(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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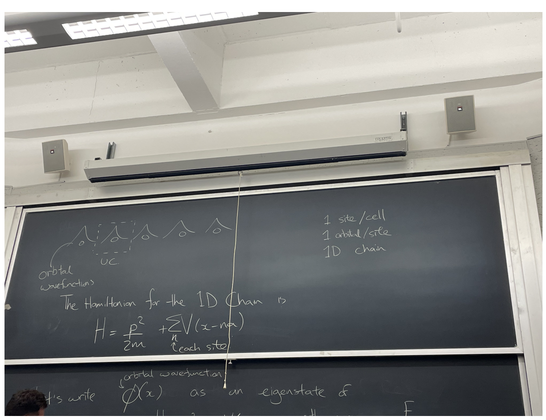
# 1 January 22, 2025:

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

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

(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

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

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

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

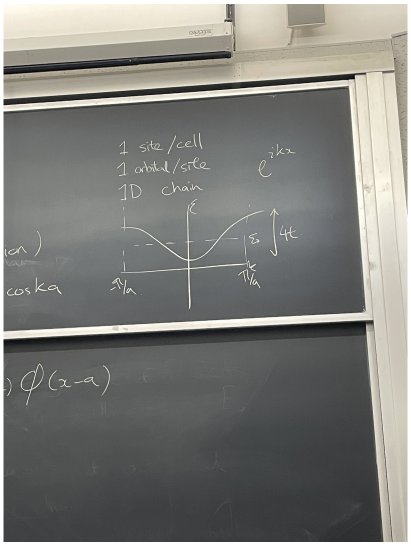
This can be interpreted as the single orbital wavefunction $\phi(x)$ being modulated by the free-electron wavefunction $e^{ikx}$.

The Energy Spectrum (or dispersion relation) is given by

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

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

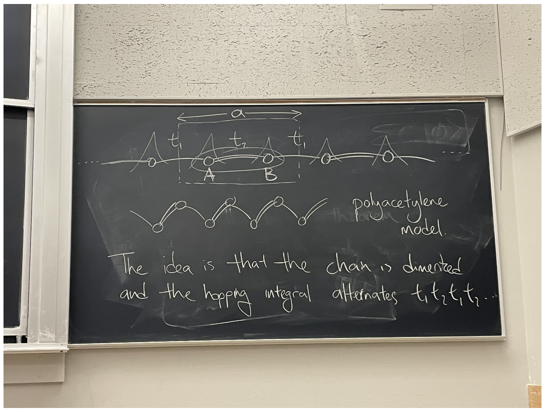
$$t \equiv \int \mathrm{d}x\ \phi(x)V(x)\phi(x - a)$$




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

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

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

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

- Taking the first of these equations, the RHS is

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

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

- Now, for the LHS,

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

- 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

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

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

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

# 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

$$N = \begin{pmatrix} \text{\# sites} \\ \text{per U.C.} \end{pmatrix} \times \begin{pmatrix} \text{\# orbitals} \\ \text{per site} \end{pmatrix} \times \begin{pmatrix} \text{\# of} \\ \text{dimensions} \end{pmatrix}$$

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

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

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 psuedospin wavefunctions

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

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

$$\vec{b}_x = \begin{pmatrix} \Delta_1(k) \\ 0 \\ 0 \end{pmatrix},\ \vec{b}_y = \begin{pmatrix} 0 \\ \Delta_2(k) \\ 0 \end{pmatrix},\ \vec{b}_z = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$
$$\text{and } \vec{b}(k) = b_x\hat{x} + b_y\hat{y} + b_z\hat{z}$$

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 anticommute 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 $\Theta$ actos 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.