta_j}$$

- Also recall that  $\ln(AB) = \ln(A) + \ln(B)$  so

$$\phi = - \sum_{j=0}^{N-1} \text{Im}(\ln(\langle u_j | u_{j+1} \rangle))$$

- But there's some subtely here. In our first definition for  $\phi$ , we have the restriction  $\phi \in [-\pi, \pi]$
- But in this summation expression, we only have equivalence between  $\phi$  values up to a phase of  $2\pi$ .
- So, we make sure that we define  $\phi$  modulo  $2\pi$  - this becomes important for equalities in our calculations.

## 6.1 Parallel Transport Gauge

Since we are free to choose a gauge (choice of phase to multiply the wavefunctions by), we can define each consecutive eigenstate along our loop as having the phase

$$|\bar{u}_0\rangle = |u_0\rangle$$

but then define  $|\bar{u}_1\rangle$  such that  $\langle \bar{u}_0 | \bar{u}_1 \rangle$  is real.

Include figure of loop with kets and bar'd kets

In this gauge, we have

$$\text{Im}(\langle u_j | u_{j+1} \rangle) = 0$$

and the eigenvectors are "parallel" in the sense taht their relative phase is zero.

Include figure of "parallel"

- However there is an awkwardness about the gauge.
- Before, we had  $|u_0\rangle \equiv |u_N\rangle$  but now,  $|\bar{u}_0\rangle \not\equiv |\bar{u}_N\rangle$ . They now differ by a phase - in fact, they differ exactly by a Berry;s phase.

### An example computation

Consider  $|\bar{u}_a\rangle = |u_a\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$  and now we need to define  $|\bar{u}_b\rangle$  in terms of  $|u_b\rangle = \begin{pmatrix} 1 \\ e^{i2\pi/3} \end{pmatrix}$  so that  $\text{Im}\langle \bar{u}_a | \bar{u}_b \rangle = 0$

Let's define  $|\bar{u}_b\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ . Then,  $\langle \bar{u}_a | \bar{u}_b \rangle = \alpha + \beta = \text{Real}$  So, then, let's define  $|\bar{u}_b\rangle = e^{-i\pi/3}|u_b\rangle$  giving us

$$\langle \bar{u}_a | \bar{u}_b \rangle = e^{-i\pi/2} + e^{i\pi/3} = 2 \cos \pi/3 = -1$$

repeating the procedure we get (**Fill in from picture**)

But now there is a discontinuity in the phase as we move along the closed path. This is what people sometimes refer to when they say we need to "unwind" the phase by  $\pi$  to go from  $|\bar{u}_N\rangle$  to  $|\bar{u}_0\rangle$ . To avoid this awkward discontinuity we can instead use the Twisted Parallel Transport Gauge.

### 6.2 Twisted Parallel Transport Gauge

In this gauge, we define

$$|\tilde{u}_j\rangle = e^{-i(\phi/N)j}|\bar{u}_j\rangle$$

This is a way of "continuously unwinding" the Berry Phase.

## 7 February 5, 2025:

Last time, we left off discussing the Twisted Parallel transport Gauge. The idea is that the phase evolves by the same amount at each step as we parallel transport.

### Twisted Parallel Transport Gauge continued...

In this gauge, we define

$$|\tilde{u}_j\rangle = e^{-i(\phi/N)j}|\bar{u}_j\rangle$$

where  $|\bar{u}_j\rangle$  is an eigenstate in the Parallel Transport Gauge and there is no discontinuity between  $|\tilde{u}_0\rangle$  and  $|\tilde{u}_N\rangle$ , like there is in parallel transport gauge.

#### 7.1 Continuous Formulation of the Berry Connection

(We're following David Vanderbilt's "Berry Phases in Electronic Structure Theory CHS" for this section.) This time instead of having discrete steps, we take our path to be parameterized by a continuous variable  $\lambda$  such that  $|u_\lambda\rangle$  traverses a closed path going from  $\lambda = 0$  to  $\lambda = 1$  i.e.

$$|u_{\lambda=0}\rangle \equiv |u_{\lambda=1}\rangle$$

We assume that  $|u_\lambda\rangle$  is a continuously differentiable function of  $\lambda$ .

