Phys 435

TOPICS IN CONDENSED MATTER

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Disclaimer

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1 Toy Model of a Solid

Todo (TC Fraser): Type up notes for first class
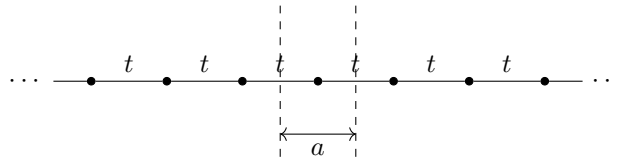
Thus far we have been discussing a toy model of a solid in one dimension. By diagonalizing the Hamiltonian we were able to determine the energy levels of the various states,

$$\varepsilon(k) = -2t\cos(ka) \tag{1.1}$$

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,

$$k = \frac{2\pi m}{Na} \qquad m = 0, \pm 1, \pm 2, \ldots$$

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,

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

The interval has a width of $\varepsilon_{\max} - \varepsilon_{\min} = 4t$ and is referred to as the allowed energy *band*.
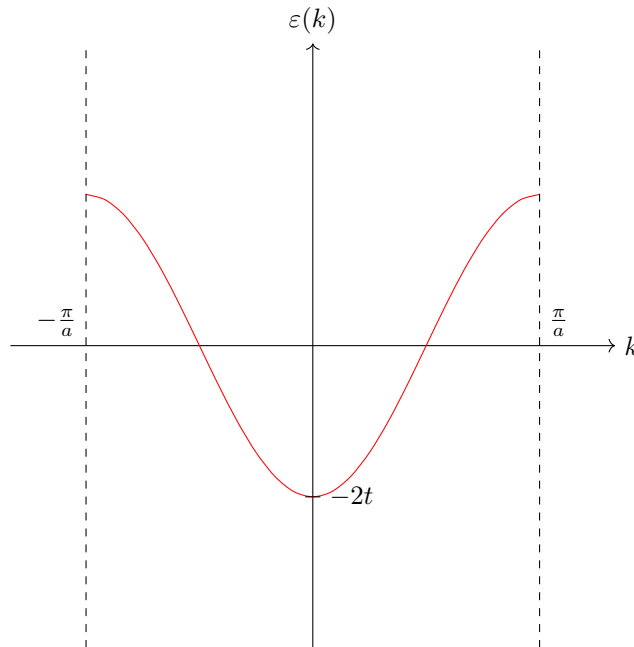
How many states does the band contain. Given that k is discrete and bounded,

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

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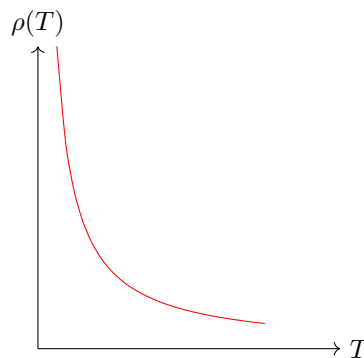
When the electrons occupy all of the lowest possible energy states, we fill all of the negative energy states and the positive energy states remain vacant. This separation defines the **Fermi energy** for this system where occurs at $\varepsilon_F = 0$. In order to find the state that corresponds to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

$$C : 1s^2 2s^2 2p^2 \qquad 4 \text{ valence electrons}$$
$$H : 1s^1$$

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.
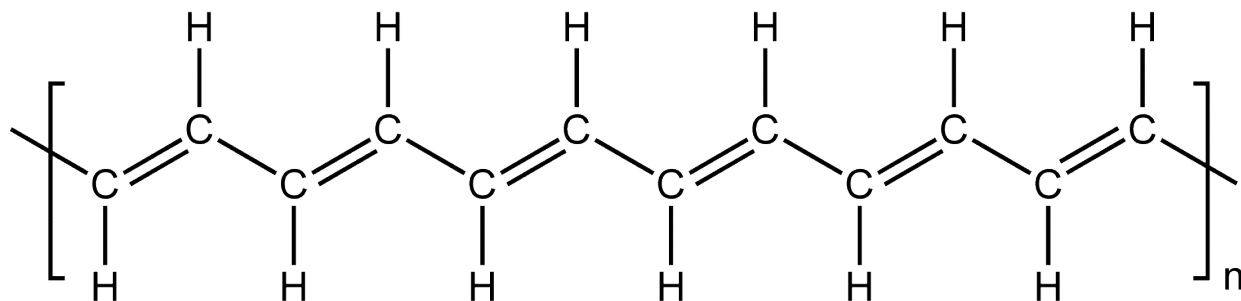
Three of the valence electrons are engaged in bonding with neighboring carbon and hydrogen atoms while the 4-th one is free to move around. As it turns out, the bonds between carbon atoms possess alternating tunneling amplitudes.
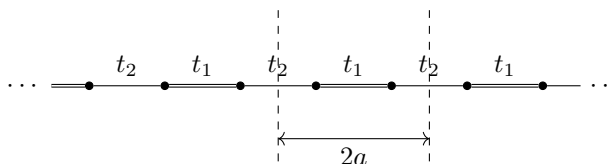
In Polyacetylene, the tunneling amplitude between the carbon atoms joined by a double bound is slightly higher $t_1 > t_2$. This is referred to as **Peierls instability**.

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

$$t_1 = t + \delta t \qquad t_2 = t - \delta t \tag{1.2}$$

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,

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

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

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

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

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

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.

