
Phys 435

TOPICS IN CONDENSED MATTER

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Table Of Contents

	Page
1 Toy Model of a Solid	4

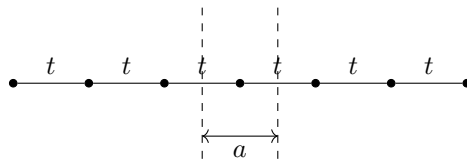
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1 Toy Model of a Solid

Todo (TC Fraser): Type up notes for first class



Thus far we have been discussing a toy model of a solid in one dimension. By diagonalizing the Hamiltonian we were able to determine the energy levels of the various states,

$$\varepsilon(k) = -2t \cos(ka) \quad (1.1)$$

Where k is the wave-vector with $p = \hbar k$ as the ordinary linear momentum. Additionally, t acts as a tunneling coefficient that dictates a tunneling *rate* (up to a constant \hbar) for the electrons in the solid. Unlike free particles, the momentum k in this toy model is confined to a discrete region.

$$-\frac{\pi}{a} \leq k < \frac{\pi}{a}$$

This interval is called the **first Brillouin zone**. To highlight this difference, we sometimes refer to p in this model as the **crystal momentum**.

Moreover, the periodic boundary conditions used restrict k to take on discrete and finite values,

$$k = \frac{2\pi m}{N} \quad m = 0, \pm 1, \pm 2, \dots$$

Where $L = Na$ is the size of the crystal, N is the number of atoms and a is the interval between two atoms in the solid.

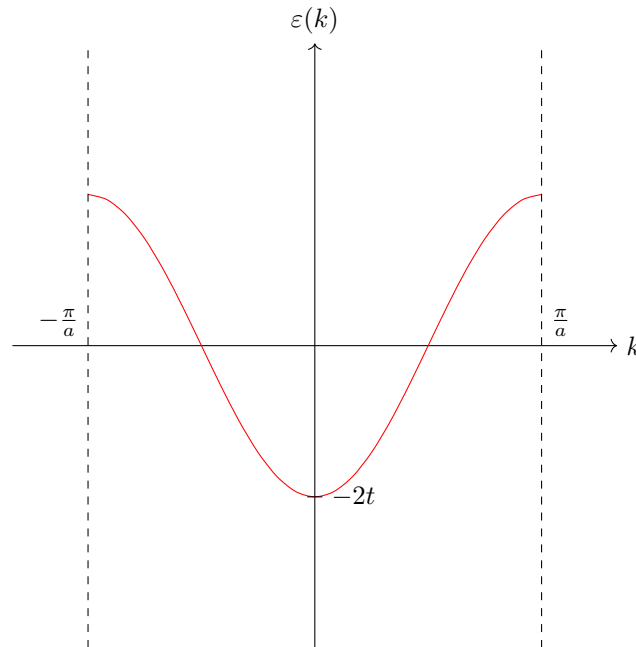
The states that diagonalized the Hamiltonian are called **Bloch states** and are denoted $|k\rangle$ where,

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_n |n\rangle e^{ikna}$$

Which is a **lattice Fourier transform**. Since k is confined to a finite interval, the energy levels are confined to a finite interval,

$$\varepsilon_{\min} = -2t \quad \varepsilon_{\max} = +2t$$

The interval has a width of $\varepsilon_{\max} - \varepsilon_{\min} = 4t$ and is referred to as the allowed energy *band*.



How many states does the band contain. Given that k is discrete and bounded,

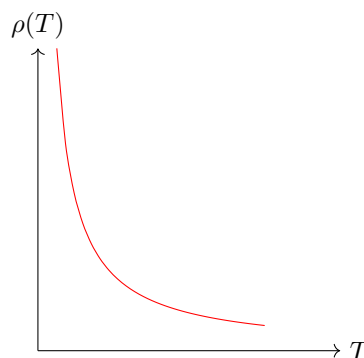
$$-\frac{\pi}{a} \leq \frac{2\pi m}{Na} = k < \frac{\pi}{a}$$

Implies,

$$-\frac{N}{2} \leq m < \frac{N}{2}$$

Therefore there are N distinct waves of m . The total number states per band is thus $2N$ where N is the number of primitive unit cells in the crystal.