Now,

$$\begin{aligned} \ln(\langle u_\lambda | u_{\lambda+d\lambda} \rangle) &= \ln \left( \langle u_\lambda | u_\lambda \rangle + d\lambda \langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle + \dots \right) \\ &= \ln(1 + d\lambda \langle u_\lambda | d_\lambda u_\lambda \rangle + \dots) \end{aligned}$$

where

$$|d_\lambda u_\lambda\rangle = \frac{d}{d\lambda} |u_\lambda\rangle$$

We taylor expand the logarithm to write

$$\ln(\langle u_\lambda | u_{\lambda+d\lambda} \rangle) \approx d\lambda \langle u_\lambda | d_\lambda u_\lambda \rangle + \underbrace{\dots}_{\text{second order terms}}$$

Since we're physicists we discard all the second order terms.

Now, summing all of these terms across our closed path

Include figure

We find

$$\phi = -\text{Im} \left( \oint_{\text{purely imaginary}} \underbrace{\langle u_\lambda | d_\lambda u_\lambda \rangle}_{\text{purely imaginary}} d\lambda \right)$$

### Why is it purely imaginary?

We have

$$\begin{aligned} \langle u_\lambda | d_\lambda u_\lambda \rangle + \langle d_\lambda u_\lambda | u_\lambda \rangle &= \frac{d}{d\lambda} \langle u_\lambda | u_\lambda \rangle = 0 \\ \implies \frac{1}{2} (\langle u_\lambda | d_\lambda u_\lambda \rangle + \langle d_\lambda u_\lambda | u_\lambda \rangle) &= \text{Re}(\langle u_\lambda | d_\lambda u_\lambda \rangle) = 0 \end{aligned}$$

That is, the real part must vanish and so it is purely imaginary. We can thus drop the Im and simply write

$$\phi = i \oint \langle u_\lambda | d_\lambda u_\lambda \rangle d\lambda = \oint \underbrace{\langle u_\lambda | i d_\lambda u_\lambda \rangle}_{\text{Berry connection}} d\lambda \quad (1)$$

The integrand

$$A(\lambda) = \langle u_\lambda | i \cdot d_\lambda u_\lambda \rangle$$

is a connection in the sense of Differential Geometry and is referred to as the Berry Connection or sometimes the Berry Potential (in analogy with the Vector Potential; both of them are **Gauge Potentials**)

### Gauge invariance?

Just like the Electromagnetic Poetntial, the Berry potential is not gauge invariant. To see this, consider a gauge transformation

$$|\tilde{u}_\lambda\rangle \rightarrow e^{-i\beta(\lambda)}|u_\lambda\rangle$$

where  $\beta(\lambda)$  is a continuous function.

Then, the Berry potential/connection transforms as

$$\begin{aligned} \tilde{A}(\lambda) &= \langle \tilde{u}_\lambda | i \cdot d_\lambda \tilde{u}_\lambda \rangle \\ &= \langle u_\lambda | e^{i\beta(\lambda)} i \frac{d}{d\lambda} (e^{-i\beta(\lambda)} |u_\lambda\rangle) \rangle \\ &= \langle u_\lambda | e^{i\beta(\lambda)} i e^{-i\beta(\lambda)} |d_\lambda u_\lambda\rangle + \langle u_\lambda | e^{i\beta(\lambda)} i (-i\beta(\lambda)) e^{-i\beta(\lambda)} \frac{d\beta}{d\lambda} |u_\lambda\rangle \rangle \\ &= \langle u_\lambda | i d_\lambda u_\lambda \rangle + \frac{d\beta}{d\lambda} \end{aligned}$$

