
Phys 435

TOPICS IN CONDENSED MATTER

University of Waterloo

Course notes by: TC Fraser
Instructor: Anton Burkov

tcfrazer@tcfrazer.com

Version: 1.0

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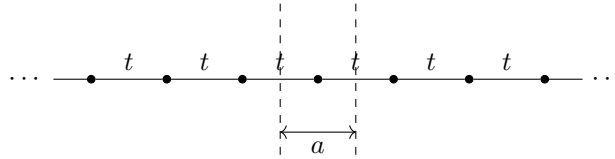
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Latest versions of all my course notes are available at **www.tcfrazer.com/coursenotes**.

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,

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

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.

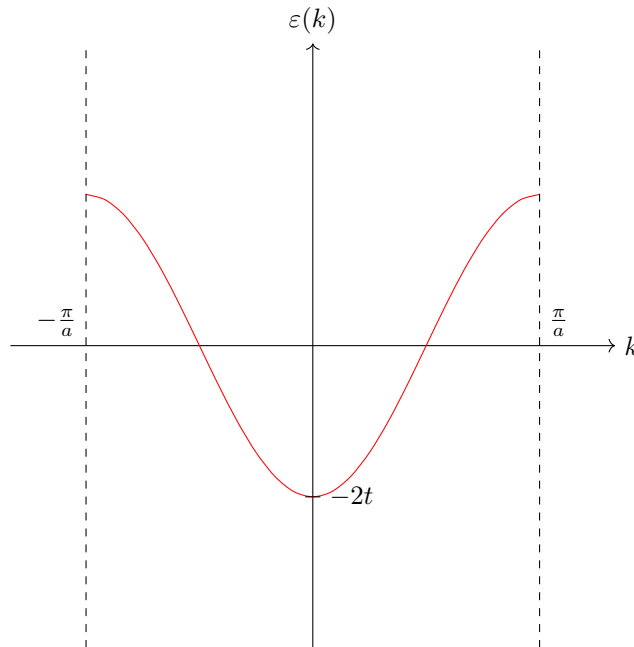
The states that diagonalized the Hamiltonian are called **Bloch states** and are denoted $|k\rangle$ where,

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

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,

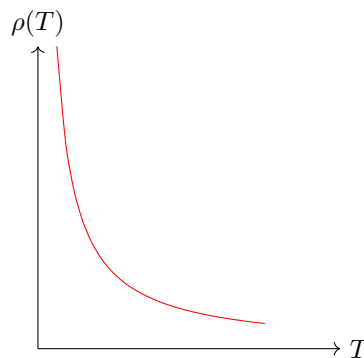
$$-\frac{\pi}{a} \leq \frac{2\pi m}{Na} = k < \frac{\pi}{a}$$

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 ,

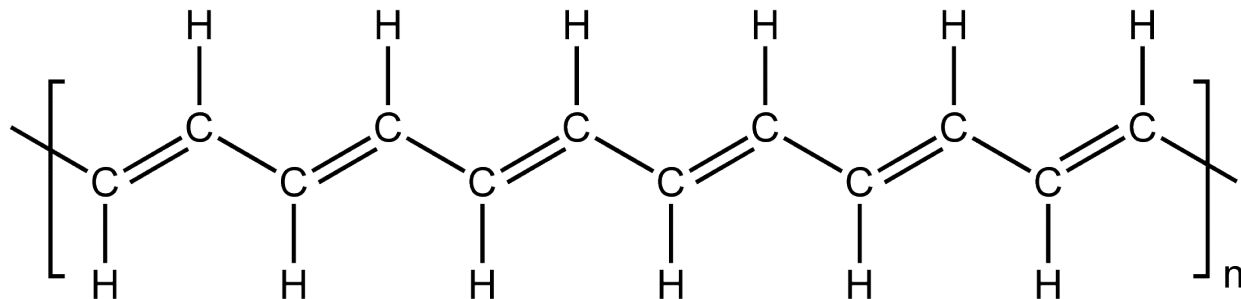
$$k_F = \frac{\pi}{2}n$$

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.

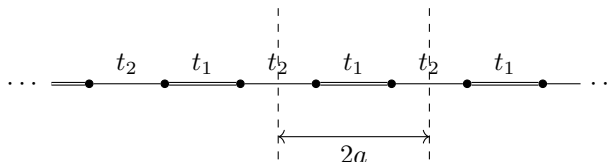
This toy model actually describes a real solid called polyacetylene. Polyacetylene consists of weakly-interacting chains of CH units.



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,

$$t_1 = t + \delta t \quad t_2 = t - \delta t \quad (1.2)$$

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,

$$\begin{aligned} H = & -t_1 \frac{1}{N} \sum_n \sum_{k, k'} |k, 2\rangle \langle k', 1| e^{-2ikna} e^{2ik'na} \\ & - t_2 \frac{1}{N} \sum_n \sum_{k, k'} |k, 2\rangle \langle k', 1| e^{-2ik(n-1)a} e^{2ik'na} \\ & - t_1 \frac{1}{N} \sum_n \sum_{k, k'} |k, 1\rangle \langle k', 2| e^{-2ikna} e^{2ik'na} \\ & - t_2 \frac{1}{N} \sum_n \sum_{k, k'} |k, 1\rangle \langle k', 2| e^{-2ikna} e^{2ik'(n-1)a} \end{aligned} \quad (1.3)$$

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

$$\frac{1}{N} \sum_n e^{-2i(k-k')na} = \delta_{k, k'} \quad (1.4)$$

Each term in eq. (1.3) contains terms of the form of eq. (1.4) which simplify H greatly,

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

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. (1.5) 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,

$$\begin{aligned} H(k) = & -t_1 \{ |2\rangle \langle 1| + |1\rangle \langle 2| \} \\ & - t_2 \{ |2\rangle \langle 1| e^{2ika} + |1\rangle \langle 2| e^{-2ika} \} \end{aligned} \quad (1.6)$$

Equation (1.6) 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,

$$\begin{aligned} \sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |\uparrow\rangle \langle \downarrow| + |\downarrow\rangle \langle \uparrow| \\ \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i|\uparrow\rangle \langle \downarrow| + i|\downarrow\rangle \langle \uparrow| \\ \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |\uparrow\rangle \langle \uparrow| - |\downarrow\rangle \langle \downarrow| \end{aligned} \quad (1.7)$$

Using the following correspondence (which we refer to as a pseudo-spin),

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

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,

$$\begin{aligned} d_x(k) &= -(t + \delta t) - (t - \delta t) \cos(2ka) \\ d_y(k) &= -(t - \delta t) \sin(2ka) \\ d_z(k) &= 0 \end{aligned} \quad (1.8)$$

Where \mathbf{d} can be written,

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

Making use of eq. (1.7), we can see that,

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

Which means that the Hamiltonian is,

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

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

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

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.

