Phys 435

TOPICS IN CONDENSED MATTER

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1   Effects of the Electronic Structure Topology

1.1   Toy Model of a Solid

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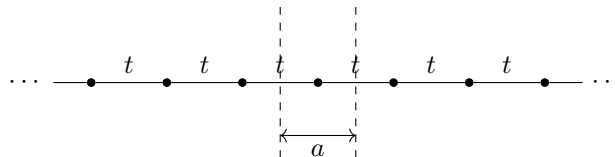
Thus far we have been discussing a toy model of a solid in one dimension. By diagonalizing the Hamiltonian we were able to determine the energy levels of the various states,

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

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.

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

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,

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

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,

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

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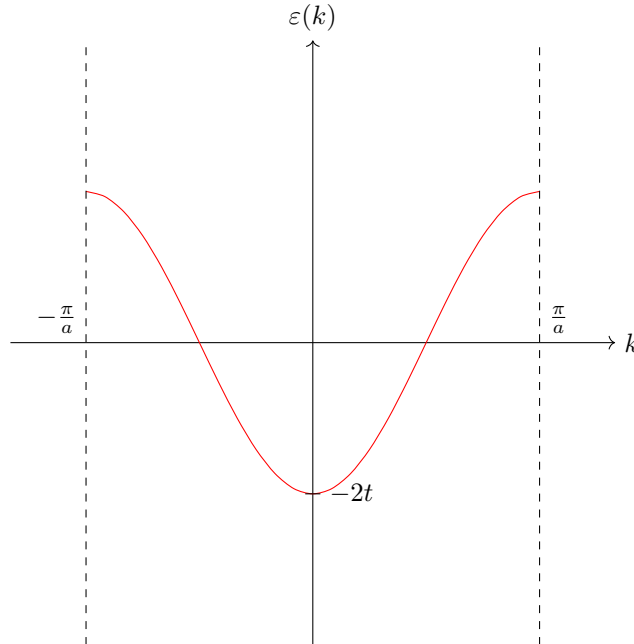
How many states does the band contain. Given that k is discrete and bounded,

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

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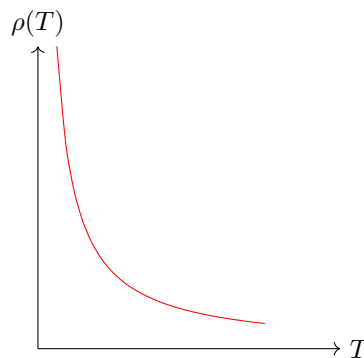
When the electrons occupy all of the lowest possible energy states, we fill all of the negative energy states and the positive energy states remain vacant. This separation defines the **Fermi energy** for this system where occurs at $\varepsilon_{\mathrm{F}} = 0$. In order to find the state that corresponds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

$$\varepsilon(k) = \varepsilon_{\mathrm{F}} = 0 \implies -2t\cos(ka) = 0$$

Therefore the value of k that solves this equation is,

$$k = \pm\frac{\pi}{2a} = \pm k_{\mathrm{F}}$$

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.

$$C : 1s^2 2s^2 2p^2 \qquad 4 \text{ valence electrons}$$
$$H : 1s^1$$
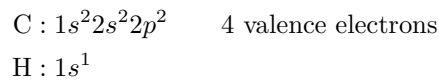
Electrons found in the inner orbitals of the atoms are tightly bound to their nuclei and therefore only the valence electrons in carbon are free to travel throughout the lattice.
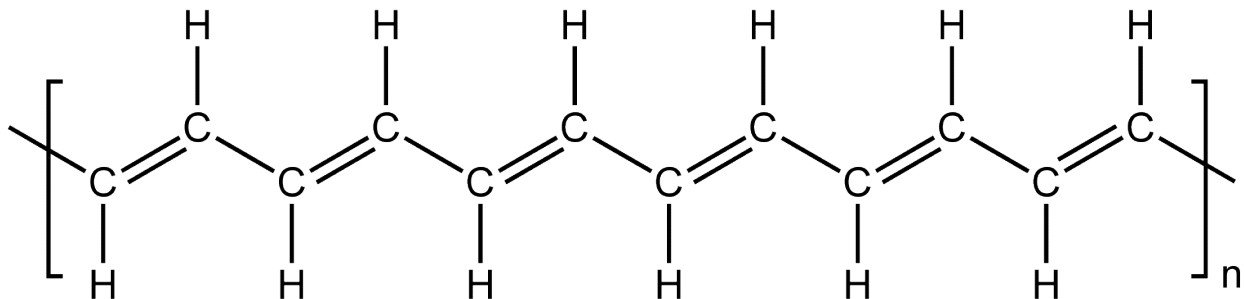
Three of the valence electrons are engaged in bonding with neighboring carbon and hydrogen atoms while the 4-th one is free to move around. As it turns out, the bonds between carbon atoms possess alternating tunneling amplitudes.
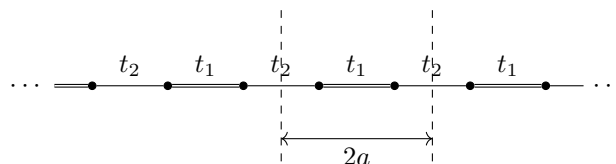
In Polyacetylene, the tunneling amplitude between the carbon atoms joined by a double bound is slightly higher $t_1 > t_2$. This is referred to as **Peierls instability**.

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,

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

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,
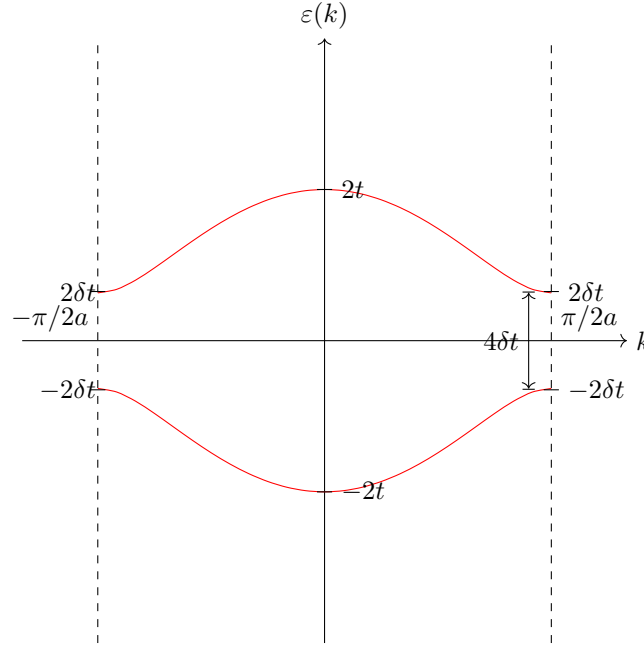
Notice that the first Brillouin zone is $\frac{\pi}{2a} \le k \le \frac{\pi}{2a}$ is *smaller* than it was previously. In this model, there is one electron per atom and thus two electrons per unit cell. Therefore there are $2N$ electrons. At zero temperature, the entire lower band is filled and the upper 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,
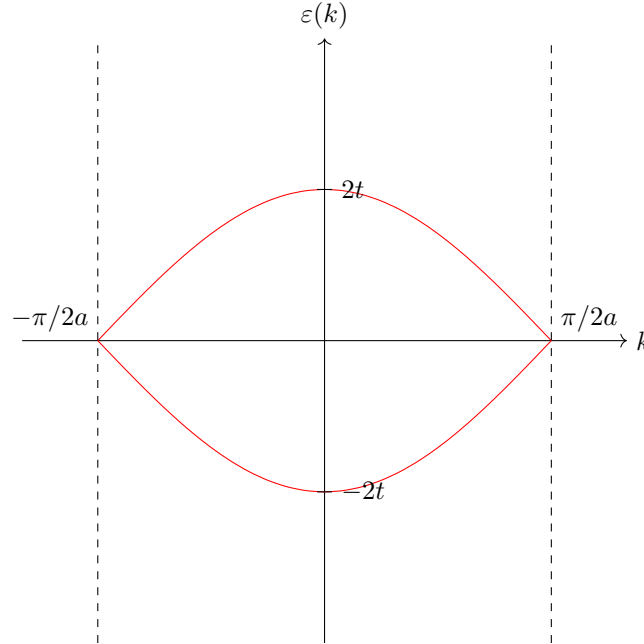
The resolution between these two plots is to notice that in the polyacetylene model, the unit cell had with $2a$ instead of a. Therefore in momentum space, the plotted values for k are bounded by $-\pi/2a \leq k \leq \pi/2a$ instead of $-\pi/a \leq k \leq \pi/a$. If one were to unravel the upper band 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