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

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

$$H(k) = -t_1\{|2\rangle\langle 1| + |1\rangle\langle 2|\}$$
$$- t_2\{|2\rangle\langle 1|e^{2ika} + |1\rangle\langle 2|e^{-2ika}\} \tag{1.6}$$

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,

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

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

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

We have that,

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

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

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

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

$$d_x(k) = -(t + \delta t) - (t - \delta t)\cos(2ka)$$
$$d_y(k) = -(t - \delta t)\sin(2ka) \tag{1.8}$$
$$d_z(k) = 0$$

Where $\boldsymbol{d}$ can be written,

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

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,

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

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

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

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:

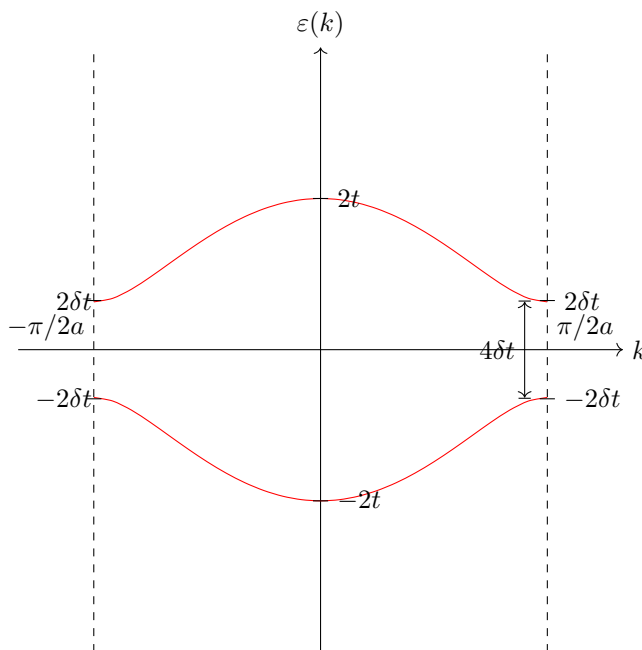*Every atom in the unit cell will give rise to a separate band.*

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

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

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 $\delta t \to 0$ one should expect to recover eq. (1.1),

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

As expected. Notice however the plot of $\epsilon(k)$ differs,
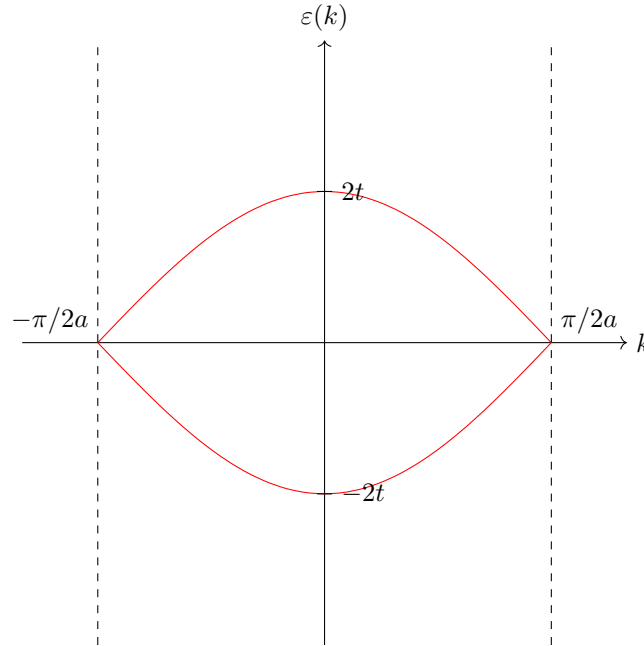
The resolution between these two plots is to notice that in the polyacetylene model, the unit cell had with $2a$ instead of a. Therefore in momentum space, the plotted values for k are bounded by $-\pi/2a \leq k \leq \pi/2a$ instead of $-\pi/a \leq k \leq \pi/a$. If one were to unravel the upper band into regions where $|k| > \pi/2a$ one would recover the initial model.
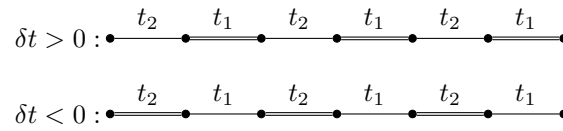
Heretofore, we have assumed that $\delta t > 0$. If however we consider $\delta t < 0$, then we transition from $t_1 > t_2$ to $t_2 > t_1$ pursuant to eq. (1.2). And our diagram is adjusted

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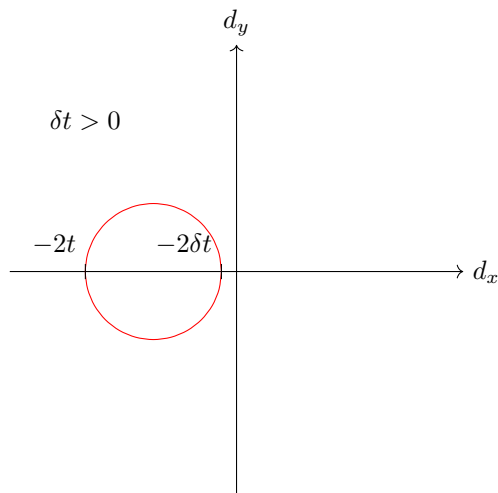
It can be seen that when $\delta t > 0$, the curve in d_x, d_y does not enclose the origin $\boldsymbol{d} = 0$. Recalling that $\varepsilon_\pm(k) = \pm|\boldsymbol{d}(k)|$, as long as $\boldsymbol{d}(k) \neq 0$, there exists a energy gap between the two bands ε_+ and ε_-. Therefore for $\delta t >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