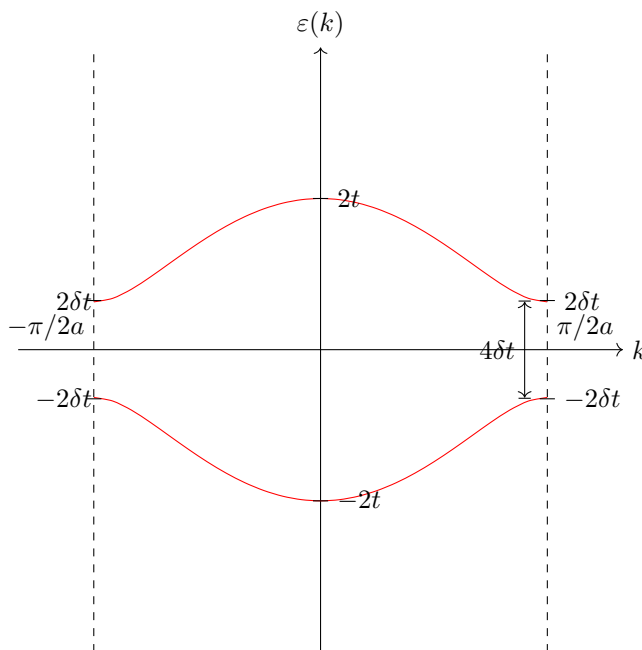
Explicitly, $|\mathbf{d}(k)|^2$ can be calculated from eq. (1.8),

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

Which makes the two bands have the form,

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

Which when plotted is,

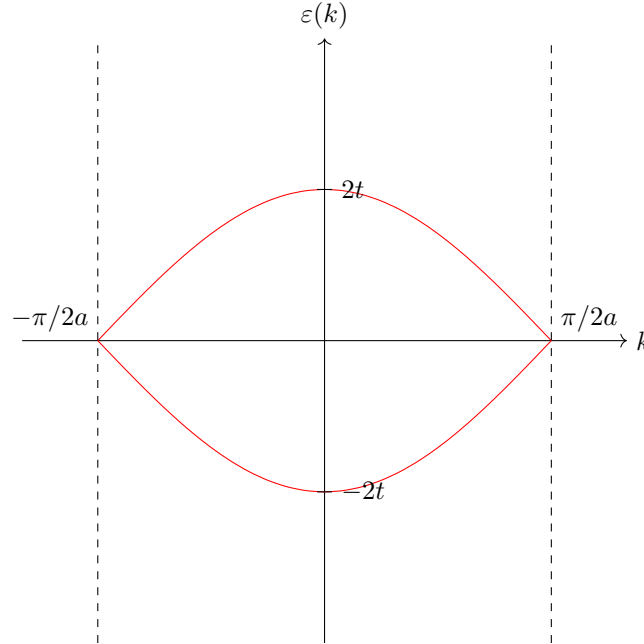


Notice that the first Brillouin zone is $\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$ is *smaller* than it was previously. In this model, there is one electron per atom and thus two electrons per unit cell. Therefore there are $2N$ electrons. At zero temperature, the entire lower band is filled and the upper band is empty. This makes polyacetylene an **insulator** because it requires an energy of at least $4\delta t$ in order to transition an electron across the Fermi surface.

In the limit of the $\delta t \rightarrow 0$ one should expect to recover eq. (1.1),

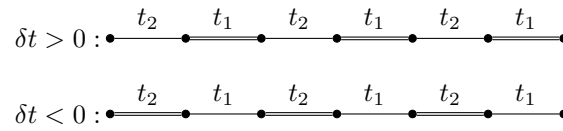
$$\lim_{\delta t \rightarrow 0} \varepsilon_{\pm}(k) = \pm 2 \lim_{\delta t \rightarrow 0} \sqrt{t^2 \cos^2(ka) + \delta t^2 \sin^2(ka)} = \pm 2t \cos(ka)$$

As expected. Notice however the plot of $\epsilon(k)$ differs,



The resolution between these two plots is to notice that in the polyacetylene model, the unit cell had with $2a$ instead of a . Therefore in momentum space, the plotted values for k are bounded by $-\pi/2a \leq k \leq \pi/2a$ instead of $-\pi/a \leq k \leq \pi/a$. If one were to unravel the upper band into regions where $|k| > \pi/2a$ one would recover the initial model.

Heretofore, we have assumed that $\delta t > 0$. If however we consider $\delta t < 0$, then we transition from $t_1 > t_2$ to $t_2 > t_1$ pursuant to eq. (1.2). And our diagram is adjusted



Therefore, the ground state of polyacetylene is doubly degenerate, corresponding to the two signs of δt . As it turns out, this difference in sign is related to topological properties in momentum space. Upon examination of eq. (1.8) one can notice \mathbf{d} 's dependence on δt . How does $\mathbf{d}(k)$ change as k goes from $-\pi/2a$ to $\pi/2a$?