Thus, it transforms as

$$\tilde{A}(\lambda) = A(\lambda) + \frac{d\beta}{d\lambda}$$

### What if we carry out a closed loop?

If we insist that  $|\tilde{u}_{\lambda=0}\rangle = |\tilde{u}_{\lambda=1}\rangle$  in the new gauge then, by the formula  $|\tilde{u}_\lambda\rangle = e^{-i\beta(\lambda)}|u_\lambda\rangle$  we must have

$$\beta(1) = \beta(0) + 2\pi \cdot m, \quad m \in \mathbb{Z}$$

Then,

$$\int_{\lambda=0}^{\lambda=1} \frac{d\beta}{d\lambda} \cdot d\lambda = \beta(1) - \beta(0) = 2\pi m$$

which means that the berry phase after gauge transformation is related to the original berry phase as

$$\begin{aligned}\tilde{\phi} &= \oint \tilde{A}(\lambda) d\lambda \\ &= \oint A(\lambda) + \frac{d\beta}{d\lambda} d\lambda \\ &= \phi + 2\pi m\end{aligned}$$

So, the Berry's Phase is invariant modulo  $2\pi$ !!

## 7.2 In the Parallel Transport Gauge...

we have

$$\bar{A}(\lambda) = \langle \bar{u}_\lambda | i d_\lambda \bar{u}_\lambda \rangle = 0$$

(the berry connection vanishes in this gauge)

So,

$$\phi = -\text{Im} (\ln \langle u_{\lambda=1} | \lambda = 0 \rangle)$$

which is the mismatch of the phases at the beginning and end of the path.

## 7.3 In the Twisted Parallel Transport Gauge...

we have

$$|\tilde{u}_j\rangle = e^{-i\phi/Nj} |\bar{u}_j\rangle$$

so

$$|\tilde{u}_\lambda\rangle = e^{-i\phi\lambda} |\bar{u}_\lambda\rangle$$

and

$$\tilde{A}(\lambda) = \langle \tilde{u}_\lambda | i d_\lambda \tilde{u}_\lambda \rangle = \text{constant across the loop}$$

## 7.4 Physical Effects of Non-trivial Berry's Phase

The Berry's Phase does indeed lead to interesting interference effects.

### Aharanov-Bohm Effect

Include figure of two paths not being individually gauge inv but difference is

While the Berry Phases accumulated along the two paths are not individually gauge invariant, their different  $\phi_B - \phi_A = \Delta\phi$  is gauge invariant. The total phase is

$$\begin{aligned}\tilde{\phi} &= \left( \int_A^B A(\lambda) d\lambda \right)_{\text{Path 1}} + \left( \int_B^A A(\lambda) d\lambda \right)_{\text{Path 2}} \\ &= \int_A^B A(\lambda) d\lambda - \int_A^B A(\lambda) d\lambda\end{aligned}$$

This is the origin of the Aharonov-Bohm Effect. ([Elaborate](#))

## 8 February 10, 2025:

### 8.1 Spin $\frac{1}{2}$ particle in a magnetic field $\mathbf{B}$

- The idea is to have eigenstate  $|u_\lambda\rangle$  (function of  $\lambda$ ) that we evolve with time adiabatically across a closed loop.
- The meaning of adiabatic is that  $|u\rangle_\lambda$  remains a good eigenstate parametrized by  $\lambda$ .
- $\lambda$  can represent any kind of continuous variable like magnetic field direction, rotations of a molecule, etc.
- As an example, spin in a magnetic field is described by Hamiltonian

$$H = \gamma \vec{S} \cdot \vec{B} = \frac{\gamma \hbar}{2} \vec{\sigma} \cdot \vec{B} = \frac{\hbar \gamma B}{2} \vec{\sigma} \cdot \hat{n}$$

Include figure

- $|u_\lambda\rangle$  describes eigenstates of  $\vec{\sigma} \cdot \hat{n}$  with spin along the direction of the magnetic field  $\vec{B}$ .
- Moving  $\hat{n}$  around a loop will define our closed path  $P$ .

Include figure with "consider one octant"

We have

$$|u_{\hat{n}}\rangle = \begin{pmatrix} \cos(\frac{\theta}{2}) \\ \sin(\frac{\theta}{2}) e^{i\phi} \end{pmatrix}$$

#### Where exactly does this come from?

Using Spherical Coordinates,

$$\hat{r} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z}$$

we can project the spin as (**what exactly does it mean to project the spin onto spherical coordinates**)

$$\vec{S} \cdot \vec{r} = \frac{\hbar}{2} (\sin \theta \cos \phi \vec{\sigma}_x + \sin \theta \sin \phi \vec{\sigma}_y + \cos \theta \vec{\sigma}_z) = S_r$$

(Fill in more from picture).