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

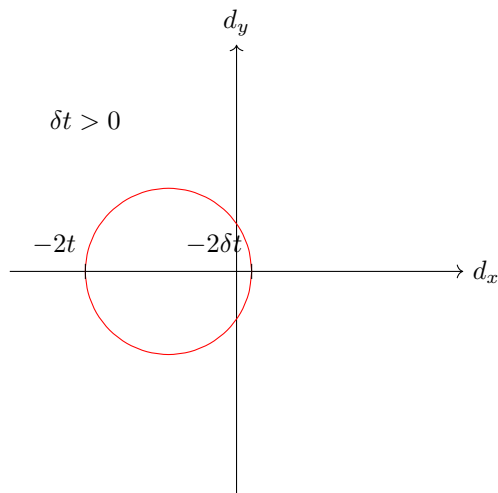Effectively, there is no possible way to continuously deform the Hamiltonian (i.e. changing δt) without merging the two energy bands.

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 $H(k) = \boldsymbol{d}(k) \cdot \boldsymbol{\sigma}$ can be expanded out explicitly,

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

$$= -(t + \delta t) + (t - \delta t) + \mathcal{O}\left((\delta k)^2\right)$$
$$\simeq -2\delta t$$

Similarly for d_y,

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

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 use rename a number of terms,

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

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. These 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 $p \to -i\hbar\partial_x$ 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,

$$|z\rangle = z_\uparrow|\uparrow\rangle + z_\downarrow|\downarrow\rangle$$
$$\sigma_z|\uparrow\rangle = +|\uparrow\rangle \qquad \sigma_z|\downarrow\rangle = -|\downarrow\rangle$$

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

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

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

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

Adjusting the constant coefficients,

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

Therefore,

$$\frac{\mathrm{d}f}{\mathrm{d}x} = -\frac{m(x)}{\hbar v_F}$$

Can be solved using,

$$f(x) = -\frac{1}{\hbar v_F}\int\limits_0^x \mathrm{d}x'm(x')$$

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

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

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

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

$$x = 0$$

$$\begin{array}{ll} \delta t < 0 & \delta t > 0 \\ m < 0 & m > 0 \end{array}$$
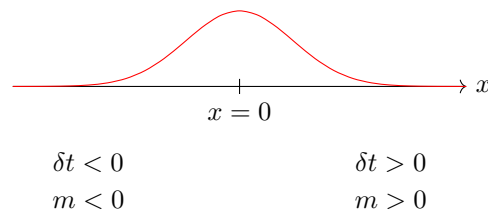
2   Higher Dimensions

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

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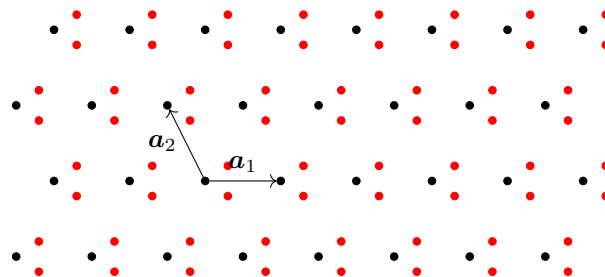
A **Bravais lattice** is all points in $\mathbb{R}^3$ ($\mathbb{R}^2, \mathbb{R}^1, \mathbb{R}^n$) such that,

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

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

$$n_1, n_2, n_3 = 0, \pm1, \pm2, \pm3, \ldots$$

Typically, the choice for $\boldsymbol{a}_i$ 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

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

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

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

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

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

Where the reciprocal lattice is defined such that,

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

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

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

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

3.2 Electronic Structure for Square Lattice

The square lattice in 2 dimensions has two primitive basis vectors $\boldsymbol{a}_1, \boldsymbol{a}_2$,
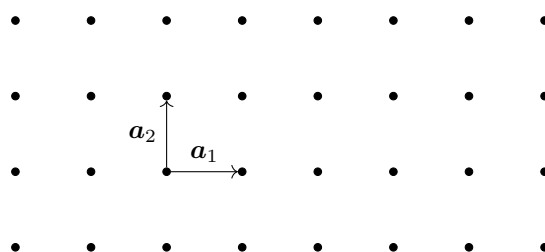
Using Cartesian coordinates,

$$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}} \qquad \boldsymbol{a}_2 = a\hat{\boldsymbol{y}}$$

The reciprocal lattice has the following form,

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\hat{\boldsymbol{x}} \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\hat{\boldsymbol{y}}$$

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

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

Where $\boldsymbol{a} \in \{\boldsymbol{a}_1, \boldsymbol{a}_2\}$. Notice that we only need to sum over terms of the form involving $\boldsymbol{R} + \boldsymbol{a}$ and not $\boldsymbol{R} - \boldsymbol{a}$. 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,

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

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

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

Therefore,

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

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

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

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

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

Therefore,

$$\boldsymbol{k} \cdot \boldsymbol{R} = (k_1 \boldsymbol{b}_1 + k_2 \boldsymbol{b}_2) \cdot (n_1 \boldsymbol{a}_1 + n_2 \boldsymbol{a}_2)$$
$$\boldsymbol{k} \cdot \boldsymbol{R} = 2\pi(k_1 n_1 + k_2 n_2)$$