$$\delta t > 0 : \overset{t_2}{\bullet\!-\!\!-\!\bullet} \overset{t_1}{\bullet\!=\!\bullet} \overset{t_2}{\bullet\!-\!\!-\!\bullet} \overset{t_1}{\bullet\!=\!\bullet} \overset{t_2}{\bullet\!-\!\!-\!\bullet} \overset{t_1}{\bullet\!=\!\bullet}$$

$$\delta t < 0 : \overset{t_2}{\bullet\!=\!\bullet} \overset{t_1}{\bullet\!-\!\!-\!\bullet} \overset{t_2}{\bullet\!=\!\bullet} \overset{t_1}{\bullet\!-\!\!-\!\bullet} \overset{t_2}{\bullet\!=\!\bullet} \overset{t_1}{\bullet\!-\!\!-\!\bullet}$$
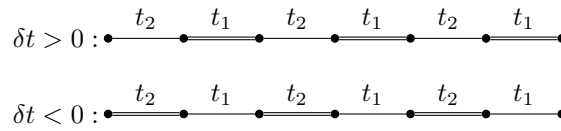
Therefore, the ground state of polyacetylene is doubly degenerate, corresponding to the two signs of δt. As it turns out, this difference in sign is related to topological properties in momentum space. Upon examination of eq. (1.8) once can notice $\boldsymbol{d}$'s dependence on δt. How does $\boldsymbol{d}(k)$ change as k goes from $-\pi/2a$ to $\pi 2a$?

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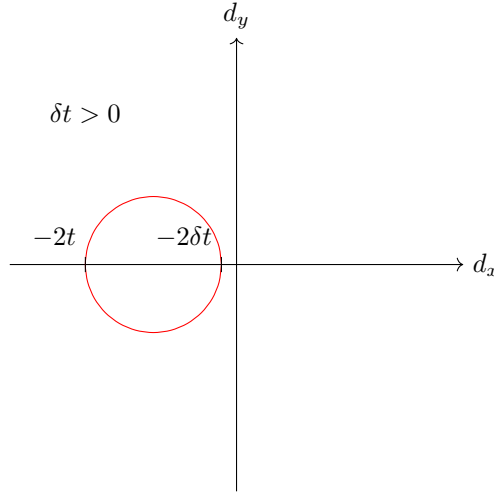$$d_y(k) = -(t - \delta t)\sin(2ka)$$

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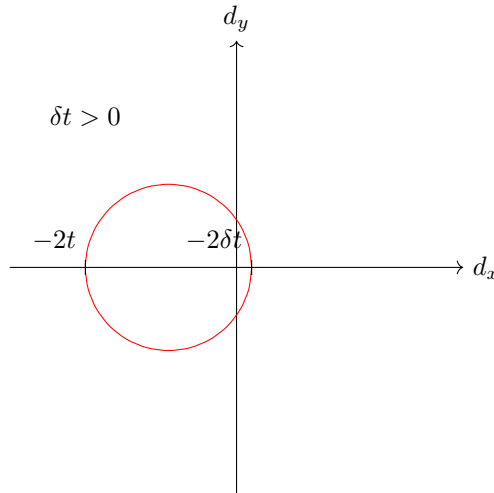
It can be seen that the origin $|\boldsymbol{d}| = 0$ is enclosed. This *topological* difference is what leads us to call the $\delta t < 0$ a **topological insulator** as apposed to an **ordinary insulator**.

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,

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

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

Similarly for d_y,

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

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

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

$$x = 0$$
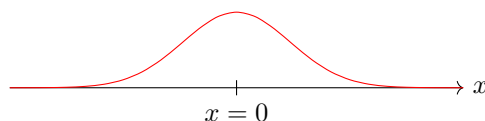
$\delta t < 0$	$\delta t > 0$
$m < 0$	$m > 0$

1.2   Higher Dimensions

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

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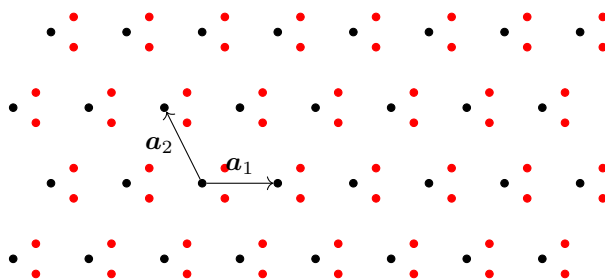
A **Bravais lattice** is all points in $\mathbb{R}^3$ ($\mathbb{R}^2, \mathbb{R}^1, \mathbb{R}^n$) such that,

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

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,

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

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.

1.3   Lattice Theory

Todo (TC Fraser): Missed a lecture

1.3.1   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.

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

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

1.3.2   Electronic Structure for Square Lattice

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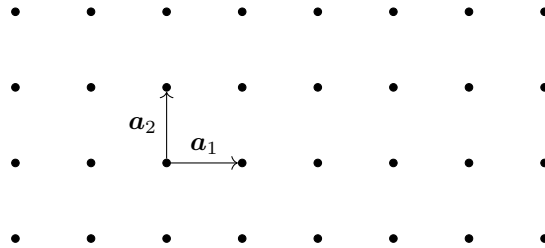
Using Cartesian coordinates,

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

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.

$$H = -t\sum_{\boldsymbol{R},\boldsymbol{a}}(|\boldsymbol{R} + \boldsymbol{a}\rangle\langle\boldsymbol{R}| + |\boldsymbol{R}\rangle\langle\boldsymbol{R} + \boldsymbol{a}|) \tag{1.9}$$