### 8.2 Calculating the Berry's Phase

Let's focus on  $|\uparrow_{\hat{n}}\rangle$ : We have

$$|\uparrow_{\hat{z}}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|\uparrow_{\hat{x}}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|\uparrow_{\hat{y}}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

**(Include calculation of  $\phi$  from image)** This is actually exact, and it doesn't matter how many discrete parts we take, we will always get the same Berry's Phase so long as the path traverses the same octant.

### 8.3 Generalization to Continuous Wavefunctions: Berry Curvature

- Suppose we have a 2D Parameter Space, spanned by  $\lambda_x$  and  $\lambda_y$ .
- Then the Berry Connection  $\vec{A}$  will also have two components:  $A_x$  and  $A_y$ .

Include figure of Parameter space.

- What are the two components?

$$A_x = \langle u_\lambda | i\partial_{\lambda_x} u_\lambda \rangle, \quad A_y = \langle u_\lambda | i\partial_{\lambda_y} u_\lambda \rangle$$

and we have

$$\phi = \oint_P \vec{A} \cdot d\vec{\lambda}$$

where  $P$  is the closed path traced in parameter space.

- The Berry Curvature is defined as the Berry Phase per unit area in  $(\lambda_x, \lambda_y)$  space, and is usually denoted by  $\Omega(\lambda)$ .
- When discretized, the Berry Curvature is like the Berry Phase per plaquette, divided by the area of the Plaquette.
- The Idea is that the closed path  $P$  in parameter space encloses some area, which can be broken down into a collection of Plaquettes. The Berry Curvature gives us the contribution of each of these plaquettes towards the Berry Phase, after we integrate over their areas.
- Given our insight from Electromagnetism, where  $\vec{B} = \nabla \times \vec{A}$ , we motivate the definition

$$\begin{aligned} \Omega(\lambda) &= \partial_x A_y - \partial_y A_x = (\nabla \times \vec{A})_z \\ &= \partial_x \langle u | i\partial_y u \rangle - \partial_y \langle u | i\partial_x u \rangle \\ &= (\langle \partial_x u | i\partial_y u \rangle + \langle u | \partial_x \partial_y u \rangle) - (\langle \partial_y u | \partial_x u \rangle + \langle u | \partial_y \partial_x u \rangle) \\ &= i (\langle \partial_x u | \partial_y u \rangle - \langle \partial_y u | \partial_x u \rangle) \\ &= i (i 2 \text{Im} (\langle \partial_x u | \partial_y u \rangle)) \end{aligned}$$

We then use Stokes' Theorem to relate the "Berry flux"  $\Phi_S$  (which is all those differential components added up over an area enclosed by path  $P$ ):

$$\begin{aligned} \Phi_S &= \int_S \vec{\Omega}(\lambda) \cdot \hat{n} dS \text{ where } \hat{n} \text{ is the unit normal to surface element } dS \\ &= \int_S \nabla \times \vec{A} \cdot \hat{n} dS \\ &= \oint_P \vec{A} \cdot d\vec{\lambda} \text{ (Stokes' Theorem)} \\ &= \phi, \text{ the Berry Phase!} \end{aligned}$$

**9 February 12, 2025:**

Missed this lecture.

## 10 February 14, 2025:

Today, we'll calculate the Berry Phase on a cylinder and a Torus, followed by some general discussion about Berry Phases over general Brillouin zones.

### 10.1 Berry Phase on a cylinder

Include figure

In this setup we have periodicity in the direction  $\nu$  but not in direction  $\mu$  i.e.

$$|u(\nu = 0, \mu_i)\rangle = |u(\nu = 1, \mu)\rangle$$

where these are identical, not just equal up to a phase.