$$d_x(k) = -(t + \delta t) - (t - \delta t) \cos(2ka)$$

$$d_y(k) = -(t - \delta t) \sin(2ka)$$

Checking specific points,

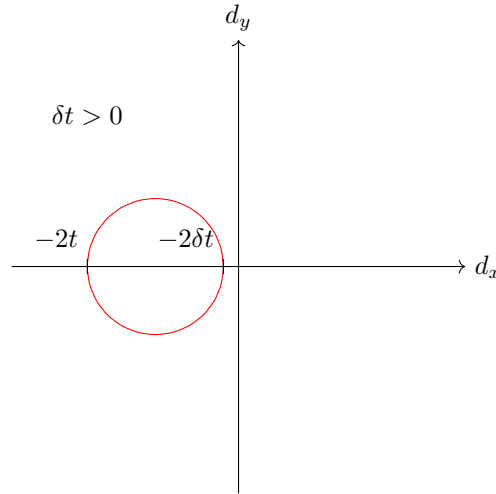
$$d_x\left(\pm \frac{\pi}{2a}\right) = -(t + \delta t) + (t - \delta t) = -2\delta t$$

$$d_y\left(\pm \frac{\pi}{2a}\right) = 0$$

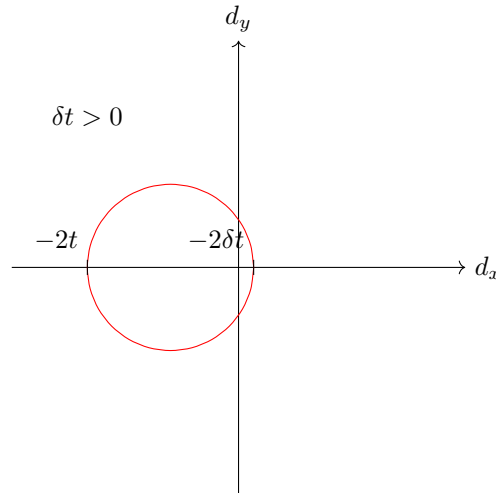
$$d_x(0) = -(t + \delta t) - (t - \delta t) = -2t$$

$$d_y(0) = 0$$

Plotted the case of $\delta t > 0$ in d_y, d_x space,



It can be seen that when $\delta t > 0$, the curve in d_x, d_y does not enclose the origin $\mathbf{d} = 0$. Recalling that $\varepsilon_{\pm}(k) = \pm|\mathbf{d}(k)|$, as long as $\mathbf{d}(k) \neq 0$, there exists a energy gap between the two bands ε_+ and ε_- . Therefore for $\delta t > 0$ polyacetylene is an ordinary insulator. However, in the case where $\delta t < 0$,



It can be seen that the origin $|\mathbf{d}| = 0$ is enclosed. This *topological* difference is what leads us to call the $\delta t < 0$ a **topological insulator** as apposed to an **ordinary insulator**.

Effectively, there is no possible way to continuously deform the Hamiltonian (i.e. changing δt) without merging the two energy bands.

An observable feature of topological insulators becomes evident for the edge states at zero energy (i.e. in the middle of a band gap). In this case of polyacetylene, these states that are closest to the band gap are those that live on the edge of the Brillouin zone where $|k - \pi/2a|$ is small. In order to explore the physics of these regions, define δk such that,

$$k = \frac{\pi}{2a} + \delta k$$

Where δk is small. In this case, the Hamiltonian $H(k) = \mathbf{d}(k) \cdot \boldsymbol{\sigma}$ can be expanded out explicitly,

$$\begin{aligned} d_x(k) &= d_x \left(\frac{\pi}{2a} + \delta k \right) \\ &= -(t + \delta t) - (t - \delta t) \cos(\pi + 2\delta k a) \\ &= -(t + \delta t) + (t - \delta t) \cos(2\delta k a) \end{aligned}$$

$$\begin{aligned}
&= -(t + \delta t) + (t - \delta t) + \mathcal{O}((\delta k)^2) \\
&\simeq -2\delta t
\end{aligned}$$

Similarly for d_y ,

$$\begin{aligned}
d_y(k) &= d_y\left(\frac{\pi}{2a} + \delta k\right) \\
&= -(t - \delta t) \sin(\pi + 2\delta k a) \\
&= (t - \delta t) \sin(2\delta k a) \\
&= (t - \delta t) 2\delta k a + \mathcal{O}((\delta k)^3) \\
&\simeq 2t\delta k a
\end{aligned}$$

Therefore,

$$H(\delta k) = -2\delta t \sigma_x + 2ta\delta k \sigma_y$$

In order to draw familiarity with systems that have been studied previously, let us rename a number of terms,

$$2\delta t = m \quad 2ta = \hbar v_F$$

Where m has units of energy and v_F has units of velocity. The Hamiltonian can now be written as,

$$H = -m\sigma_x + \hbar v_F \delta k \sigma_y$$

Since $\hbar \delta k$ has units of momentum, we simply label it p . Then the Hamiltonian can be written as,

$$H = v_F p \sigma_y - m \sigma_x$$

Which is identical to the Dirac equation (1D) for a *relativistic* particle of *mass* m and velocity v_F in place of the speed of light c . This velocity v_F is called the **Fermi velocity**.

$$\varepsilon_{\pm}(p) = \pm \sqrt{v_F^2 p^2 + m^2}$$

Consider the interface between 2 polyacetylene samples $\delta t > 0$ and $\delta t < 0$. In the position basis $p \rightarrow -i\hbar \partial_x$ we can write our Dirac Hamiltonian as,

$$H = -i\hbar v_F \sigma_y \partial_x - m(x) \sigma_x$$

Where m has an x dependence.

$$H\psi = E\psi$$

With $E = 0$ localized near $x = 0$.

$$[-i\hbar v_F \sigma_y \partial_x - m(x) \sigma_x] \psi(x) = 0$$

Therefore we should look for a solution of the form,

$$\psi(x) = e^{f(x)} \sigma_y |z\rangle$$

Where $|z\rangle$ is written in σ_z basis,

$$\begin{aligned}
|z\rangle &= z_{\uparrow} |\uparrow\rangle + z_{\downarrow} |\downarrow\rangle \\
\sigma_z |\uparrow\rangle &= +|\uparrow\rangle \quad \sigma_z |\downarrow\rangle = -|\downarrow\rangle
\end{aligned}$$

Using $\sigma_y^2 = \mathbf{1}$ and $\sigma_x \sigma_y = i\sigma_z$,

$$\left[i\hbar v_F \sigma_y \frac{df}{dx} + im(x) \sigma_z \right] e^{f(x)} |z\rangle = 0$$

Dropping the exponential $e^{f(x)}$,

$$\left[i\hbar v_F \sigma_y \frac{df}{dx} + im(x)\sigma_z \right] |z\rangle = 0$$

Adjusting the constant coefficients,

$$\left[\frac{df}{dx} + \frac{m(x)}{\hbar v_F} \sigma_z \right] |z\rangle = 0$$

Therefore,

$$\frac{df}{dx} = -\frac{m(x)}{\hbar v_F}$$

Can be solved using,

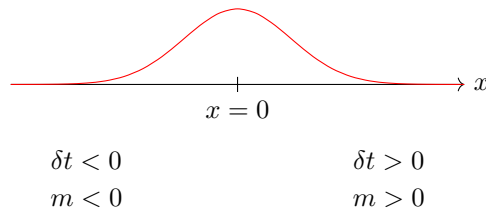
$$f(x) = -\frac{1}{\hbar v_F} \int_0^x dx' m(x')$$