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

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

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

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

Therefore eq. (3.1) becomes,

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

Recognize a cosine term,

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

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

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

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

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

Likewise at the Brillouin zone corners,

$$\max\{\varepsilon(\boldsymbol{k})\} = \varepsilon_{\max} = 4t$$
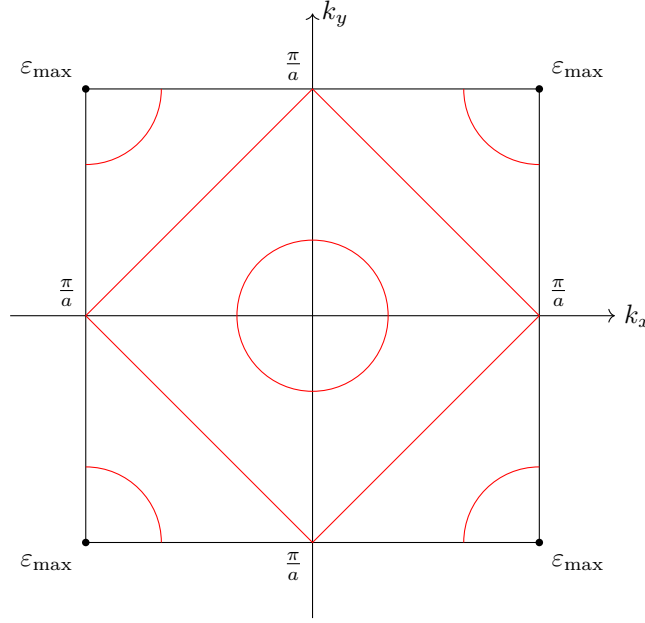
Expanding $\boldsymbol{k}$ near the minimum,

$$\varepsilon(\boldsymbol{k}) \simeq -4t + ta^2\left(k_x^2 + k_y^2\right) = -4t + ta^2 k^2 \tag{3.3}$$

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

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

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

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

Where the effective mass is,

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

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

The Fermi surface in this model can be calculated by setting $\varepsilon(\boldsymbol{k}) = \varepsilon_{\mathrm{F}}$,

$$\varepsilon(\boldsymbol{k}) = -4t + \frac{\hbar^2 k^2}{2m^*} = \varepsilon_{\mathrm{F}}$$

Therefore,

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

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

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

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

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

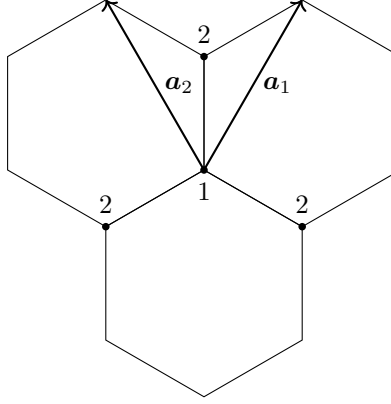For a half-filled band, $\varepsilon_{\mathrm{F}} = 0$, the Fermi surface is depicted above.

3.3   Graphene

The primitive unit vectors for Graphene are,

$$\boldsymbol{a}_1 = \frac{a}{2}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{a}_2 = \frac{a}{2}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \tag{3.4}$$

Whereas the reciprocal lattice is,

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \tag{3.5}$$

The nearest neighbor Hamiltonian becomes,

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

In the reciprocal lattice,

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

Therefore the Hamiltonian becomes,

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

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

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

$$H(\boldsymbol{k}) = -t\left[|2\rangle\langle1|\left(1 + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{i\boldsymbol{k}\cdot\boldsymbol{a}_2}\right) + |1\rangle\langle2|\left(1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_1} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a}_2}\right)\right]$$

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

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

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

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

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

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

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 $\boldsymbol{k}$ which is expressed via the reciprocal lattice vectors $\boldsymbol{b}_1, \boldsymbol{b}_2$ in terms of the Cartesian vectors $\boldsymbol{a}_1, \boldsymbol{a}_2$.

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

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

Recalling eqs. (3.4) and (3.5),

$$\boldsymbol{a}_1 = \frac{a}{2}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{a}_2 = \frac{a}{2}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right)$$

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right)$$

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

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

Inverting this system gives,

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

Therefore,

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

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

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

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 $\boldsymbol{k}_{\pm}$,

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

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

At either of these points,

$$|\boldsymbol{d}(\boldsymbol{k}_{\pm})| = \sqrt{d^{x2}(\boldsymbol{k}) + d^{y2}(\boldsymbol{k})} = 0$$

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,

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right)$$

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

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

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

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

We are now able to plot the first Brillouin zone.
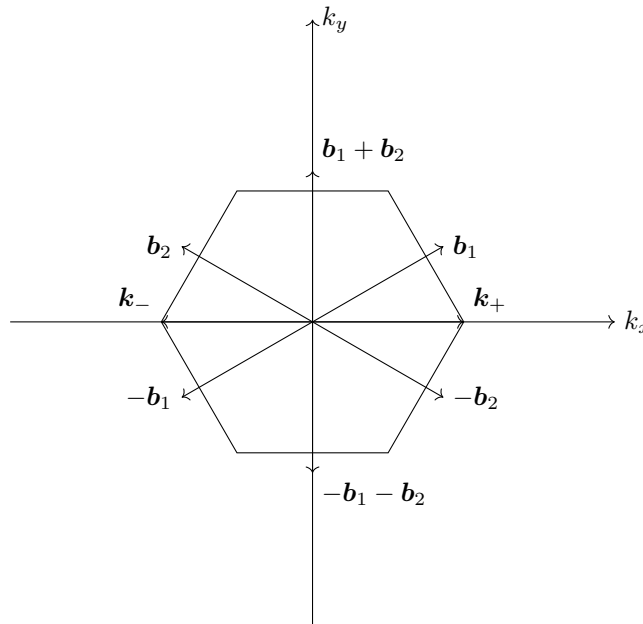
The first Brillouin zone for graphene forms a hexagonal lattice with the corners obtained from $\boldsymbol{k}_\pm$ by adding $\pm b_1, \pm b_2$,

$$\boldsymbol{G} = m_1\boldsymbol{b}_2 + m_2\boldsymbol{b}_2$$

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 $\boldsymbol{k} = \boldsymbol{k}_\pm$. If we expand $H(\boldsymbol{k})$ near $\boldsymbol{k}_\pm$ to first order,