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. (1.9) 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. (1.9) becomes,

$$H = -t\sum_{\boldsymbol{R},\boldsymbol{a}}\sum_{\boldsymbol{k},\boldsymbol{k}'}\left(|\boldsymbol{k}\rangle\langle\boldsymbol{k}'|e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{a})}e^{i\boldsymbol{k}'\cdot\boldsymbol{R}} + |\boldsymbol{k}\rangle\langle\boldsymbol{k}'|e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}e^{i\boldsymbol{k}'\cdot(\boldsymbol{R}+\boldsymbol{a})}\right) \tag{1.10}$$

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. (1.9) 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,

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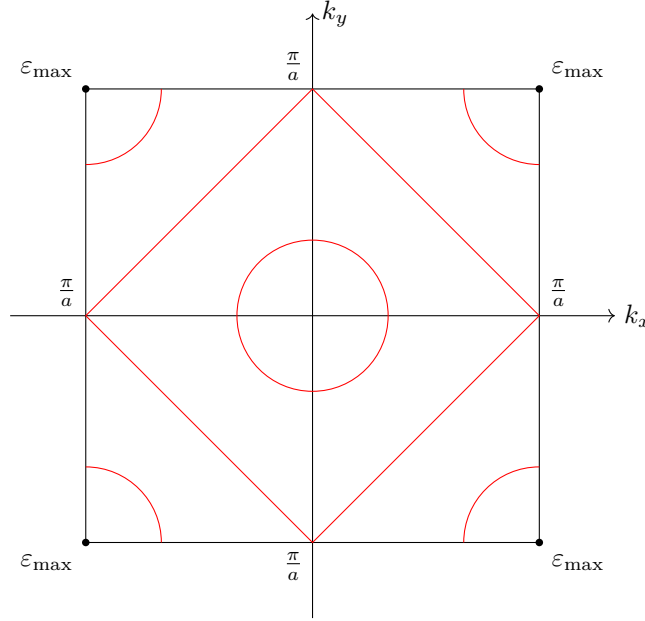
Expanding $\boldsymbol{k}$ near the minimum,

$$\varepsilon(\boldsymbol{k}) \simeq -4t + ta^2\left(k_x^2 + k_y^2\right) = -4t + ta^2 k^2 \tag{1.11}$$

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. (1.11) that this equation only defines the Fermi surface near the minimum energy level. In general,

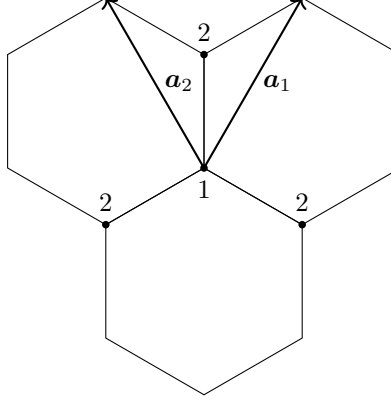$$\varepsilon(\boldsymbol{k}) = -2t(\cos(k_x a) + \cos(k_y a))$$

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

1.3.3   Graphene

The primitive unit vectors for Graphene are,

$$\boldsymbol{a}_1 = \frac{a}{2}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{a}_2 = \frac{a}{2}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \tag{1.12}$$

Whereas the reciprocal lattice is,

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\left(\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \qquad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(-\hat{\boldsymbol{x}} + \sqrt{3}\hat{\boldsymbol{y}}\right) \tag{1.13}$$

The nearest neighbor Hamiltonian becomes,

$$H = -t\sum_{\boldsymbol{R}}(|\boldsymbol{R},2\rangle\langle\boldsymbol{R},1| + |\boldsymbol{R}-\boldsymbol{a}_1,2\rangle\langle\boldsymbol{R},1| + |\boldsymbol{R}-\boldsymbol{a}_2,2\rangle\langle\boldsymbol{R},1| + \text{h.c.}) \tag{1.14}$$

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. (1.12) and (1.13),

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

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

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,

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

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. (1.13) 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.
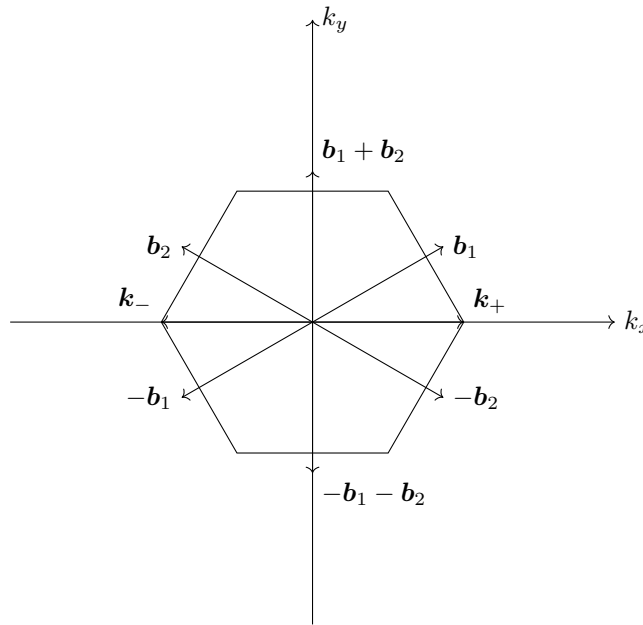
The first Brillouin zone for graphene forms a hexagonal lattice with the corners obtained from $\boldsymbol{k}_\pm$ by adding $\pm b_1, \pm b_2$,

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

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,

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

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

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,

$$H_{\pm}(\boldsymbol{k}) = \hbar v_{\mathrm{F}}(\pm k_x \sigma^x + k_y \sigma^y) \tag{1.15}$$

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. (1.15), eq. (1.15) 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. (1.15) 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,
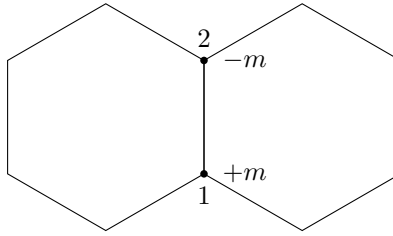
Which effectively corresponds to adding the following term to the original Hamiltonian,

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

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,

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

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

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 $m = 0$,

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

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,

$$H(\boldsymbol{k}) = \hbar v_{\mathrm{F}}(k_x \tau^z \sigma^x + k_y \sigma^y) \tag{1.16}$$

1.4   Spin-Orbit Interactions

What are the symmetries of eq. (1.16)? 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. (1.16) can we written,

$$\pi^\dagger H(\boldsymbol{k})\pi = H(\boldsymbol{k}) \tag{1.17}$$

$$\Theta H(\boldsymbol{k})\Theta^{-1} = H(\boldsymbol{k}) \tag{1.18}$$

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

$$\pi^\dagger \tau^z \pi = -\tau^z \tag{1.19}$$

$$\Theta \tau^z \Theta^{-1} = -\tau^z \tag{1.20}$$

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. (1.17) and (1.18),

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

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

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

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

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. (1.17) and (1.18),

$$\pi^\dagger \sigma^z \pi = -\sigma^z \qquad \Theta \sigma^z \Theta^{-1} = \sigma^z \tag{1.21}$$

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. (1.14). If we include *next-nearest neighbor* terms, it is possible to recover symmetries. Upon examination of eq. (1.21) and eqs. (1.19) and (1.20) 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,

$$H(\boldsymbol{k}) = \hbar v_{\mathrm{F}}(k_x \tau^z \sigma^x + k_y \sigma^y) + \Delta_{\mathrm{SO}} \tau^z \sigma^z S^z \tag{1.22}$$