Where $m(0) = 0$. Altogether, the solution ψx can be written,

$$\psi(x) = e^{-\frac{1}{\hbar v_F} \int_0^x dx' m(x')} \sigma_y |\uparrow\rangle$$

Since $\sigma_y |\uparrow\rangle = i|\downarrow\rangle$,

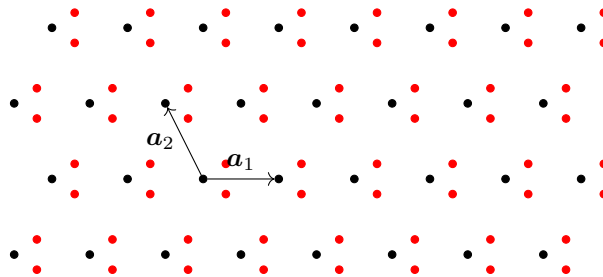
$$\psi(x) = ie^{-\frac{1}{\hbar v_F} \int_0^x dx' m(x')} |\downarrow\rangle$$



2 Higher Dimensions

A crystal is an infinite, periodic array of identical groups of atoms,

crystal = (basis, Bravais lattice)



A **Bravais lattice** is all points in \mathbb{R}^3 ($\mathbb{R}^2, \mathbb{R}^1, \mathbb{R}^n$) such that,

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

Where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the primitive translation vectors of the Bravais lattice. Moreover the coefficients n_1, n_2, n_3 are integers,

$$n_1, n_2, n_3 = 0, \pm 1, \pm 2, \pm 3, \dots$$

Typically, the choice for \mathbf{a}_i is not unique. However, the best choice for the primitive transition vectors is typically the one that exhibits the most symmetry.

The **primitive unit cell** is the parallelepiped defined by the primitive translation vectors.

A special type of unit cell, usually the most convenient, is the **Wigner-Seitz unit cell**. A WS unit cell is the region of space about a BL point that are closer to this point than to any other BL point.

3 Lattice Theory

Todo (TC Fraser): Missed a lecture

3.1 Reciprocal Lattice

The reciprocal lattice

$$e^{i\mathbf{G} \cdot \mathbf{P}} = 1$$

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3$$

Specifically, the honeycomb lattice had the following primitive translation vectors,

$$\mathbf{a}_1 = \frac{a}{2} (\hat{x} + \sqrt{3}\hat{y})$$

$$\mathbf{a}_2 = \frac{a}{2} (-\hat{x} + \sqrt{3}\hat{y})$$

Where the reciprocal lattice is defined such that,

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$$

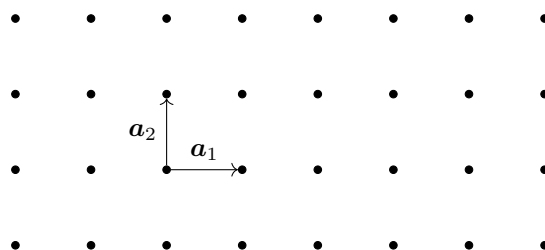
Which means \mathbf{b}_1 and \mathbf{b}_2 take on the following form.

$$\mathbf{b}_1 = \frac{2\pi}{\sqrt{3}a} (\hat{y} + \sqrt{3}\hat{x})$$

$$\mathbf{b}_2 = \frac{2\pi}{\sqrt{3}a} (\hat{y} - \sqrt{3}\hat{x})$$

3.2 Electronic Structure for Square Lattice

The square lattice in 2 dimensions has two primitive basis vectors $\mathbf{a}_1, \mathbf{a}_2$,



Using Cartesian coordinates,

$$\mathbf{a}_1 = a\hat{x} \quad \mathbf{a}_2 = a\hat{y}$$

The reciprocal lattice has the following form,

$$\mathbf{b}_1 = \frac{2\pi}{a} \hat{x} \quad \mathbf{b}_2 = \frac{2\pi}{a} \hat{y}$$

The Hamiltonian for this system in the nearest neighbor approximation can be written as the sum over all possible transitions with tunneling coefficient t .

$$H = -t \sum_{\mathbf{R}, \mathbf{a}} (|\mathbf{R} + \mathbf{a}\rangle \langle \mathbf{R}| + |\mathbf{R}\rangle \langle \mathbf{R} + \mathbf{a}|) \quad (3.1)$$

Where $\mathbf{a} \in \{\mathbf{a}_1, \mathbf{a}_2\}$. Notice that we only need to sum over terms of the form involving $\mathbf{R} + \mathbf{a}$ and not $\mathbf{R} - \mathbf{a}$. If we were to include those terms, we would double-count all each of the possible transitions. In order to diagonalize eq. (3.1) we use the familiar Fourier transform but here we apply it as a vector change of coordinates,

$$|\mathbf{R}\rangle = \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k} | \mathbf{R} \rangle$$

Where $\langle \mathbf{k} | \mathbf{R} \rangle$ is normalized in the usual fashion,

$$\langle \mathbf{k} | \mathbf{R} \rangle = \frac{1}{\sqrt{N}} e^{i\mathbf{k} \cdot \mathbf{R}}$$

Therefore,

$$|\mathbf{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} |\mathbf{k}\rangle e^{i\mathbf{k} \cdot \mathbf{R}}$$

In the reciprocal lattice, \mathbf{k} can be written as,

$$\mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2$$

Where $k_{1,2}$ is bounded,

$$-\frac{1}{2} \leq k_{1,2} < \frac{1}{2}$$

Therefore,

$$\begin{aligned} \mathbf{k} \cdot \mathbf{R} &= (k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2) \cdot (n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2) \\ \mathbf{k} \cdot \mathbf{R} &= 2\pi(k_1 n_1 + k_2 n_2) \end{aligned}$$