The components of the Berry Curvature, as discussed earlier, are given by

$$\Omega_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

**Note.** Note that a choice has been made as to which derivative comes first. So, we'll label the Berry Flux  $\Phi^{\mu\nu}$  and Chern Number  $C^{\mu\nu}$  by the same convention since, for example, their signs depend on the order of  $\mu$  and  $\nu$ . This is why we write the ordering explicitly.

Now we can think about the Berry Flux

$$\begin{aligned}\Phi^{\mu\nu} &= \oint_{\text{cylinder}} \Omega^{\mu\nu} d\nu d\mu \\ &= \int_{\mu_i}^{\mu_f} d\mu \int_0^1 d\nu (\partial_\mu A_\nu - \partial_\nu A_\mu)\end{aligned}$$

Recall that we have periodicity in the  $\nu$  index. Because of this periodicity, going from  $\nu = 0$  to  $\nu = 1$  brings us back to the same state, and the second term of the integration disappears (**Understand this better**) giving us

$$\begin{aligned}\Phi^{\mu\nu} &= \int_0^1 d\nu \int_{\mu_i}^{\mu_f} \partial_\nu A_\mu d\mu \\ &= \int_{\mu_i}^{\mu_f} \underbrace{\partial_\mu \left( \int_0^1 A_\nu d\nu \right)}_{\text{Berry Phase}} d\mu\end{aligned}$$

So,

$$\begin{aligned}\Phi^{\mu\nu} &= \int_{\mu_i}^{\mu_f} \phi^\nu d\mu \\ &= \phi^\nu(\mu_f) - \phi^\nu(\mu_i)\end{aligned}$$

where  $\phi^\nu$  denotes the Berry Phase in the closed path along the  $\nu$  direction.

So, when working on a cylinder, the flux only depends on the phases at the ends of the cylinder.

Include figure

## 10.2 Berry Phase on a Torus

In this case, the state at  $\mu_i = 0$  and at  $\mu_f = 1$  is identical except for a phase modulo  $2\pi$ .

Include figure

- The difference in Berry Phase can only be  $2\pi m$ . (**Why, precisely?**)
- The Berry flux therefore also have to be  $2\pi m$ , because of the expression derived above.
- The Chern Number (berry flux integrated over a closed surface) has to be an integer multiple of  $2\pi C^{\mu\nu}$ , thus we identify

$$C^{\mu\nu} = m$$

as the Chern number of a torus.

**Note.** If we reversed the order in which we take the paths (namely,  $\nu$  first and then  $\mu$ ), the Chern number picks up a minus sign

$$C^{\mu\nu} = -C^{\nu\mu}$$

## 10.3 Integrating over a Brillouin Zone

Bloch states  $|\psi_{n,k}\rangle$  are labelled by their momentum  $k$  and their band index  $n$ . We know that these states take the form

$$|\psi_{n,k}\rangle = e^{ikx} |u_{nk}\rangle$$

where  $e^{ikx}$  is just a plane wave and  $|u_{n,k}\rangle$  is periodic over the unit-cell.

**Note.** One way to think about  $|u_{n,k}\rangle$  is as a periodic function equal to the orbital wavefunction when  $k = 0$ .

What do we mean by "periodic over the unit-cell"?

$$u_{n,k}(\vec{r}) = u_{n,k}(\vec{r} + \vec{R})$$

where  $\vec{R}$  is the lattice constant.

- Assume that each band  $n$  is isolated so they don't cross. Why? Because we want to make use of Adiabaticity (crossings involve degeneracies which are not adiabatic).
- The Berry Phase is going to involve inner products which look like

$$\begin{aligned} \langle \psi_{n,k} | \psi_{n,k+\delta k} \rangle &= \int_{-\infty}^{\infty} dx \psi_{n,k}^* \psi_{n,k+\delta k} \\ &\quad \int_{-\infty}^{\infty} dx e^{-i\delta k x} u_{n,k}^*(x) u_{n,k+\delta k}(x) \end{aligned}$$

- Note that since  $u_{n,k}(x)$  and  $u_{n,k+\delta k}$  are both periodic over the Unit Cell, so is their product. It will be the same number per unit cell added over all the unit cells.