Suppose now that we have 1 electron per atom (instead of 1 electron in total). We recall the **Pauli principle** which states that only 1 electron can occupy a given state in a band. Since there are N electrons and $2N$ states, the band is *half-filled*.



When the electrons occupy all of the lowest possible energy states, we fill all of the negative energy states and the positive energy states remain vacant. This separation defines the **Fermi energy** for this system where occurs at $\varepsilon_F = 0$. In order to find the state that corresponds to this upper limit one needs to solve,

$$\varepsilon(k) = \varepsilon_F = 0 \implies -2t \cos(ka) = 0$$

Therefore the value of k that solves this equation is,

$$k = \pm \frac{\pi}{2a} = \pm k_F$$

Where k_F is given a special name: the **Fermi wave-vector** (Fermi momentum).

$$|k| < k_F : \text{filled states}$$

$$|k| > k_F : \text{empty states}$$

The **Fermi surface** defines the surface in momentum space separating the filled states from the unfilled states. Most of the observed properties of metals follow from the existence of the Fermi surface.

This concept is so important that it is worth measuring the volume in momentum space corresponding to the filled states. This is the volume enclosed by the Fermi surface. In this example, the volume in momentum space is characterized by the $2k_F$ interval. Since $k = 2\pi m/Na$, the volume per single k -value is $2\pi/Na$. Letting n be the density of electrons, we can compute the total number of electrons:

$$nNa = 2 \frac{2k_F}{2\pi/Na}$$

Which allows one to calculate k_F ,

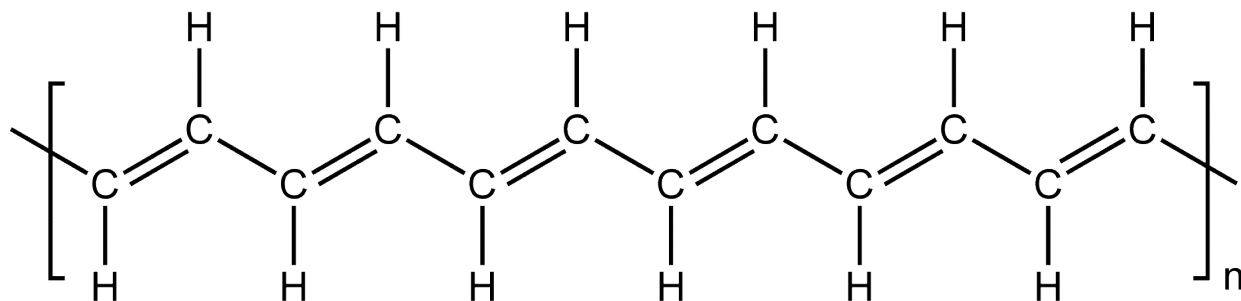
$$k_F = \frac{\pi}{2}n$$

Which makes sense for this model because there is one electron per atom making $n = 1/a$. This result is called **Luttinger's theorem** which states that the volume enclosed by the Fermi surface (sometimes called the Fermi sea) is directly proportional to the electron density.

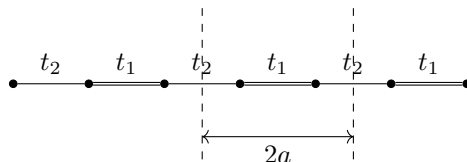
This toy model actually describes a real solid called polyacetylene. Polyacetylene consists of weakly-interacting chains of CH units.



Electrons found in the inner orbitals of the atoms are tightly bound to their nuclei and therefore only the valence electrons in carbon are free to travel throughout the lattice.