Using the $|\mathbf{k}\rangle$ basis, eq. (3.1) becomes,

$$H = -t \sum_{\mathbf{R}, \mathbf{a}} \sum_{\mathbf{k}, \mathbf{k}'} \left(|\mathbf{k}\rangle \langle \mathbf{k}'| e^{-i\mathbf{k} \cdot (\mathbf{R} + \mathbf{a})} e^{i\mathbf{k}' \cdot \mathbf{R}} + |\mathbf{k}\rangle \langle \mathbf{k}'| e^{-i\mathbf{k} \cdot \mathbf{R}} e^{i\mathbf{k}' \cdot (\mathbf{R} + \mathbf{a})} \right) \quad (3.2)$$

Using a multi-dimensional version of eq. (1.4),

$$\frac{1}{N} \sum_{\mathbf{R}} e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}} = \delta_{\mathbf{k}, \mathbf{k}'}$$

Therefore eq. (3.1) becomes,

$$H = -t \sum_{\mathbf{k}, \mathbf{a}} |\mathbf{k}\rangle \langle \mathbf{k}| (e^{-i\mathbf{k} \cdot \mathbf{a}} + e^{i\mathbf{k} \cdot \mathbf{a}})$$

Recognize a cosine term,

$$H = -2t \sum_{\mathbf{k}, \mathbf{a}} |\mathbf{k}\rangle \langle \mathbf{k}| \cos(\mathbf{k} \cdot \mathbf{a})$$

The energy levels (as indexed by \mathbf{k}) can now be read off easily,

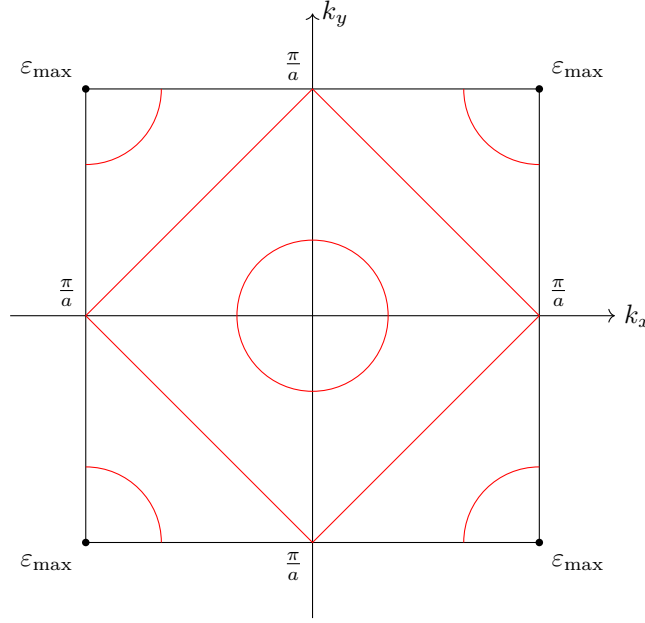
$$\varepsilon(\mathbf{k}) = -2t \sum_{\mathbf{a}} \cos(\mathbf{k} \cdot \mathbf{a}) = -2t [\cos(k_x a) + \cos(k_y a)]$$

Clearly, $\varepsilon(\mathbf{k})$ has minimum when $k_x = k_y = 0$. Therefore,

$$\min\{\varepsilon(\mathbf{k})\} = \varepsilon_{\min} = -4t$$

Likewise at the Brillouin zone corners,

$$\max\{\varepsilon(\mathbf{k})\} = \varepsilon_{\max} = 4t$$



Expanding \mathbf{k} near the minimum,

$$\varepsilon(\mathbf{k}) \simeq -4t + ta^2(k_x^2 + k_y^2) = -4t + ta^2k^2 \quad (3.3)$$

Notice that this looks like the dispersion of a free electron. Recall that for a free electron,

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$$

Therefore we can define an effective mass m^* as follows,

$$\varepsilon(\mathbf{k}) - \varepsilon_{\min} = ta^2k^2 = \frac{\hbar^2 k^2}{2m^*}$$

Where the effective mass is,

$$m^* = \frac{\hbar^2}{2ta^2}$$

In conclusion, electrons near the minimum energy level ε_{\min} behave like free particles with effective mass m^* .

The Fermi surface in this model can be calculated by setting $\varepsilon(\mathbf{k}) = \varepsilon_F$,

$$\varepsilon(\mathbf{k}) = -4t + \frac{\hbar^2 k^2}{2m^*} = \varepsilon_F$$

Therefore,

$$\frac{\hbar^2 k^2}{2m^*} = \varepsilon_F - \varepsilon_{\min}$$

Defines the equation of a circle in k_x, k_y space with radius,

$$k_F = \sqrt{\frac{2m^*}{\hbar^2}(\varepsilon_F - \varepsilon_{\min})}$$

Recall from eq. (3.3) that this equation only defines the Fermi surface near the minimum energy level. In general,

$$\varepsilon(\mathbf{k}) = -2t(\cos(k_x a) + \cos(k_y a))$$

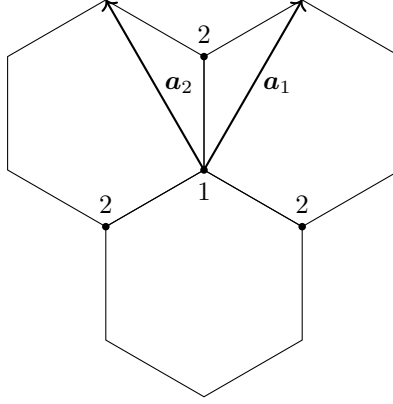
For a half-filled band, $\varepsilon_F = 0$, the Fermi surface is depicted above.

3.3 Graphene

The primitive unit vectors for Graphene are,

$$\mathbf{a}_1 = \frac{a}{2}(\hat{x} + \sqrt{3}\hat{y}) \quad \mathbf{a}_2 = \frac{a}{2}(-\hat{x} + \sqrt{3}\hat{y}) \quad (3.4)$$

Whereas the reciprocal lattice is,



$$\mathbf{b}_1 = \frac{2\pi}{a}(\hat{x} + \sqrt{3}\hat{y}) \quad \mathbf{b}_2 = \frac{2\pi}{a}(-\hat{x} + \sqrt{3}\hat{y}) \quad (3.5)$$

The nearest neighbor Hamiltonian becomes,

$$H = -t \sum_{\mathbf{R}} (|\mathbf{R}, 2\rangle\langle\mathbf{R}, 1| + |\mathbf{R} - \mathbf{a}_1, 2\rangle\langle\mathbf{R}, 1| + |\mathbf{R} - \mathbf{a}_2, 2\rangle\langle\mathbf{R}, 1| + \text{h.c.}) \quad (3.6)$$