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. (1.22) 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 ($1 \to 1$ and $2 \to 2$ tunneling),
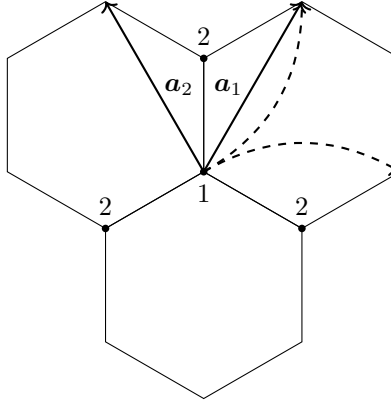
The additional terms to eq. (1.14) can be expressed as,

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

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. (1.22), 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,

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

$$\{\varepsilon(\boldsymbol{k})\}_{\tau^z = -1} \equiv \varepsilon_-(\boldsymbol{k}) = \pm\sqrt{\hbar^2 v_{\mathrm{F}}^2 (k_x^2 + k_y^2) + (m - \Delta_{\mathrm{SO}})^2} \tag{1.23}$$

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. (1.23). 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 $k_y = 0$.

$$H(0) = i\hbar v_{\text{F}}\frac{\partial}{\partial x}\sigma^x + m(x)\sigma^z \tag{1.24}$$

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

$$\psi(x) = e^{f(x)\sigma^x}|z\rangle \tag{1.25}$$

Substituting eq. (1.25) into eq. (1.24) 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,

$$\psi(x) = e^{-\frac{1}{\hbar v_{\text{F}}}\int_0^x \mathrm{d}x'm(x')}|\sigma^y = -1\rangle \tag{1.26}$$

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. (1.26) is know in high energy physics as the Jackiv-Relli soliton. If we consider $k_y \neq 0$, differs from eq. (1.24). 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,

$$\varepsilon(k_y) = -\hbar v_{\text{F}}k_y \tag{1.27}$$
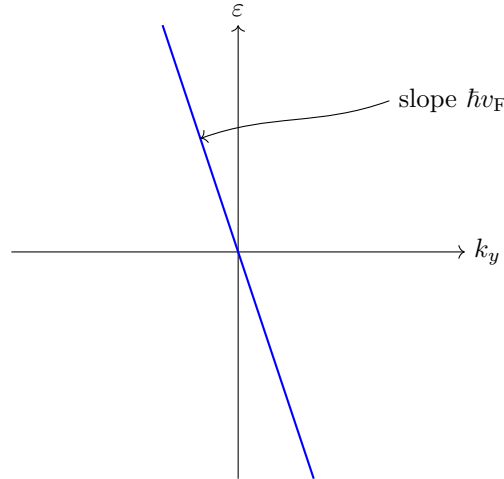
We refer to this type of dispersion as **chiral dispersion**. To understand why we refer to this as chiral dispersion, recall some properties of relativistic quantum mechanics. The velocity of free electrons is,

$$\varepsilon(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m} \tag{1.28}$$

This can be derived using classical intuition,

$$\boldsymbol{v} = \frac{\boldsymbol{p}}{m} = \frac{\hbar \boldsymbol{k}}{m} \tag{1.29}$$

Of course, eq. (1.28) and eq. (1.29) only hold for free electrons. More generally, we can define the **group velocity**,

$$\boldsymbol{v} = \frac{1}{\hbar} \boldsymbol{\nabla}_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \tag{1.30}$$

For eq. (1.27) 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.
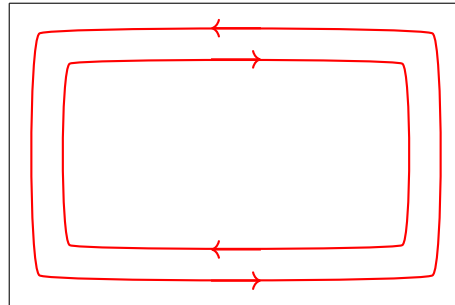
This metal produces the **quantum spin hall effect**. We can define the current density $\boldsymbol{j}$,

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

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,

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

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*.

1.5   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**:
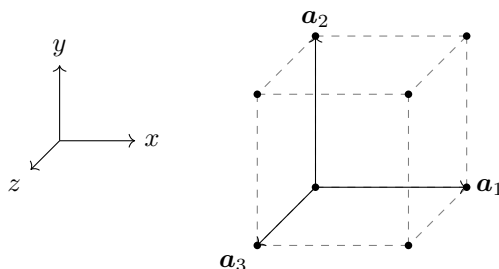
$$\boldsymbol{a}_1 = a\hat{\boldsymbol{x}} \quad \boldsymbol{a}_2 = a\hat{\boldsymbol{y}} \quad \boldsymbol{a}_3 = a\hat{\boldsymbol{z}}$$

2. **Body-centered Cubic (bcc)**: Todo: Draw

3. **Face-centered Cubic (fcc)**:

$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) \quad \boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}) \quad \boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})$$
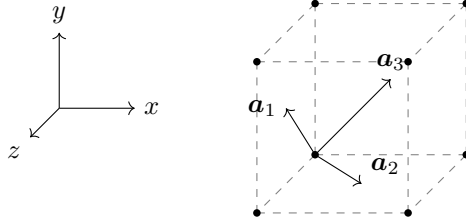
4. **Diamond Structure**: Todo: Draw

$$\hat{\boldsymbol{r}} = \frac{Q}{4}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) \quad \boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}) \quad \boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})$$

The Diamond structure is a generalization of the graphene lattice in 3D. The nearest-neighbor hopping Hamiltonian is as follows,

$$H_1 = -\sum_{\boldsymbol{R}}(t|\boldsymbol{R},1\rangle\langle\boldsymbol{R},2| + t|\boldsymbol{R}+\boldsymbol{a}_1,1\rangle\langle\boldsymbol{R},2| + t|\boldsymbol{R}+\boldsymbol{a}_2,1\rangle\langle\boldsymbol{R},2| + t|\boldsymbol{R}+\boldsymbol{a}_3,1\rangle\langle\boldsymbol{R},2| + \text{h.c.}) \tag{1.31}$$

While the second-nearest neighbor terms are numerous. In fact there are 24 terms similar to the one below.

$$H_2 = i\frac{8\Delta_{\text{SO}}}{a^2}\sum_{\boldsymbol{R}}|\boldsymbol{R}+\boldsymbol{a}_1,1\rangle\langle\boldsymbol{R},1|\boldsymbol{S}\cdot(\boldsymbol{r}\times\boldsymbol{a}_1) + \dots$$

It is to explore the first nearest-neighbor hopping Hamiltonian in the case where the tunneling amplitudes in eq. (1.31) are perturbed a small amount $t \mapsto t + \delta t$. When $\delta t = 0$ there are 3 band-touching point in the BZ. When $\delta t \neq 0$ we have,

$$H = -\delta t\sigma^x + tak_z\sigma^y - 2\Delta_{\text{SO}}a\sigma^z S^x k_x + 2\Delta_{\text{SO}}a\sigma^z S^y k_y$$

Where th Pauli spin $\boldsymbol{\sigma}$ describes the degree of freedom associated with localization to atoms 1 or 2. The $\boldsymbol{S}$ spin is the intrinsic spin of the electron. The dispersion relation can be calculated as well,

$$\varepsilon_\pm(\boldsymbol{k}) = \pm\sqrt{t^2a^2k_z^2 + 4\Delta_{\text{SO}}^2a^2\left(k_x^2 + k_y^2\right) + \delta t^2}$$

1.6　Quantum Hall Effect

In this subsection we will discuss the Quantum Hall Effect. Specifically we will look at the Quantum Hall Effect in a 2-dimensional electron gas (2DEG) when subjected to a magnetic field. 2DEG arise at heterointerfaces; interfaces between two different semiconductor materials. Semiconductors are insulators with a small band gap $< 1\,\text{eV}$.