Three of the valence electrons are engaged in bonding with neighboring carbon and hydrogen atoms while the 4-th one is free to move around. As it turns out, the bonds between carbon atoms possess alternating tunneling amplitudes.



In Polyacetylene, the tunneling amplitude between the carbon atoms joined by a double bond is slightly higher $t_1 > t_2$. This is referred to as **Peierls instability**.

Since this deviation is only slight, let $2\delta t = t_1 - t_2$ such that,

$$t_1 = t + \delta t \quad t_2 = t - \delta t$$

Another important difference is that the primitive unit cell has size $2a$ (instead of a). This two atom basis can be arranged on a lattice with lattice constant $2a$. This is referred to as a **Bravais lattice**. Notationally, we can describe any crystal as,

$$\text{crystal} = (\text{basis}, \text{Bravais lattice})$$

To describe an electron in this lattice, we need two indices: one to describe the unit cell the electron is in and one to describe which atom (1 or 2) the electron is located at. Therefore the Hamiltonian needs to characterize a number of possible transitions,

- $|n, 2\rangle\langle n, 1|, |n, 1\rangle\langle n, 2|$ tunneling within a unit cell (forward, backward)
- $|n-1, 2\rangle\langle n, 1|, |n, 1\rangle\langle n-1, 2|$ tunneling between unit cells (forward, backward)

$$H = \sum_n \{-t_1 |n, 2\rangle\langle n, 1| - t_2 |n-1, 2\rangle\langle n, 1| - t_1 |n, 1\rangle\langle n, 2| - t_2 |n, 1\rangle\langle n-1, 2|\}$$

Just as before, we need to write $|n, \alpha\rangle$ in the momentum basis,

$$|n, \alpha\rangle = \sum_k |k, \alpha\rangle \langle k, \alpha | n, \alpha\rangle$$

Where $\langle k, \alpha | n, \alpha\rangle$ is written as,

$$\langle k, \alpha | n, \alpha\rangle = \frac{1}{\sqrt{N}} e^{-2ikna}$$

It is important to note that here N does not represent the total number of atoms; N is the total number of unit cells (equivalently the total number of distinct $|n, \alpha\rangle$ states for *fixed* α). Moreover the extra factor of 2 in the exponential is due to the increases unit cell size. In momentum space, the Hamiltonian can be written,

$$\begin{aligned} H = & -t_1 \frac{1}{N} \sum_n \sum_{k, k'} |k, 2\rangle\langle k', 1| e^{-2ikna} e^{2ik'na} \\ & - t_2 \frac{1}{N} \sum_n \sum_{k, k'} |k, 2\rangle\langle k', 1| e^{-2ik(n-1)a} e^{2ik'na} \\ & - t_1 \frac{1}{N} \sum_n \sum_{k, k'} |k, 1\rangle\langle k', 2| e^{-2ikna} e^{2ik'na} \\ & - t_2 \frac{1}{N} \sum_n \sum_{k, k'} |k, 1\rangle\langle k', 2| e^{-2ikna} e^{2ik'(n-1)a} \end{aligned} \quad (1.2)$$

One again we need to make use of the following identity,

$$\frac{1}{N} \sum_n e^{-2i(k-k')na} = \delta_{k, k'} \quad (1.3)$$

Each term in eq. (1.2) contains terms of the form of eq. (1.3) which simplify H greatly,

$$\begin{aligned} H = & -t_1 \sum_k \{|k, 2\rangle\langle k, 1| + |k, 1\rangle\langle k, 2|\} \\ & - t_2 \sum_k \{|k, 2\rangle\langle k, 1| e^{2ika} + |k, 1\rangle\langle k, 2| e^{-2ika}\} \end{aligned} \quad (1.4)$$