- However, since the product of the  $u$  functions is constant over each UC, the presence of the  $e^{i\delta kx}$  averages this integral to zero. **So, this definition of the inner product is not useful.**
- If we instead define the inner product to be over a unit cell, we still have a problem: the  $e^{-i\delta kx}$  has different values if we define the integral to be over  $[0, a]$  versus  $[-a/2, a/2]$ .
- So, in order to study the Berry Phase, instead of using the full Bloch Wavefunction  $|\psi_{n,k}\rangle$ , we study the cell periodic part of the wavefunction:  $|u_{n,k}\rangle$ . This way, the inner product is not averaged to zero, and the choice of unit cell does not matter.

$$\begin{aligned} \langle u_{n,k} | u_{n,k+\delta k} \rangle &= \int_0^a dx u_{n,k}^*(x) u_{n,k+\delta k}(x) \\ \implies \langle u_{n,k} | u_{n,k} \rangle &= \int_0^a dx u_{n,k}^*(x) u_{n,k}(x) = 1 \end{aligned}$$

**Note.** Something to note is that  $|u_{n,k}\rangle$  is an eigenstate of the momentum-dependent Hamiltonian

$$H|\psi_{n,k}\rangle = E_n(k)|\psi_{n,k}\rangle$$

defined by

$$H_k = e^{-ikx} H e^{ikx}$$

i.e.

$$H_{n,k}|u_{n,k}\rangle = E_{n,k}|u_{n,k}\rangle$$

We are now ready to define the Berry Phase and Curvature.

- We have

$$\begin{aligned} \phi_k &= \oint_P \vec{A}_n(k) \cdot d\vec{k}, \quad \vec{A}_n = \begin{pmatrix} A_{n,k_x} \\ A_{n,k_y} \\ A_{n,k_z} \end{pmatrix} \text{ where} \\ A_{n\mu} &= \langle u_{n,k} | i\partial_\mu u_{n,k} \rangle \end{aligned}$$

The Berry Curvature is

$$\Omega_{n,\nu\mu}(\vec{k}) = \partial_\mu A_{n\nu}(\vec{k}) - \partial_\nu A_{n\mu}(\vec{k}) = -2\text{Im} \left( \langle \partial_\mu u_{n,\vec{k}} | \partial_\nu u_{n,\vec{k}} \rangle \right)$$

## **11 February 17, 2025: No lecture**

President's day!

## **12 Watch recorded lecture**

### **13 Watch recorded lecture**

## 14 February 24, 2025:

Last time, we spoke about the symmetries of Graphene. To recap a bit,

### 14.1 Symmetries of Graphene

- Time Reversal:  $H(\vec{k}) \xrightarrow{\mathcal{T}} H^*(-\vec{k})$
- Inversion:

$$\begin{aligned}\psi_k(r) &\xrightarrow{\mathcal{I}} \sigma_x \psi_{-k}(r) \\ H(\vec{k}) &\xrightarrow{\mathcal{I}} \sigma_x \mathcal{H}(-\vec{k}) \sigma_X\end{aligned}$$

Include figure

- We will show today that the hamiltonian describing graphene  $H(\vec{k})$  is both time-reversal symmetric and inversion-symmetric.

### 14.2 The Graphene Hamiltonian

From the last lecture, we have the Bloch Hamiltonian

$$H(\vec{k}) = \begin{pmatrix} \epsilon_0 & \Delta(\vec{k}) \\ \Delta(\vec{k}) & \epsilon_0 \end{pmatrix}$$

Just as we did with the SSH Model, we will try to write this Hamiltonian as some sort of spinor function or dot product.

