$$|\psi_n(k)\rangle = \sum_x u_{n,\alpha}(k)\, \frac{e^{i k x}}{\sqrt{2\pi/a}} \left| x \right\rangle \tag{3.209}$$

$$c_k^\dagger \left| G \right\rangle = \sum_x u_{n,\alpha}(k)\, \frac{e^{i k x}}{\sqrt{2\pi/a}}\, c_j^\dagger \left| G \right\rangle \tag{3.210}$$

Compare with

$$c_k^\dagger = \sum_j \frac{e^{i k x_j}}{\sqrt{2\pi/a}}\, c_j^\dagger \tag{3.211}$$

we find that $u_k = 1$.

So we know immediately that

$$\mathcal{A} = \mathcal{F} = 0 \tag{3.212}$$

There is no Hall effect.

3.12.2. Discrete Fourier transform and Fourier series

Consider a discrete function f_i, $i = 1, 2, 3 \ldots$N

Assuming periodic boundary condition $f_{N+i} = f_i$

For large system $N \to \infty$, different boundary conditions are believe to give the same results (But there are exceptions, e.g. the edge states in topological states of matter).

$$f_j = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k\, e^{i k a j} \tag{3.213}$$

$$\tilde{f}_k = \frac{1}{\sqrt{N}} \sum_j f_j\, e^{-i k a j} \tag{3.214}$$

- Same as j, k is also a discrete variable.

This is because $f_{N+i} = f_N$

$$f_{j+N} = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k\, e^{i k (a j + a N)} = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k\, e^{i k a j}\, e^{i k a N} \tag{3.215}$$

$$f_j = \frac{1}{\sqrt{N}} \sum_k \tilde{f}_k\, e^{i k a j} \tag{3.216}$$

Compare the two equations, we find that $e^{i k a N}=1$, which implies

$$k = \frac{2\pi m}{N a} = \frac{2\pi m}{L} \tag{3.217}$$

For infinite systems, $L \to \infty$, the discrete sum turns into an integral.

- Same as j, k also have a periodicity, and the periodicity is also N.

$$\tilde{f}_{k_m}\, e^{i k_m a j} = \tilde{f}_{k_m}\, e^{i \frac{2\pi}{N a} m a j} = \tilde{f}_{k_m}\, e^{i \frac{2\pi}{N} m j} \tag{3.218}$$

$$\tilde{f}_{k_{m+N}}\, e^{i k_{m+N} a j} = \tilde{f}_{k_{m+N}}\, e^{i \frac{2\pi}{N a}(m+N) a j} = \tilde{f}_{k_{m+N}}\, e^{i \frac{2\pi}{N a} m a j}\, e^{i \frac{2\pi}{N a} N a j} = \tilde{f}_{k_{m+N}}\, e^{i \frac{2\pi}{N} m j}\, e^{i 2\pi j} = \tilde{f}_{k_{m+N}}\, e^{i \frac{2\pi}{N} m j} \tag{3.219}$$

$$\tilde{f}_{k_m} = \tilde{f}_{k_{m+N}} \tag{3.220}$$

$$m = -\frac{N}{2}, -\frac{N}{2} + 1, \ \ldots \frac{N}{2} - 1, \tag{3.221}$$

$$k = -\frac{\pi}{L}, -\frac{\pi}{L} + 1\times\frac{2\pi}{L}, -\frac{\pi}{L} + 2\times\frac{2\pi}{L}, \ \ldots \frac{\pi}{L} - \frac{2\pi}{L}, \tag{3.222}$$

- Identities:

$$\frac{1}{N}\sum_k e^{i k a j} e^{-i k a j'} = \delta_{j,j'} \tag{3.223}$$

$$\frac{1}{N}\sum_j e^{i k a j} e^{-i k' a j} = \delta_{k,k'} \tag{3.224}$$

3.12.3. Example: a two-band model in 1D

$$H = -t\sum_i \left(a_i^\dagger b_i + b_i^\dagger a_{i+1} + h.c.\right) + V_a\sum_i a_i^\dagger a_i + V_b\sum_i b_i^\dagger b_i \tag{3.225}$$