$Al_xGa_{1-x}As$　　　　　　　　　　GaAs

ε_F
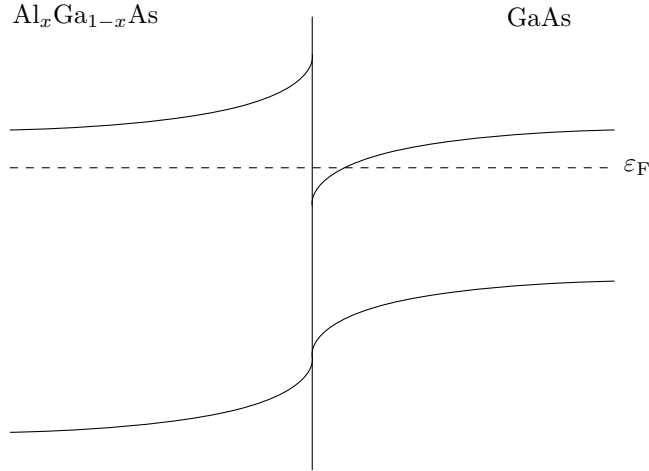
We place the 2DEG in the xy-plane and subject it to a magnetic field in the z-direction $\boldsymbol{B} = B\hat{\boldsymbol{z}}$. If the electrons are classical particles of charge $-e$ and mass m,

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \boldsymbol{F}_{\mathrm{L}} = -\frac{e}{c}\boldsymbol{v} \times \boldsymbol{B} \qquad \boldsymbol{v} = \frac{\boldsymbol{p}}{m}, \boldsymbol{v} = \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}$$

Solving these equations yields,

$$m\frac{\mathrm{d}^2\boldsymbol{r}}{\mathrm{d}t^2} = -\frac{e}{c}\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} \times \boldsymbol{B}$$

Therefore we obtain a two dimensional system of coupled ordinary differentiable equations,

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\frac{eB}{mc}\frac{\mathrm{d}y}{\mathrm{d}t}$$
$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} = \frac{eB}{mc}\frac{\mathrm{d}x}{\mathrm{d}t}$$

Where the frequency $\omega_C = \frac{eB}{mc}$ is the cyclotron frequency. In order to solve this system, introduce a complex parameter $z = x + iy$ such that,

$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = i\omega_x\frac{\mathrm{d}z}{\mathrm{d}t}$$

$$z(t) = z_0 - \frac{iv_0}{\omega_C}e^{i\omega_c t}$$

Which is circular motion with frequency ω_C. Therefore if we need to model the average time between collisions with impurities, the simplest description involves a decrease in momentum with characteristic time τ.

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -e\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}\right) - \frac{\boldsymbol{p}}{\tau}$$

Therefore without a magnetic field we have,

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = \frac{-\boldsymbol{p}}{t} \implies \boldsymbol{p}(t) = \boldsymbol{p}(0)e^{-t/\tau}$$

In general,

$$m\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = -\frac{m\boldsymbol{v}}{\tau} - e\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}\right)$$

Assuming that $\boldsymbol{E}$ and $\boldsymbol{B}$ are time-independent, we can look for the time-independent steady state solution corresponds to a fixed $\boldsymbol{v}$,

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = 0 \implies \boldsymbol{v} = -\frac{e\tau}{m}\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v} \times \boldsymbol{B}\right)$$

The electron $\boldsymbol{v}$ is connect to the current density $\boldsymbol{j}$ through the following equation we have seen before,

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

Where n is the electron density and e is the electric charge. Therefore,

$$\boldsymbol{j} = \frac{e^2 n \tau}{m}\left(\boldsymbol{E} - \frac{e\tau}{mc}\boldsymbol{j} \times \boldsymbol{B}\right)$$

In the absence of a magnetic field $\boldsymbol{B}$, we recover Ohm's law,

$$\boldsymbol{j} = \frac{e^2 n \tau}{m}\boldsymbol{E}$$

Where the proportionality is the conductivity σ,

$$\sigma = \frac{e^2 n \tau}{m}$$

Todo: Missed the start of this lecture The electric field in the conduction is,

$$\boldsymbol{E} = \frac{\boldsymbol{j}}{\sigma} = \frac{1}{nec}\boldsymbol{B} \times \boldsymbol{j}$$

Component-wise,

$$E_x = \frac{1}{\sigma}j_x + \frac{B}{nec}j_y$$
$$E_y = \frac{1}{\sigma}j_y - \frac{B}{nec}j_x$$

If there is no current in the y-direction ($j_y = 0$) we have,

$$E_y = -\frac{B}{nec}j_x \qquad \frac{E_y}{Bj_x} = -\frac{1}{nec} = -R_H$$
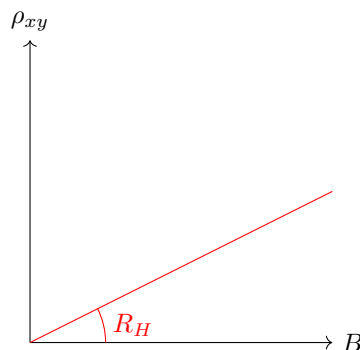
The last equality is a definition of the **Hall coefficient** R_H

$$R_H = \frac{1}{nec}$$

Notice that the Hall coefficient only depends on the density of the electrons and other fundamental constants. Now we introduce the **resistivity tensor**,

$$\rho\begin{pmatrix} 1/\sigma & BR_H \\ -BR_H & 1/\sigma \end{pmatrix}$$

We refer to this as the **classical Hall effect**.

In reality, the classical Gall effect occurs at weak magnetic fields or in dirty samples. If we let $1/\tau$ characterize the impurity scattering rate, our classical Hall effect is relevant in the domain where,

$$\omega_C \tau \ll 1$$

Recall that the cyclotron frequency is ω_C,

$$\omega_C = \frac{eB}{mc}$$

If $\omega_C \tau \ll 1$, the electron will be scatter many times before being able to complete a single circular orbit; i.e. if the period of the circular motion of the electron is greater than the mean-free time, then we can model the electrons as a classical particle.

In we have $\omega_C \tau \gg 1$, then the classical Hall effect is no longer the dominant feature. If the circular motion of the electrons becomes quantized, we need to consider the **quantum Hall effect**. The quantum aspects of the electron need to be considered in really clean materials or in high magnetic fields.