In the reciprocal lattice,

$$|\mathbf{R}, \alpha\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} |\mathbf{k}, \alpha\rangle e^{-i\mathbf{k} \cdot \mathbf{R}}$$

Therefore the Hamiltonian becomes,

$$H = -\frac{t}{N} \sum_{\mathbf{R}} \sum_{\mathbf{K}, \mathbf{K}'} \left(|\mathbf{k}, 2\rangle\langle\mathbf{k}, 1| e^{-i\mathbf{k} \cdot \mathbf{R}} e^{i\mathbf{k}' \cdot \mathbf{R}} + |\mathbf{k}, 2\rangle\langle\mathbf{k}, 1| e^{-i\mathbf{k} \cdot (\mathbf{R} - \mathbf{a}_1)} e^{i\mathbf{k}' \cdot \mathbf{R}} + |\mathbf{k}, 2\rangle\langle\mathbf{k}, 1| e^{-i\mathbf{k} \cdot (\mathbf{R} - \mathbf{a}_2)} e^{i\mathbf{k}' \cdot \mathbf{R}} + \text{h.c.} \right)$$

$$H = -t \sum_{\mathbf{k}} [|\mathbf{k}, 2\rangle\langle\mathbf{k}, 1| (1 + e^{i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot \mathbf{a}_2}) + |\mathbf{k}, 1\rangle\langle\mathbf{k}, 2| (1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{-i\mathbf{k} \cdot \mathbf{a}_2})]$$

We have now diagonalized H in terms of the momentum wave-vector index \mathbf{k} . Letting $H = \sum_{\mathbf{k}} H(\mathbf{k})$ where,

$$H(\mathbf{k}) = -t [|\mathbf{k}, 2\rangle\langle\mathbf{k}, 1| (1 + e^{i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot \mathbf{a}_2}) + |\mathbf{k}, 1\rangle\langle\mathbf{k}, 2| (1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{-i\mathbf{k} \cdot \mathbf{a}_2})]$$

Invoking pseudo-spin states $|1\rangle = |\uparrow\rangle$ and $|2\rangle = |\downarrow\rangle$ we can write,

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

Where $\mathbf{d}(\mathbf{k})$ is,

$$\begin{aligned} d^x(\mathbf{k}) &= -t[1 + \cos(\mathbf{k} \cdot \mathbf{a}_1) + \cos(\mathbf{k} \cdot \mathbf{a}_2)] \\ d^y(\mathbf{k}) &= -t[\sin(\mathbf{k} \cdot \mathbf{a}_1) + \sin(\mathbf{k} \cdot \mathbf{a}_2)] \\ d^z(\mathbf{k}) &= 0 \end{aligned}$$

The eigenvalues of $H(\mathbf{k})$ are then the usual,

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

Since we have 1 electron per carbon atom, there are 2 electrons per unit cell which means that the ε_- band is completely filled while the ε_+ is empty. For this configuration, the conduction band is empty and thus graphene is an insulator.

In order to analyze the electronic structure of graphene, we need to rewrite \mathbf{k} which is expressed via the reciprocal lattice vectors $\mathbf{b}_1, \mathbf{b}_2$ in terms of the Cartesian vectors $\mathbf{a}_1, \mathbf{a}_2$.

$$\mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2$$

$$\mathbf{k} \cdot \mathbf{a}_1 = (k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2) \cdot \mathbf{a}_1 = 2\pi k_1 \quad \mathbf{k} \cdot \mathbf{a}_2 = 2\pi k_2$$

Recalling eqs. (3.4) and (3.5),

$$\mathbf{a}_1 = \frac{a}{2} (\hat{x} + \sqrt{3}\hat{y}) \quad \mathbf{a}_2 = \frac{a}{2} (-\hat{x} + \sqrt{3}\hat{y})$$

$$\mathbf{b}_1 = \frac{2\pi}{a} (\hat{x} + \sqrt{3}\hat{y}) \quad \mathbf{b}_2 = \frac{2\pi}{a} (-\hat{x} + \sqrt{3}\hat{y})$$

We can now write k_x, k_y in terms of k_1, k_2 ,

$$k_x = \frac{2\pi}{\sqrt{3}a} (k_1 - k_2) \quad k_y = \frac{2\pi}{\sqrt{3}a} (k_1 + k_2)$$

Inverting this system gives,

$$k_1 = \frac{a}{4\pi} (k_x + \sqrt{3}k_y) \quad k_2 = \frac{a}{4\pi} (-k_x + \sqrt{3}k_y)$$

Therefore,

$$\begin{aligned} d^x(\mathbf{k}) &= -t[1 + \cos(2\pi k_1) + \cos(2\pi k_2)] \\ &= -t \left[1 + 2 \cos\left(\frac{k_x a}{2}\right) + \cos\left(\frac{\sqrt{3}k_y a}{2}\right) \right] \end{aligned}$$

Similarly for $d^y(\mathbf{k})$,

$$d^y(\mathbf{k}) = 2t \cos\left(\frac{k_x a}{2}\right) \sin\left(\frac{\sqrt{3}k_y a}{2}\right)$$

By examining these equations it can be seen that there are two points (and only two points) in the first Brillouin zone where both d^x and d^y vanish simultaneously. We label these points as \mathbf{k}_{\pm} ,

$$\mathbf{k}_+ = (k_{+,x}, k_{+,y}) = \left(\frac{4\pi}{3a}, 0\right)$$

$$\mathbf{k}_- = (k_{-,x}, k_{-,y}) = \left(-\frac{4\pi}{3a}, 0\right)$$

At either of these points,

$$|\mathbf{d}(\mathbf{k}_{\pm})| = \sqrt{d^x{}^2(\mathbf{k}) + d^y{}^2(\mathbf{k})} = 0$$

Therefore, the gap between the ε_+ band and the ε_- closes at only two points. Since graphene is an insulator and does not have a Fermi surface (meaning its not *not* a metal) we refer to graphene, and materials that share these features, as **semimetals**.