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

To first order,

$$d_\pm^x(\delta\boldsymbol{k}) \simeq \pm\frac{\sqrt{3}}{2}ta\delta k_x$$

$$d_\pm^y(\delta\boldsymbol{k}) \simeq \pm\frac{\sqrt{3}}{2}ta\delta k_y$$

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

$$v_{\mathrm{F}} = \frac{\sqrt{3}ta}{2\hbar}$$

Then we can write the Hamiltonian as,

$$H_\pm(\boldsymbol{k}) = \hbar v_\mathrm{F}(\pm k_x \sigma^x + k_y \sigma^y) \tag{3.7}$$

Where here k_x and k_y refer to δk_x and δk_y. This is done by shifting coordinates such that $\boldsymbol{k}_\pm = 0$ 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 $\boldsymbol{k}_\pm$ is,

$$\varepsilon(\boldsymbol{k}) = \pm \hbar v_\mathrm{F} k$$

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

One question we can ask is what can we do to graphene in order to open a gap between $\boldsymbol{k}_-$ and $\boldsymbol{k}_+$. 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,
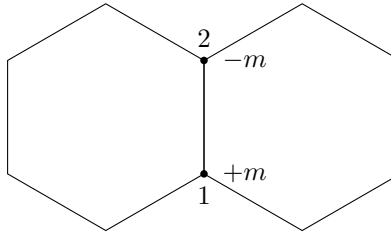
Which effectively corresponds to adding the following term to the original Hamiltonian,

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

Applying the Fourier transform yields the following,

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

Which further adjusts the dispersion relationship,

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

Therefore,

$$H_\pm(\boldsymbol{k}) = \hbar v_\mathrm{F}(\pm k_x \sigma^x + k_y \sigma^y) + m\sigma^z$$

$$\varepsilon_\pm(\boldsymbol{k}) = \pm\sqrt{\hbar^2 v_\mathrm{F} k^2 + m^2}$$

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 $m = 0$,

$$H_\pm(\boldsymbol{k}) = \hbar v_\mathrm{F}(\pm k_x \sigma^x + k_y \sigma^y)$$

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,

$$H(\boldsymbol{k}) = \hbar v_\mathrm{F}(k_x \tau^z \sigma^x + k_y \sigma^y) \tag{3.8}$$

4   Spin-Orbit Interactions

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 we written,

$$\pi^\dagger H(\boldsymbol{k})\pi = H(\boldsymbol{k}) \tag{4.1}$$

$$\Theta H(\boldsymbol{k})\Theta^{-1} = H(\boldsymbol{k}) \tag{4.2}$$

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

$$\pi^\dagger \tau^z \pi = -\tau^z \tag{4.3}$$

$$\Theta \tau^z \Theta^{-1} = -\tau^z \tag{4.4}$$

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. (4.1) and (4.2),

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

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

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

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

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. (4.1) and (4.2),

$$\pi^\dagger \sigma^z \pi = -\sigma^z \qquad \Theta \sigma^z \Theta^{-1} = \sigma^z \tag{4.5}$$

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. (4.5) and eqs. (4.3) and (4.4) 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) $\boldsymbol{S}$. Spin $\boldsymbol{S}$ is parity even and time-reversal odd,

$$\pi^\dagger \boldsymbol{S} \pi = \boldsymbol{S} \qquad \Theta \boldsymbol{S} \Theta^{-1} = -\boldsymbol{S}$$

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

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

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

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

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,

$$H(\boldsymbol{k}) = \hbar v_\mathrm{F}(k_x\tau^z\sigma^x + k_y\sigma^y) + \Delta_\mathrm{SO}\tau^z\sigma^z S^z \tag{4.6}$$

Where Δ_SO is refered 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 $\boldsymbol{B} = \boldsymbol{v} \times \boldsymbol{E}/c$ which tends to be small as $B \propto c^{-1}$. Additionally, $\boldsymbol{E}$ grows for heavier and heavier atoms. This magnetic field acts on the spin in the usual manner $H \propto \boldsymbol{B}\cdot\boldsymbol{S}$. This is encapsulated in eq. (4.6) as $\tau^z\sigma^z$ is coupled with the spin S^z.