To study the quantum Hall effect, consider free quantum particles of charge $-e$ in the xy-plane in a magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ pointing in the $\hat{\boldsymbol{z}}$ direction. In the absence of a magnetic field, we have the relation $\boldsymbol{p} = m\boldsymbol{v}$ which makes the Hamiltonian,

$$H = -\frac{\hbar^2 \nabla^2}{2m}$$

However, a magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ we have,

$$m\boldsymbol{v} = \boldsymbol{p} + \frac{e}{c}\boldsymbol{A}$$

Therefore the Hamiltonian for a charged particle in a magnetic field is,

$$H = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} + \frac{e}{c}\boldsymbol{A}\right)^2 - \boldsymbol{\mu} \cdot \boldsymbol{B}$$

Where $\boldsymbol{\mu}$ is the magnetic dipole moment. For simplicity, we neglect $\boldsymbol{\mu}$ for now. Therefore, the Hamiltonian of interest is,

$$H = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} + \frac{e}{c}\boldsymbol{A}\right)^2 \tag{1.32}$$

Where we wish to find the energy eigenstates ψ where $H\psi = E\psi$. Moreover, the magnetic field is determined by $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ leaving a **gauge invariance** in the choice of $\boldsymbol{A}$,

$$\boldsymbol{A} \to \boldsymbol{A} + \boldsymbol{\nabla}f$$

The gauge choice we will used is called the **Landau gauge**.

$$\boldsymbol{A} = xB\hat{\boldsymbol{y}}$$

Therefore,

$$(\boldsymbol{\nabla} \times \boldsymbol{A})_z = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = B$$

Analogously the x, y components of $\boldsymbol{\nabla} \times \boldsymbol{A}$ are as follows,

$$(\boldsymbol{\nabla} \times \boldsymbol{A})_x = \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = 0$$

$$(\boldsymbol{\nabla} \times \boldsymbol{A})_y = \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} = 0$$

Therefore eq. (1.32) becomes,

$$H = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} + \frac{e}{c}\boldsymbol{A}\right)^2$$

$$= \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} + \frac{e\boldsymbol{B}}{c}\times\hat{\boldsymbol{y}}\right)^2$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} + \frac{eB}{c}x\right)^2 \tag{1.33}$$

Notice that H is not invariant with respect to translations along the x-direction but *is* invariant with respect to translations along the y-direction. Translation symmetries give rise to wave functions that are also momentum eigenstates. If the energy eigenstates $\psi(x,y)$ are thus functions of x,y and have the following form,

$$H\psi(x,y) = E\psi(x,y)$$

Symmetry analysis suggests we should expect ψ to the separable into a plane wave solution with non-trivial x-dependence $\varphi(x)$.

$$\psi(x,y) = e^{iky}\varphi(x)$$

With k to be determined. Substituting this ansatz into eq. (1.33) yields,

$$E\psi(x,y) = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2}e^{iky} + \frac{1}{2m}\left(\hbar k + \frac{eB}{c}x\right)^2\varphi e^{iky}$$

Canceling φ,

$$E\varphi = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} + \frac{1}{2m}\left(\hbar k + \frac{eB}{c}x\right)^2\varphi \tag{1.34}$$

Gives us a 1D differential equation. For convenience of notation we introduce the **magnetic length** ℓ,

$$\ell = \sqrt{\frac{\hbar c}{eB}}$$

Additionally re-use the classical cyclotron frequency,

$$\omega_C = \frac{eB}{mc}$$

Using these constants, eq. (1.34) can we re-expressed as,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} + \frac{m\omega_C^2}{2}\left(x + k\ell^2\right)^2\varphi = E\varphi$$

At this stage, it should be clear that this Hamiltonian is nothing more than a 1D Harmonic oscillator with frequency ω_C and centered at $x - k\ell^2$. The solution for the quantum harmonic oscillator can be found in a number of undergraduate quantum theory textbooks. Therefore the energy level for the n-th state for fixed k can be written as,

$$E_{nk} = \hbar\omega_C\left(n + \frac{1}{2}\right) \qquad n = 0,1,2,\ldots$$

We refer to these energy levels as **Landau levels**. Every Landau level is degenerate with respect to all the different values of k. Since E_{nk} is independent of k, we say that E_{nk} has degeneracies in k. Because of this, Landau levels are analogous to bands in a crystal.

Todo: Missed 2 lectures

1.6.1   Conclusion

The topological features of electronic structures we have considered thus far are genuine manifestations of quantum mechanics on macroscopic scales. For example, resistivity in the Quantum Hall effect,

$$\rho_{xy} = \frac{h}{e^2\nu}$$

Has dependence on Planck's constant h which indicates that it has no classical counterpart. This is in contrast with the Classical Hall effect,

$$\rho_{xy} = \frac{B}{nec}$$

which does not rely on quantum mechanics whatsoever. This concludes the first focus of this course and one of the major ideas in condensed matter physics: the effects of the electronic structure topology on macroscopic scales.

2   Electron-electron Interactions

Heretofore, we have consider materials where electrons are modeled as moving in a atomic lattice in *isolation*. In essence, the electrons are treated as being non-interacting. This approximation was well-founded as many material properties can be seen as consequences of non-interacting electrons and in most cases, electron interactions are negligible.

However, in specific cases the electron interactions yield interesting physics. For example Landau Fermi liquid theory, magnetism and superconductivity all require a description of electronic interactions.

In particular, **ferro-magnetism** is the appearance of *spontaneous* macroscopic magnetic momentum in certain materials at sufficiently low temperature T. For a material magnetic field H, the magnetization M is

$$M = \chi H$$

Where χ is the **magnetic susceptibility**.

- $\chi > 0$ para-magnets

- $\chi < 0$ dia-magnets

Ferromagnets are distinct from both para and dia-magnets in that they possess magnetic fields $M \neq 0$ even in the absence of H. It is this feature we are referring to when we say that ferromagnets produce magnetic fields *spontaneously.*

Unlike materials with completely filled shells (which have zero spin), materials that have incompletely filled d-shells (such as iron) have non-zero spin,

$$\text{Fe} : 3\text{d}^6 4\text{s}^2$$
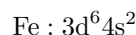
Hund's rule states that atomic orbitals are filled in such a way as to *maximize* the total spin. Equivalently, any incompletely filled atomic orbital will always have non-zero total spin. If any incompletely filled shell has non-zero spin why are d-shells important? d-shells are important to magnetism because the electrons in higher orbital shells are spaced farther apart. This permits the electrons to have a stronger notion of localization for specific positions around atoms.