Already we can see that unlike the previous model, the Hamiltonian is not yet diagonalize. At this point, we have only *partially* diagonalized the Hamiltonian with respect to the index of the unit cell. What remains is

to diagonalize the Hamiltonian with respect to the index of the *atom* within a single unit cell (i.e. $\alpha = 1, 2$). In order to do this, notice that eq. (1.4) can be written as,

$$H = \sum_k H(k)$$

Where $H(k)$ is a k dependent Hamiltonian. We will focus on this Hamiltonian henceforth.

$$\begin{aligned} H(k) = & -t_1 \{|k, 2\rangle\langle k, 1| + |k, 1\rangle\langle k, 2|\} \\ & - t_2 \{|k, 2\rangle\langle k, 1|e^{2ika} + |k, 1\rangle\langle k, 2|e^{-2ika}\} \end{aligned}$$

For convenience, we will drop reference to k within the states,

$$\begin{aligned} H(k) = & -t_1 \{|2\rangle\langle 1| + |1\rangle\langle 2|\} \\ & - t_2 \{|2\rangle\langle 1|e^{2ika} + |1\rangle\langle 2|e^{-2ika}\} \end{aligned} \quad (1.5)$$

Equation (1.5) has the Hamiltonian of a 2 level system. Therefore we can model this system as a spin-1/2 system using the **Pauli matrices**. Recall,

$$\begin{aligned} \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow| \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \end{aligned} \quad (1.6)$$

Using the following correspondence,

$$|1\rangle = |\uparrow\rangle \quad |2\rangle = |\downarrow\rangle$$

We have that,

$$\begin{aligned} H(k) = & -[(t + \delta t) + (t - \delta t)e^{-2ika}]|\uparrow\rangle\langle\downarrow| \\ & - [(t + \delta t) + (t - \delta t)e^{2ika}]|\downarrow\rangle\langle\uparrow| \end{aligned}$$

We now elect to write $e^{\pm 2ika}$ in terms of sines and cosines and isolate the real and imaginary components,

$$\begin{aligned} H(k) = & -[(t + \delta t) + (t - \delta t)\cos(2ka)]|\uparrow\rangle\langle\downarrow| \\ & + i(t - \delta t)\sin(2ka)|\uparrow\rangle\langle\downarrow| + \text{h.c.} \end{aligned}$$

Where ‘h.c.’ refers to the Hermitian conjugate the the preceding terms. At this stage, we define some notation,

$$\begin{aligned} d_x(k) &= -(t + \delta t) - (t - \delta t)\cos(2ka) \\ d_y(k) &= -(t - \delta t)\sin(2ka) \\ d_z(k) &= 0 \end{aligned}$$

Where \vec{d} can be written,

$$\vec{d}(k) = (d_x(k), d_y(k), d_z(k))$$

Making use of eq. (1.6), we can see that,

$$|\uparrow\rangle\langle\downarrow| = \frac{1}{2}(\sigma_x + i\sigma_y)$$

Which means that the Hamiltonian is,

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

This system is *equivalent* to a spin-1/2 particle in a magnetic field of the form $\vec{d}(k)$. The eigenstates of $H(k)$ correspond to $\langle \vec{\sigma} \rangle$ along \vec{d} or in the opposite direction to \vec{d} ,

$$\varepsilon_{\pm}(k) = \pm |\vec{d}(k)|$$

This is contrasting to the previous model; before we had a *single* energy band pursuant to eq. (1.1), but here we have *two energy bands*. This result can be generalized to the following observation:

Every atom in the unit cell will give rise to a separate band.

Explicitly, $|\vec{d}(k)|^2$ has the value,

$$|\vec{d}(k)|^2 = d_x^2(k) + d_y^2(k) + d_z^2(k) = 4t^2 \cos^2(ka) + 4\delta t^2 \sin^2(ka)$$

Which makes the two bands have the form,

$$\varepsilon_{\pm} = \pm 2\sqrt{t^2 \cos^2(ka) + \delta t^2 \sin^2(ka)}$$

Which when plotted is,