Recalling eq. (3.5) again,

$$\mathbf{b}_1 = \frac{2\pi}{a} (\hat{x} + \sqrt{3}\hat{y}) \quad \mathbf{b}_2 = \frac{2\pi}{a} (-\hat{x} + \sqrt{3}\hat{y})$$

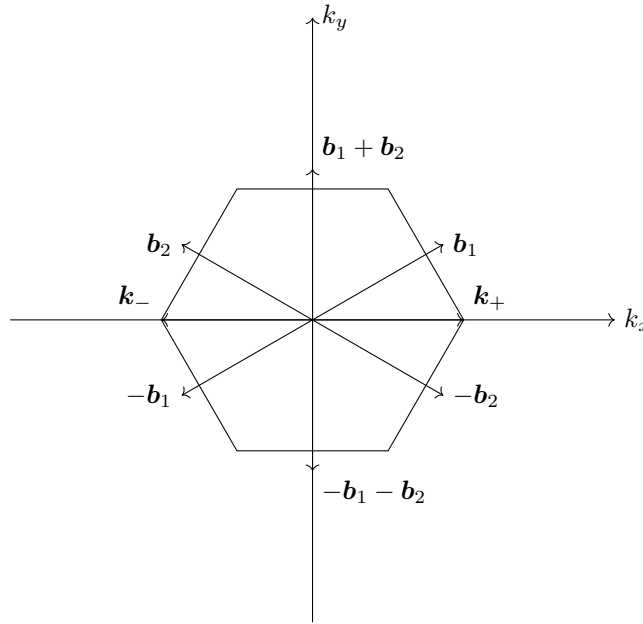
We can compute the lengths of \mathbf{b}_1 and \mathbf{b}_2 ,

$$|\mathbf{b}_1| = |\mathbf{b}_2| = \frac{2\pi}{a} \sqrt{1 + \frac{1}{3}} = \frac{4\pi}{\sqrt{3}a}$$

Therefore \mathbf{b}_1 makes an angle of $\theta = \pi/6$ with the x -axis,

$$\cos \theta = \frac{\mathbf{b}_1 \cdot \hat{x}}{|\mathbf{b}_1|} = \frac{\frac{2\pi}{a}}{\frac{4\pi}{\sqrt{3}a}} = \frac{\sqrt{3}}{2} \implies \theta = \frac{\pi}{6}$$

We are now able to plot the first Brillouin zone.



The first Brillouin zone for graphene forms a hexagonal lattice with the corners obtained from \mathbf{k}_\pm by adding $\pm \mathbf{b}_1, \pm \mathbf{b}_2$,

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2$$

In graphene, the upper and lower band are *not* separated by a band gap (sometimes $\varepsilon_+ > \varepsilon_-$ and sometimes $\varepsilon_+ < \varepsilon_-$). The crossing points are precisely the two points where $\mathbf{k} = \mathbf{k}_\pm$. If we expand $H(\mathbf{k})$ near \mathbf{k}_\pm to first order,

$$k_x = k_{x,\pm} + \delta k_x \quad k_y = k_{y,\pm} + \delta k_y$$

To first order,

$$d^x_\pm(\delta \mathbf{k}) \simeq \pm \frac{\sqrt{3}}{2} t a \delta k_x$$

$$d^y_\pm(\delta \mathbf{k}) \simeq \pm \frac{\sqrt{3}}{2} t a \delta k_y$$

For both the x and y directions, the leading coefficient $\frac{\sqrt{3}}{2} t a$ has units of speed times \hbar . We again call this the Fermi velocity,

$$v_F = \frac{\sqrt{3} t a}{2 \hbar}$$

Then we can write the Hamiltonian as,

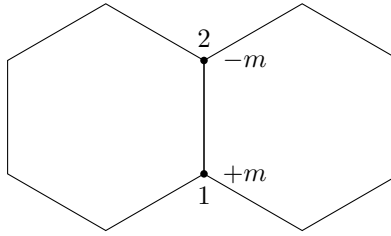
$$H_{\pm}(\mathbf{k}) = \hbar v_F(\pm k_x \sigma^x + k_y \sigma^y) \quad (3.7)$$

Where here k_x and k_y refer to δk_x and δk_y . This is done by shifting coordinates such that $\mathbf{k}_{\pm} = 0$ for each of the $+$, $-$ cases. Upon examination of eq. (3.7), eq. (3.7) takes the form of a 2D Dirac Hamiltonian for a massless relativistic particle in 2D. The energies near the touching points \mathbf{k}_{\pm} is,

$$\varepsilon(\mathbf{k}) = \pm \hbar v_F k$$

Where $k = \sqrt{k_x^2 + k_y^2}$. This means that $\varepsilon(\mathbf{k})$ has linear dispersion near \mathbf{k}_{\pm} .

One question we can ask is what can we do to graphene in order to open a gap between \mathbf{k}_{-} and \mathbf{k}_{+} . In order words, how can we give the electron in eq. (3.7) an effective mass. This can be accomplished by introducing a discrepancy between the atoms labeled 1 and the atoms labeled 2 within a unit cell. As an example, we can add energies $\pm m$ to the atoms as follows,



Which effectively corresponds to adding the following term to the original Hamiltonian,

$$H' = m \sum_{\mathbf{R}} (|\mathbf{R}, 1\rangle \langle \mathbf{R}, 1| - |\mathbf{R}, 2\rangle \langle \mathbf{R}, 2|)$$

Applying the Fourier transform yields the following,

$$H' = m \sum_{\mathbf{k}} (|\mathbf{k}, 1\rangle \langle \mathbf{k}, 1| - |\mathbf{k}, 2\rangle \langle \mathbf{k}, 2|)$$

Which further adjusts the dispersion relationship,

$$H'(\mathbf{k}) = m(|1\rangle \langle 1| - |2\rangle \langle 2|) = m\sigma^z$$

Therefore,

$$H_{\pm}(\mathbf{k}) = \hbar v_F(\pm k_x \sigma^x + k_y \sigma^y) + m\sigma^z$$

$$\varepsilon_{\pm}(\mathbf{k}) = \pm \sqrt{\hbar^2 v_F^2 k^2 + m^2}$$

This opens up a band gap of size $2m$. Therefore clean graphene ($m = 0$) is a semimetal due to inversion symmetry but becomes an insulator for $m > 0$.