The combination of incompletely filled d-shells and Hund's rule implies that there is a non-zero atomic **magnetic moments μ**,

$$\boldsymbol{\mu} = g\mu_B \boldsymbol{S}$$

Where μ_B is the **Bohr magneton**,

$$\mu_B = \frac{e\hbar}{2mc}$$

And $g \approx 2$. Therefore,

$$\mu \sim g\mu_B \sim \frac{e\hbar}{mc}$$

The most obvious source interactions are magnetic dipole interactions

$$U_{\text{dip}} = \frac{1}{r^3}(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - 3(\boldsymbol{\mu}_1 \cdot \hat{\boldsymbol{r}})(\boldsymbol{\mu}_2 \cdot \hat{\boldsymbol{r}}))$$

Recalling the Bohr radius a_0,

$$a_0 = \frac{\hbar^2}{mc^2}$$

We can write U_{dip} in terms of a distance r,

$$U_{\text{dip}} \sim \frac{(g\mu_B)^3}{r^3} = \left(\frac{e\hbar}{mc}\right)^2 \frac{1}{r^3} = \left(\frac{e^2}{\hbar c}\right)^2 \frac{e^2}{a_0}\left(\frac{a_0}{r}\right)^3$$

Where the coefficients are related to the dimensionless **Fine structure constant** α,

$$\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}$$

Using this constant,

$$U_{\text{sip}} \sim \alpha^2 \frac{e^2}{a_0}\left(\frac{a_0}{r}\right)^3$$

For typical atomic separations $r \sim a_0$, we have $U_{\text{dip}} \sim \alpha^2 \frac{e^2}{a_0} \sim 10^{-4}\,\text{eV}$ which corresponds to temperatures $T \sim U_{\text{dip}}/k_B \sim 1\,\text{K}$. This result is odd because we know that the critical temperature for iron is,

$$\text{Fe} : T_c = 1043\,\text{K}$$

Therefore dipole-dipole interactions can *not* be the source of ferro-magnetism.

For ordinary electron-electron Coulomb interactions e^2/a_0 is the typical Coulomb interaction energy between electrons on neighboring atoms.

$$\frac{e^2}{a_0} \sim 1\,\text{eV} \qquad T \sim 10^4\,\text{K}$$

This is much closer to the critical temperature for iron, therefore we conclude that ordinary Coulumb interactions are responsible for ferro-magnetism. This result is surprising because the Coulumb potential does not know about magnetic fields; instead the effects of spin (in combination with $V(\boldsymbol{r})$) will give rise to ferro-magnetism.

Consider 2 electrons on two atomic orbitals $\varphi_1(\boldsymbol{r}_1)$ and $\varphi_2(\boldsymbol{r}_2)$ with the same energy. The Coulomb potential is,

$$V(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$$

In general the wave-function for the two electrons will depend on positions $\boldsymbol{r}_1, \boldsymbol{r}_2$ for the two electrons and spin values $\sigma_i \in \{\uparrow, \downarrow\}$. This position and spin wave-functions are separable,

$$\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2) = \psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\chi(\sigma_1, \sigma_2)$$

Since the electrons are Fermions the wave-function must be antisymmetric with respect to the exchange of the two particles,

$$\psi(\boldsymbol{r}_2\sigma_2, \boldsymbol{r}_1\sigma_1) = -\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)$$

Therefore we have two possibilities for the antisymmetry of ψ,

1. $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is antisymmetric:
$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = -\psi(\boldsymbol{r}_2, \boldsymbol{r}_1)$$
$$\chi(\sigma_1, \sigma_2) = +\chi(\sigma_2, \sigma_1)$$

2. $\chi(\sigma_1, \sigma_2)$ is antisymmetric:
$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = +\psi(\boldsymbol{r}_2, \boldsymbol{r}_1)$$
$$\chi(\sigma_1, \sigma_2) = -\chi(\sigma_2, \sigma_1)$$

Since the potential $V(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ is independent of the spin, the total spin of two electrons is a conserved quantity. In using this observation, it is convenient to not label the individual spins σ_1, σ_2 (which are not conserved) but instead the total spin S and its projection onto the z-axis M.

$$|\sigma_1, \sigma_2\rangle \mapsto |S, M\rangle$$

If the total number states has to be conserved ($|\sigma_1, \sigma_2\rangle \in \mathcal{H}^2 \otimes \mathcal{H}^2 \implies |S, M\rangle \in \mathcal{H}^2 \otimes \mathcal{H}^2$), then the four spin states,

$$|\uparrow, \uparrow\rangle \quad |\uparrow, \downarrow\rangle \quad |\downarrow, \uparrow\rangle \quad |\downarrow, \downarrow\rangle$$

Map to 4 possible values for S, M. The z component of the spin can take on any value from $1, 0, -1$ but the total magnitude of the spin must be either $0, 1$.

$$|0, 0\rangle \quad |1, 1\rangle \quad |1, 0\rangle \quad |1, -1\rangle$$

Notice that these four states form and orthonormal basis for $\mathcal{H}^2 \otimes \mathcal{H}^2$. Explicitly these $|S, M\rangle$ states can be written as superpositions of the $|\sigma_1, \sigma_2\rangle$ states,

$$|1, 1\rangle = |\uparrow, \uparrow\rangle$$
$$|1, -1\rangle = |\downarrow, \downarrow\rangle$$
$$|1, 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle + |\uparrow, \downarrow\rangle)$$
$$|0, 0\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\uparrow, \downarrow\rangle)$$

Importantly, each state $|S, M\rangle$ where the total spin S is $S = 1$ is *symmetric* with respect to the interchange of two electrons and the the spin $S = 0$ state is *antisymmetric*. This anti-symmetry couples the spin states to the orbital components of the wave function. Since the spin $S = 1$ states are symmetric, the wavefunction in position space with $S = 1$ must be anti-symmetric,

$$\psi_{1M}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\sqrt{2}}(\varphi_1(\boldsymbol{r}_1)\varphi_2(\boldsymbol{r}_2) - \varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2))|1, M\rangle$$

Analogously,

$$\psi_{00}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\sqrt{2}}(\varphi_1(\boldsymbol{r}_1)\varphi_2(\boldsymbol{r}_2) + \varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2))|0, 0\rangle$$

In order to determine the correction to the energy values due to the Coulomb interactions, use perturbation theory. Specifically, the ψ_{1M} states are 3-fold degenerate in position space but are distinct when spin states are included. Recalling that the corrections can be computed by calculating the matrix elements of the corrections V,

$$\langle 1, M|V|1, M\rangle = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 \frac{1}{\sqrt{2}}(\varphi_1^*(\boldsymbol{r}_1)\varphi_2^*(\boldsymbol{r}_2) - \varphi_2^*(\boldsymbol{r}_1)\varphi_1^*(\boldsymbol{r}_2))V(\boldsymbol{r}_1 - \boldsymbol{r}_2)\frac{1}{\sqrt{2}}(\varphi_1(\boldsymbol{r}_1)\varphi_2(\boldsymbol{r}_2) - \varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2))$$

$$= \frac{1}{2}\int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1 - \boldsymbol{r}_2)\left[|\varphi_1(\boldsymbol{r}_1)|^2|\varphi_2(\boldsymbol{r}_2)|^2 + |\varphi_1(\boldsymbol{r}_2)|^2|\varphi_2(\boldsymbol{r}_1)|^2 + \cdots\right.$$

$$\left.\cdots - \varphi_1^*(\boldsymbol{r}_1)\varphi_2^*(\boldsymbol{r}_2)\varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2) - \varphi_2^*(\boldsymbol{r}_1)\varphi_1^*(\boldsymbol{r}_2)\varphi_1(\boldsymbol{r}_1)\varphi_2(\boldsymbol{r}_2)\right]$$

Recognize that since the potential only depends on the distance $|\boldsymbol{r}_1, \boldsymbol{r}_2|$, our integral over $\boldsymbol{r}_1, \boldsymbol{r}_2$ counts each term twice. Therefore,

$$\langle 1, M|V|1, M\rangle = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1 - \boldsymbol{r}_2)\left[|\varphi_1(\boldsymbol{r}_1)|^2|\varphi_2(\boldsymbol{r}_2)|^2 - \varphi_1^*(\boldsymbol{r}_1)\varphi_2^*(\boldsymbol{r}_2)\varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2)\right]$$