In order to formally introduce the $\Delta_\mathrm{SO}\tau^z\sigma^z S^z$ term into the Hamiltonian, we need to include next nearest-neighbor tunneling ($1 \rightarrow 1$ and $2 \rightarrow 2$ tunneling),
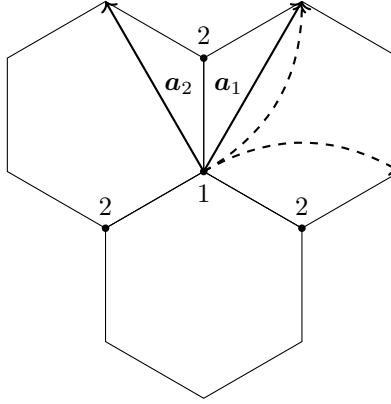
The additional terms to eq. (3.6) can be expressed as,

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

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

In order to study the effect Δ_SO in eq. (4.6), we will include a massive term $m\sigma^z$ and study the following,

$$H(\boldsymbol{k}) = \hbar v_\mathrm{F}(k_x\tau^z\sigma^x + k_y\sigma^y) + \Delta_\mathrm{SO}\tau^z\sigma^z S^z + m\sigma^z$$

Specifically for our analysis, we will look at the affect on $S^z = 1$ spin up ($\uparrow$) spins. The associated Hamiltonian for $S^z = 1$ has two bands $\tau^z = \pm 1$,

$$\{H(\boldsymbol{k})\}_{\tau^z=+1} \equiv H_+(\boldsymbol{k}) = \hbar v_\mathrm{F}(k_x\sigma^x + k_y\sigma^y) + (m + \Delta_\mathrm{SO})\sigma^z$$

$$\{H(\boldsymbol{k})\}_{\tau^z=-1} \equiv H_+(\boldsymbol{k}) = \hbar v_\mathrm{F}(-k_x\sigma^x + k_y\sigma^y) + (m - \Delta_\mathrm{SO})\sigma^z$$

Therefore the dispersion relations are distinct for each value of τ^z,

$$\{\varepsilon(\boldsymbol{k})\}_{\tau^z=+1} \equiv \varepsilon_+(\boldsymbol{k}) = \pm\sqrt{\hbar^2 v_\mathrm{F}^2\left(k_x^2 + k_y^2\right) + (m + \Delta_\mathrm{SO})^2}$$

$$\{\varepsilon(\boldsymbol{k})\}_{\tau^z=-1} \equiv \varepsilon_-(\boldsymbol{k}) = \pm\sqrt{\hbar^2 v_\mathrm{F}^2\left(k_x^2 + k_y^2\right) + (m - \Delta_\mathrm{SO})^2} \tag{4.7}$$

In the very large m limit $m \gg \Delta_{\text{SO}}$, the energy cost $(+m)$ for electrons being localized at sites of type 1 is much higher than the energy cost $(-m)$ associated with sites of type 2. Therefore all of the electrons will localize to sites of type 2. Therefore in this case, the electrons can not propagate between sites because the atoms of type 1 are in the way. We refer to these as **non-topological insulators** or sometimes *atomic* insulators.

In contrast to this, in the region where $m \approx \Delta_{\text{SO}}$ we have interesting behaviors for eq. (4.7). Since the band gap associated with the contribution from $\varepsilon_-(\boldsymbol{k})$ is $2|m - \Delta_{\text{SO}}|$, the band gap closes when m transitions between $m > \Delta_{\text{SO}}$ and $m < \Delta_{\text{SO}}$.

- $m > \Delta_{\text{SO}}$: Trivial insulator

- $m = \Delta_{\text{SO}}$: Transition point/semimetal

- $m < \Delta_{\text{SO}}$: Topological insulator

We have already seen this behavior for graphene in which $m = 0$ defined a semimetal, and $m > 0$ defined a topological insulator form of graphene. Recall the Hamiltonian of graphene had the following form,

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

The unit vector of $\boldsymbol{d}$ is,

$$\hat{\boldsymbol{d}}(\boldsymbol{k}) = \frac{\boldsymbol{d}(\boldsymbol{k})}{|\boldsymbol{d}(\boldsymbol{k})|}$$

Which can be thought of as a map from the first Brillouin zone ($\boldsymbol{k}$) to the surface of a unit sphere $\hat{\boldsymbol{d}}$. Interpreting the mappings in the way always one to understand the topological differences between ordinary and topological insulators.

Near the band touching points $\boldsymbol{k}_\pm$ we have,

$$\hat{\boldsymbol{d}}(\boldsymbol{k}_+) = \frac{(\hbar v_{\text{F}} k_x, \hbar v_{\text{F}} k_y, m + \Delta_{\text{SO}})}{\sqrt{\hbar^2 v_{\text{F}}^2 (\boldsymbol{k}_x^2 + \boldsymbol{k}_y^2) + (m + \Delta_{\text{SO}})^2}}$$

$$\hat{\boldsymbol{d}}(\boldsymbol{k}_-) = \frac{(-\hbar v_{\text{F}} k_x, \hbar v_{\text{F}} k_y, m - \Delta_{\text{SO}})}{\sqrt{\hbar^2 v_{\text{F}}^2 (\boldsymbol{k}_x^2 + \boldsymbol{k}_y^2) + (m + \Delta_{\text{SO}})^2}}$$

Clearly for the case of $m > \Delta_{\text{SO}}$,

$$\boldsymbol{d}(\boldsymbol{k}_-) \cdot \hat{\boldsymbol{z}} = m - \Delta_{\text{SO}} > 0$$

Therefore $d^z(\boldsymbol{k}_-)$ is always positive. This is also true for $d(\boldsymbol{k})$. Therefore $\boldsymbol{d}(\boldsymbol{k})$ only covers the *upper* hemisphere of the unit sphere as $\boldsymbol{k}$ covers the whole Brillouin zone.