Returning to the case of $m = 0$,

$$H_{\pm}(\mathbf{k}) = \hbar v_F(\pm k_x \sigma^x + k_y \sigma^y)$$

The ' \pm ' can be thought of as a two component degree of freedom. Because there are two components, we can think of ' \pm ' as another pseudo-spin value τ .

$$\tau^z = |+\rangle \langle +| - |-\rangle \langle -|$$

$$\tau^y = -i(|+\rangle \langle -| - |-\rangle \langle +|)$$

$$\tau^x = |+\rangle \langle -| + |-\rangle \langle +|$$

Which means that the Hamiltonian can be written without the ' \pm ' as a single matrix,

$$H(\mathbf{k}) = \hbar v_F(k_x \tau^z \sigma^x + k_y \sigma^y) \quad (3.8)$$

What are the symmetries of eq. (3.8). We must have the following:

1. Time Reversal Symmetry
2. Inversion Symmetry

In order to facilitate discussions, we introduce two operators; the **inversion (parity) operator** π and **time-reversal operator** Θ . The symmetries of eq. (3.8) can be written,

$$\pi^\dagger H(\mathbf{k})\pi = H(\mathbf{k}) \quad (3.9)$$

$$\Theta H(\mathbf{k})\Theta^{-1} = H(\mathbf{k}) \quad (3.10)$$

Since τ^z refers to the two band touching points (coordinates in momentum space), τ^z changes sign under both symmetries,

$$\pi^\dagger \tau^z \pi = -\tau^z \quad (3.11)$$

$$\Theta \tau^z \Theta^{-1} = -\tau^z \quad (3.12)$$

Furthermore, $k_{x,y,z}$ represent momentum and is thus time and parity odd,

$$\pi^\dagger k_{x,y,z} \pi = -k_{x,y,z}$$

$$\Theta k_{x,y,z} \Theta^{-1} = -k_{x,y,z}$$

Therefore we must conclude that σ^x is even under these symmetries and σ^y is odd pursuant to eqs. (3.9) and (3.10),

$$\pi^\dagger \sigma^y \pi = -\sigma^y$$

$$\Theta \sigma^y \Theta^{-1} = -\sigma^y$$

$$\pi^\dagger \sigma^x \pi = +\sigma^x$$

$$\Theta \sigma^x \Theta^{-1} = +\sigma^x$$

This is intuitive because σ refers to the spatial location of atoms 1 and 2 oriented in the y direction. If we were to include the massive term $m\sigma^z$ we break symmetry in eqs. (3.9) and (3.10),

$$\pi^\dagger \sigma^z \pi = -\sigma^z \quad \Theta \sigma^z \Theta^{-1} = \sigma^z \quad (3.13)$$

Specifically, $m\sigma^z$ breaks inversion symmetry. This is intuitive because m adds spatial discrepancies between 1 and 2. Can we open a gap in graphene without breaking time-reversal or inversion symmetries?

Interestingly, this lack of symmetry is an artifact of the simplistic model introduced by eq. (3.6). If we include *next-nearest neighbor* terms, it is possible to recover symmetries. Upon examination of eq. (3.13) and eqs. (3.11) and (3.12) we find that $\tau^z \sigma^z$ is invariant under inversion,

$$\pi^\dagger \tau^z \sigma^z \pi = \tau^z \sigma^z$$

But $\tau^z \sigma^z$ is not invariant under time-reversal,

$$\Theta \tau^z \sigma^z \Theta^{-1} = -\tau^z \sigma^z$$

Other component that is missing from our model is the real spin of the electron (not pseudo-spin) \mathbf{S} . Spin \mathbf{S} is parity even and time-reversal odd,

$$\pi^\dagger \mathbf{S} \pi = \mathbf{S} \quad \Theta \mathbf{S} \Theta^{-1} = -\mathbf{S}$$

$$S^z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|$$

$$S^x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$$

Upon adding this term, $\tau^z \sigma^z S^z$ maintains the desired symmetries,

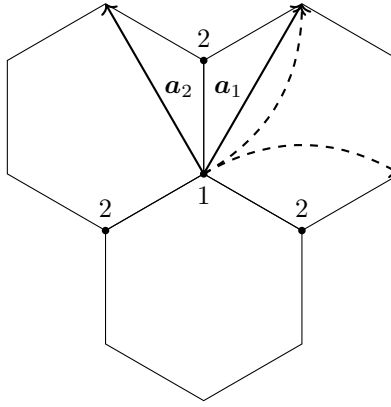
$$\pi^\dagger \tau^z \sigma^z S^z \pi = \tau^z \sigma^z S^z \quad \Theta \tau^z \sigma^z S^z \Theta^{-1} = \tau^z \sigma^z S^z$$

This was discovered by Kane and Mele (2005) and their paper gave rise to the field of topological insulators. Therefore the true graphene Hamiltonian can be written as,

$$H(\mathbf{k}) = \hbar v_F (k_x \tau^z \sigma^x + k_y \sigma^y) + \Delta_{\text{SO}} \tau^z \sigma^z S^z \quad (3.14)$$

Where Δ_{SO} is referred to as the **spin-orbit interaction**. The origin of the Δ_{SO} term is due to the following process. When the valence electrons have the ability to tunnel between atoms, some of the atoms in the crystal lattice become ionized. The electric field of ionized atoms is felt as a magnetic field in the rest frame of the electrons. Effectively this magnetic field has strength $\mathbf{B} = \mathbf{v} \times \mathbf{E}/c$ which tends to be small as $B \propto c^{-1}$. Additionally, \mathbf{E} grows for heavier and heavier atoms. This magnetic field acts on the spin in the usual manner $H \propto \mathbf{B} \cdot \mathbf{S}$. This is encapsulated in eq. (3.14) as $\tau^z \sigma^z$ is coupled with the spin S^z .

In order to formally introduce the $\Delta_{\text{SO}} \tau^z \sigma^z S^z$ term into the Hamiltonian, we need to include next nearest-neighbor tunneling ($1 \rightarrow 1$ and $2 \rightarrow 2$ tunneling),



The additional terms to eq. (3.6) can be expressed as,

$$H = \dots - it' (|\mathbf{R} + \mathbf{a}_1 - \mathbf{a}_2, 1\rangle \langle \mathbf{R}, 1| - |\mathbf{R}, 1\rangle \langle \mathbf{R} + \mathbf{a}_1 - \mathbf{a}_2, 1|) \dots$$

Which has tunneling amplitude it' . The intermediate negative sign is due to the tunneling amplitude being imaginary which switches signs under conjugation.