Let's set  $\epsilon_0 = 0$  and expand  $\Delta(\vec{k})$  out as

$$\Delta(\vec{k}) = t \sum_{n=1}^3 \cos(\vec{k} \cdot \vec{\delta}_n) + it \sum_{n=1}^3 \sin(\vec{k} \cdot \vec{\delta}_n)$$

Then we can write the Hamiltonian as

$$\begin{aligned}H(\vec{k}) &= t \left[ \sigma_x \sum_{n=1}^3 \cos(\vec{k} \cdot \vec{\delta}_n) - \sigma_y \sum_{n=1}^3 \sin(\vec{k} \cdot \vec{\delta}_n) \right] \\ &= \vec{\sigma} \cdot \vec{b}\end{aligned}$$

where

$$\vec{b} = t \sum_{n=1}^3 \cos(\vec{k} \cdot \vec{\delta}_n) - t \sum_{n=1}^3 \sin(\vec{k} \cdot \vec{\delta}_n)$$

or equivalently

$$\vec{b} = t \begin{pmatrix} \sum_{n=1}^3 \cos(\vec{k} \cdot \vec{\delta}_n) \\ -\sum_{n=1}^3 \sin(\vec{k} \cdot \vec{\delta}_n) \\ 0 \end{pmatrix}$$

- Note that  $b_x$  is even in  $\vec{k}$ :  $b_x(-\vec{k}) = b_x(\vec{k})$  and  $b_y$  is odd in  $\vec{k}$ :  $b_y(-\vec{k}) = -b_y(\vec{k})$
- So, our hamiltonian is

$$\boxed{H(\vec{k}) = \sigma_x b_x(\vec{k}) + \sigma_y b_y(\vec{k})}$$

### 14.3 Time-Reversal

Let's show that  $H(\vec{k})$  is invariant under time-reversal i.e.  $H(\vec{k}) = H^*(-\vec{k})$

$$\begin{aligned} H^*(-\vec{k}) &= (\sigma_x b_x(-\vec{k}) + \sigma_y b_y(-\vec{k}))^* \\ &= (\sigma_x b_x(k) - \sigma_y b_y(k))^* \\ &= \sigma_x b_x(\vec{k}) + \sigma_y b_y(\vec{k}) \\ &= H(\vec{k}) \end{aligned}$$

### 14.4 Inversion Symmetry

Now let's show that  $H(\vec{k})$  is invariant under inversion i.e.  $H(\vec{k}) = \sigma_x H(-\vec{k}) \sigma_x$

$$\begin{aligned} H(\vec{k}) \sigma_x &= b_x(\vec{k}) - i\sigma_z b_y \text{ Using the commutation relations for } \sigma_i \\ \implies \sigma_x H(\vec{k}) \sigma_x &= \sigma_x b_x - i\sigma_x \sigma_z b_y \\ &= \sigma_x b_x(\vec{k}) - \sigma_y b_y(\vec{k}) \\ &= \sigma_x b_x(-\vec{k}) + \sigma_y b_y(-\vec{k}) \\ &= H(-\vec{k}) \end{aligned}$$

So, inversion symmetry checks out too!

### 14.5 Chiral Symmetry

Just like the SSH Model Hamiltonian, since there is no  $\sigma_z$  component it immediately follows from the Pauli Matrices Commutation rules that

$$\sigma_z H(\vec{k}) \sigma_z = -H(-\vec{k})$$

This guarantees that if there is an eigenstate energy  $E$ , there is another eigenstate with energy  $-E$ .

#### How could we introduce a $\sigma_z$ component?

- Add second neighbor hoppings
- Consider multiorbital systems

## 14.6 Berry Phases in Graphene

Last week we discussed how Berry's Phases vanishes for a time-reversal symmetric (TRS) system. However, Graphene still displays topological behavior which is "hidden away" in the Band structure. In fact it was one of the first materials discussed as a topological material.

To see Topological Behavior, we need a bandgap (turns out there are gapless topological materials too but that's far beyond our scope).

To get a better grip on the Topological Properties of Graphene, let's see its eigenstates and Band Structure.

## 14.7 Graphene's Eigenstates

Famously, graphene has gapless "Dirac-like" eigenstates.

### Where is graphene gapless in $k$ -space?

If we want the gaps to vanish, that's equivalent to saying  $|\vec{b}(\vec{k})| = 0$ . So we just need to look for points in  $k$ -space which satisfy this condition.

(Had to leave lecture; ask Rainer or Josh for their notes.)