In difference to this is the case for $m < \Delta_{\text{SO}}$. $d^z(\boldsymbol{k}_-)$ is always negative which means that $\hat{\boldsymbol{d}}(\boldsymbol{k})$ is able to cover the entire sphere.

Given this observation, we can define the following **topological invariant** that characterizes the difference between topological insulators and ordinary insulators. This quantity is the integer $n \in \{0, 1\}$ defined as,

$$n = \frac{1}{4\pi} \int_{\text{BZ}} \mathrm{d}^2 k \, \hat{\boldsymbol{d}} \cdot \left(\partial_{k_x} \hat{\boldsymbol{d}} \times \partial_{k_y} \hat{\boldsymbol{d}} \right) = \begin{cases} 1 & \text{Topological Insulators} \\ 0 & \text{Normal Insulators} \end{cases}$$

Where $\int_{\text{BZ}}$ refers to an integration over the entire Brillouin zone (BZ).

Topological insulators behave exactly like insulators except that electrons near the band touching points have the potential to transition to the upper band and permit conduction. In order to study this in detail, it s sufficient to consider the Hamiltonian component associated with the topological terms,

$$H_-(\boldsymbol{k}) = \hbar v_{\text{F}}(-k_x \sigma^x + k_y \sigma^y) + (m - \Delta_{\text{SO}})\sigma^z$$

Where the coefficient in front of σ^z differs in sign depending on whether or not the insulator is topological or not. Let us assume that we have a material that transitions from a topological insulator to an ordinary insulator by letting $m(x)$ denote the coefficient in front of σ^z as it varies along the x-direction.

$$m(x) = m - \Delta_{\text{SO}}$$

Since k_x no-longer corresponds to plane wave solutions to the Schrodinger equation, we replace k_x with its representation in position space,

$$k_x \mapsto -i\frac{\partial}{\partial x}$$

And solve $H(k_y)$,

$$H(k_y) = i\hbar v_{\text{F}}\frac{\partial}{\partial x}\sigma^x + \hbar v_{\text{F}}k_y\sigma^y + m(x)\sigma^z$$

As a preliminary exercise, we can solve the Schrodinger equation for the case of $k_y = 0$.

$$H(0) = i\hbar v_{\text{F}}\frac{\partial}{\partial x}\sigma^x + m(x)\sigma^z \tag{4.8}$$

For the zero energy eigenstate we require $H\psi = 0$. This suggests the following ansatz solution (for some unspecified $|z\rangle$),

$$\psi(x) = e^{f(x)\sigma^x}|z\rangle \tag{4.9}$$

Substituting eq. (4.9) into eq. (4.8) and making use of the fact that $\sigma^z\sigma^x = i\sigma^y$,

$$\left(i\hbar v_{\text{F}}\frac{\mathrm{d}f}{\mathrm{d}x} + im(x)\sigma^y\right)e^{f(x)}|z\rangle = 0$$

Therefore,

$$\left(\frac{\mathrm{d}f}{\mathrm{d}x} + \frac{m(x)}{\hbar v_{\text{F}}}\sigma^y\right)|z\rangle = 0$$

If we choose $|z\rangle$ such that $\sigma^y|z\rangle = |z\rangle$.

$$\frac{\mathrm{d}f}{\mathrm{d}x} = -\frac{m(x)}{\hbar v_{\text{F}}} \implies f(x) = -\frac{1}{\hbar v_{\text{F}}}\int_0^x \mathrm{d}x'm(x')$$

Therefore,

$$\psi(x) = e^{-\frac{1}{\hbar v_{\text{F}}}\int_0^x \mathrm{d}x'm(x')}\sigma^x|z\rangle$$

What is $\sigma^x|z\rangle$?

$$\sigma^y\sigma^x|z\rangle = -\sigma^x\sigma^y|z\rangle = -\sigma^x|z\rangle$$

Therefore $\sigma^x|z\rangle$ is an eigenstate of σ^y with eigenvalue -1. Therefore,

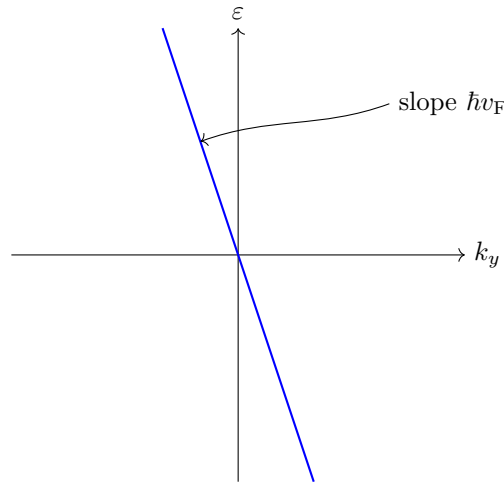$$\psi(x) = e^{-\frac{1}{\hbar v_{\text{F}}}\int_0^x \mathrm{d}x'm(x')}|\sigma^y = -1\rangle \tag{4.10}$$

This is the zero-energy eigenstate of the Hamiltonian localized at $x = 0$ for the special case of $k_y = 0$. The eigenstate of eq. (4.10) is know in high energy physics as the Jackiv-Relli soliton. If we consider $k_y \neq 0$, differs from eq. (4.8). In this case,

$$H(k_y)\psi(x) = \hbar v_{\text{F}}k_y\sigma^y\psi(x) = -\hbar v_{\text{F}}k_y\psi(x)$$