Similarly, we can calculate the matrix element for $|0, 0\rangle$ (the elements $\langle 0, 0|V|1, M\rangle$ are zero),

$$\langle 0, 0|V|0, 0\rangle = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1 - \boldsymbol{r}_2)\left[|\varphi_1(\boldsymbol{r}_1)|^2|\varphi_2(\boldsymbol{r}_2)|^2 + \varphi_1^*(\boldsymbol{r}_1)\varphi_2^*(\boldsymbol{r}_2)\varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2)\right]$$

Notice that $\langle 0,0|V|0,0\rangle$ differs from $\langle 1,M|V|1,M\rangle$ by the sign in the second set of terms. To facilitate discussions, let $\mathcal{C}$ define the **Coulomb integral $\mathcal{C}$**,

$$\mathcal{C} = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1-\boldsymbol{r}_2)\left[|\varphi_1(\boldsymbol{r}_1)|^2|\varphi_2(\boldsymbol{r}_2)|^2\right]$$

Which is shared by both matrix elements and is a equivalent to a classical measurement of a Coulomb energy,

$$\mathcal{C} = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1-\boldsymbol{r}_2)\rho_1(\boldsymbol{r}_1)\rho_2(\boldsymbol{r}_2)$$

The differing integral is called the **exchange integral $\mathcal{J}$**,

$$\mathcal{J} = \int\int \mathrm{d}^3r_1\mathrm{d}^3r_2 V(\boldsymbol{r}_1-\boldsymbol{r}_2)[\varphi_1^*(\boldsymbol{r}_1)\varphi_2^*(\boldsymbol{r}_2)\varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2)]$$

In conclusion,

$$\langle 0,0|V|0,0\rangle = \mathcal{C} + \mathcal{J} \qquad \langle 1,M|V|1,M\rangle = \mathcal{C} - \mathcal{J}$$

The state with higher (or lower) energy correction will depend on the sign of $\mathcal{J}$. If $\mathcal{J} > 0$, this leads to alignment of the individual spins and to ferro-magnetism. Recalling $\psi_{1M}(\boldsymbol{r}_1,\boldsymbol{r}_2)$,

$$\psi_{1M}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{\sqrt{2}}(\varphi_1(\boldsymbol{r}_1)\varphi_2(\boldsymbol{r}_2) - \varphi_2(\boldsymbol{r}_1)\varphi_1(\boldsymbol{r}_2))|1,M\rangle$$

It can be seen that if we let $\boldsymbol{r}_1 = \boldsymbol{r}_2$ the antisymmetry forces,

$$\psi_{1M}(\boldsymbol{r}_1,\boldsymbol{r}_1) = 0$$

Therefore the probability of both electrons being found in the same place is zero and therefore the Coulomb interaction (which would normally tend to ∞ as $\boldsymbol{r}_1 \to \boldsymbol{r}_2$). Therefore the electrons tend toward their minimal energy state which corresponds to aligning their spins $S = 1$. An alternative way of seeing this is to consider $\mathcal{J}$ in the case where $\boldsymbol{r}_1 = \boldsymbol{r}_2$, $\mathcal{J}$ tends toward $\mathcal{C}$ which is positive.

Let $\boldsymbol{S} = \boldsymbol{S}_1 + \boldsymbol{S}_2$ be the total spin operator for the two electrons. Therefore,

$$\boldsymbol{S}^2 = (\boldsymbol{S}_1 + \boldsymbol{S}_2)^2 = \boldsymbol{S}_1^2 + \boldsymbol{S}_2^2 + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$

Therefore the corrective energy is proportional to the product $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$,

$$H = -\mathcal{J}\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$

Which is minimized for aligned spins $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 > 0$. This result can be generalized to any number of electron spins using the **Heisenberg model**,

$$H = -\frac{1}{2}\mathcal{J}\sum_{\langle ij\rangle}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_B\boldsymbol{B}\cdot\sum_i\boldsymbol{S}_i \tag{2.1}$$

Where $\langle ij\rangle$ denotes nearest neighbor terms, the factor of $1/2$ avoids double-counting the interactions, and $\mathcal{J}$ forms a coupling constant proportional to,

$$\mathcal{J} \sim V\psi^2 \sim \frac{e^2}{a_0}$$

And the μ_B terms is simply the ordinary magnetic moment coupling. It is important to note that the nearest-neighbor approximation permits one to assume that $\mathcal{J}$ is a constant (depending only on the distance between nearest neighbors). The Heisenberg model eq. (2.1) is one of the simplest examples of a **quantum many-body problem** which are notoriously difficult to solve and are typically only approximated at best. One such approximation is called **mean-field theory**.

2.1   Mean-field Theory of the Heisenberg Model

Mean-field theory approximations of the Heisenberg model begin by re-writing the spins $\boldsymbol{S}_i$ as,

$$\boldsymbol{S}_i = \boldsymbol{S}_i - \langle \boldsymbol{S}_i \rangle + \langle \boldsymbol{S}_i \rangle$$

Therefore the spin product $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ includes many terms,

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = (\boldsymbol{S}_i - \langle \boldsymbol{S}_i \rangle + \langle \boldsymbol{S}_i \rangle) \cdot (\boldsymbol{S}_j - \langle \boldsymbol{S}_j \rangle + \langle \boldsymbol{S}_j \rangle)$$

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j = (\boldsymbol{S}_i - \langle \boldsymbol{S}_i \rangle) \cdot (\boldsymbol{S}_j - \langle \boldsymbol{S}_j \rangle) + \boldsymbol{S}_i \cdot \langle \boldsymbol{S}_j \rangle + \boldsymbol{S}_j \cdot \langle \boldsymbol{S}_i \rangle - \langle \boldsymbol{S}_i \rangle \cdot \langle \boldsymbol{S}_j \rangle \tag{2.2}$$

The mean-field approximation assumes that the deviations of $\boldsymbol{S}_i$ from their mean $\langle \boldsymbol{S}_i \rangle$ is small,

$$\boldsymbol{S}_i = \langle \boldsymbol{S}_i \rangle + \mathcal{O}\left((\boldsymbol{S}_i)^2 \right)$$

Therefore we can neglect the first term in eq. (2.2) for being quadratic in the deviation,

$$\boldsymbol{S}_i \cdot \boldsymbol{S}_j \simeq \boldsymbol{S}_i \cdot \langle \boldsymbol{S}_j \rangle + \boldsymbol{S}_j \cdot \langle \boldsymbol{S}_i \rangle - \langle \boldsymbol{S}_i \rangle \cdot \langle \boldsymbol{S}_j \rangle$$

Therefore eq. (2.1) becomes,

$$H = -\frac{1}{2}\mathcal{J} \sum_{\langle ij \rangle} [\boldsymbol{S}_i \cdot \langle \boldsymbol{S}_j \rangle + \boldsymbol{S}_j \cdot \langle \boldsymbol{S}_i \rangle - \langle \boldsymbol{S}_i \rangle \cdot \langle \boldsymbol{S}_j \rangle] - g\mu_B \boldsymbol{B} \cdot \sum_i \boldsymbol{S}_i$$