Which means $\psi(x)$ is an eigenstate of $H(k_y)$ with energy $-\hbar v_{\text{F}}k_y$. The dispersion relation is,

$$\varepsilon(k_y) = -\hbar v_{\text{F}}k_y \tag{4.11}$$

We refer to this type of dispersion as **chiral dispersion**. To understand why we refer to this as chiral dispersion, recall some properties of relativistic quantum mechanics. The velocity of free electrons is,

$$\varepsilon(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m} \tag{4.12}$$

This can be derived using classical intuition,

$$\boldsymbol{v} = \frac{\boldsymbol{p}}{m} = \frac{\hbar\boldsymbol{k}}{m} \tag{4.13}$$

Of course, eq. (4.12) and eq. (4.13) only hold for free electrons. More generally, we can define the **group velocity**,

$$\boldsymbol{v} = \frac{1}{\hbar}\boldsymbol{\nabla}_{\boldsymbol{k}}\varepsilon(\boldsymbol{k}) \tag{4.14}$$

For eq. (4.11) we have,

$$\boldsymbol{v} = -v_{\mathrm{F}}\hat{\boldsymbol{y}}$$

Which means that all the electrons move in one direction. This is in contrast with an ordinary conductor where electrons have the ability to propagate in point directions subject to an external potential.

Using alternating external potentials V_y we can construct and consider a 2D metal where the electrons move in alternating directions.
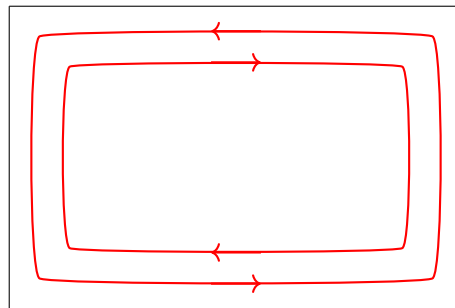
This metal produces the **quantum spin hall effect**. We can define the current density $\boldsymbol{j}$,

$$\boldsymbol{j} = -en\boldsymbol{v}$$

Where n is the density of the electrons which can be written as a integral over momentum space. Doing so gives the current where the electrons move to the right as,

$$I_R = -e \int v_{\mathrm{F}} n_{\mathrm{F}}(\varepsilon_k)\frac{\mathrm{d}k_x}{2\pi}$$

Where $k = 2\pi n/L$ and $2\pi/L$ is the volume in momentum space corresponding to a single quantum state.

$$\frac{1}{L}\frac{\mathrm{d}k_x}{\frac{2\pi}{L}} = \frac{\mathrm{d}k_x}{2\pi}$$

IF we convert this integral from an integral over momentum space to and integral over energies,

$$\varepsilon = \hbar v_\mathrm{F} k_x \implies \mathrm{d}k_x = \frac{\mathrm{d}\varepsilon}{\hbar v_\mathrm{F}}$$

Therefore the current is,

$$I_R = -e v_\mathrm{F} \frac{1}{2\pi \hbar v_\mathrm{F}} \int_{-\infty}^{\varepsilon_{FR}} \mathrm{d}\varepsilon = -\frac{e}{h} \int_{-\infty}^{\varepsilon_{FR}} \mathrm{d}\varepsilon$$

Where ε_{FR} is the Fermi energy for the right-traveling electrons. The current for the electrons traveling to the left is opposite in sign,

$$I_L = \frac{e}{h} \int_{-\infty}^{\varepsilon_{FL}} \mathrm{d}\varepsilon$$

Therefore the net current is,

$$I = I_R + I_L = -\frac{e}{h} \int_{\varepsilon_{FL}}^{\varepsilon_{FR}} \mathrm{d}\varepsilon = -\frac{e}{h}(\varepsilon_{FR} - \varepsilon_{FL}) = -\frac{e^2}{h}V_y$$

The conductivity is,

$$\frac{I}{V_y} = -\frac{e^2}{h}$$

The interesting feature of this conductivity is that is only depends on the fundamental constants e, h. As it turns out, measurements of this conductivity represent our most precise measurements of e and h. An excellent external resource is a book by R.B. Laughlin called *Different Universe*. An important thing to remember that this analysis only applies for a particular spin value. In this case we analyzed spin up states $S^z = +1$. In general we have,

$$\sigma_{xy}^{\uparrow} = -\frac{e^2}{h} \qquad \sigma_{xy}^{\downarrow} = +\frac{e^2}{h}$$

Which means that we can construct a **spin current**,

$$\sigma_{xy}^{S} = \frac{1}{2}\left(\sigma_{xy}^{\uparrow} - \sigma_{xy}^{\downarrow}\right) = -\frac{e^2}{h}$$

Effectively, if we have an equal number of electrons moving to the right and the left but each direction is biased to a particular spin, we can have a buildup of spin up electrons on the right and spin down electrons on the left. This is the analogue of *spin voltage*.

5   Bravais Lattices in 3D

There are a number of typical Bravais lattices in three dimensions. The simplest one is the simple cubic.

1. **Simple Cubic**:
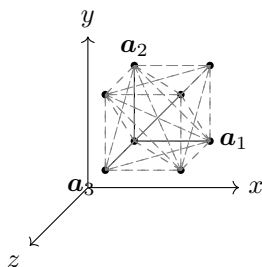
$$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}} \quad \boldsymbol{a}_2 = a\hat{\boldsymbol{y}} \quad \boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$$

2. **Body-centered Cubic**:

$$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}} \quad \boldsymbol{a}_2 = a\hat{\boldsymbol{y}} \quad \boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$$