Position of a sites in the jth unit cells:

$$r = a\times j + r_a \tag{3.226}$$

Position of b sites in the jth unit cells:

$$r = b\times j + r_b \tag{3.227}$$

$$a_k = \frac{1}{\sqrt{N}}\sum_i a_i\, e^{i k x} \tag{3.228}$$

$$a_i = \frac{1}{\sqrt{N}}\sum_k a_k\, e^{-i k x} \tag{3.229}$$

$$b_k = \frac{1}{\sqrt{N}}\sum_i a_i\, e^{i k x} \tag{3.230}$$

$$b_i = \frac{1}{\sqrt{N}}\sum_k a_k\, e^{-i k x} \tag{3.231}$$

$$\begin{aligned}\sum_j a_j^\dagger b_j = \sum_j \frac{1}{\sqrt{N}}\sum_k a_k^\dagger\, e^{-i k (a j+r_a)}\, \frac{1}{\sqrt{N}}\sum_{k'} b_{k'}\, e^{i k' (a j+r_b)} = \frac{1}{N}\sum_k\sum_{k'} a_k^\dagger b_{k'}\sum_j e^{-i k (a j+r_a)}\, e^{i k' (a j+r_b)} = \\ \sum_k\sum_{k'} a_k^\dagger b_{k'}\,\frac{1}{N}\sum_j e^{-i (k-k') a j}\, e^{-i k r_a}\, e^{i k' r_b} = \sum_k\sum_{k'} a_k^\dagger b_{k'}\,\delta_{k,k'}\, e^{-i k r_a}\, e^{i k' r_b} = \sum_k a_k^\dagger b_k\, e^{i k (r_b - r_a)}\end{aligned} \tag{3.232}$$

$$\sum_j b_j^\dagger a_{j+1} = \sum_k a_k^\dagger b_k\, e^{i k (r_a - r_b)} \tag{3.233}$$

Assume that $r_b - r_a = \frac{a}{2}$

$$\sum_j a_j^\dagger b_j = \sum_k a_k^\dagger b_k\, e^{i k a/2} \tag{3.234}$$

$$\sum_j b_j^\dagger a_{j+1} = \sum_k b_k^\dagger a_k\, e^{i k a/2} \tag{3.235}$$

We also know that

$$\sum_i a_i^\dagger a_i = \sum_k a_k^\dagger a_k \tag{3.236}$$

Therefore, in the k-space, the Hamiltonian looks like

$$\begin{aligned}H = -t\sum_k \left(a_k^\dagger b_k\, e^{i k a/2} + b_k^\dagger a_k\, e^{i k a/2} + b_k^\dagger a_k\, e^{-i k a/2} + a_k^\dagger b_k\, e^{-i k a/2}\right) + V_a\sum_k a_k^\dagger a_k + V_b\sum_k b_k^\dagger b_k = \\ -2t\sum_k\left[\left(a_k^\dagger b_k\cos\left(\frac{k a}{2}\right) + b_k^\dagger a_k\cos\left(\frac{k a}{2}\right)\right) + V_a a_k^\dagger a_k + V_b b_k^\dagger b_k\right]\end{aligned} \tag{3.237}$$

We can write it in a matrix form:

$$H = \sum_k \left(a_k^\dagger,\ b_k^\dagger\right) \begin{pmatrix} V_a & -2\,t\,\cos\left(\frac{k\,a}{2}\right) \\ -2\,t\cos\left(\frac{k\,a}{2}\right) & V_b \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.238}$$

- For any tight-binding models with two quantum states per unit cell, the Hamiltonian can be written in terns of a two-by-two matrix in the k space like this:

$$H = \sum_k \left(a_k^\dagger,\ b_k^\dagger\right) \mathcal{H}(k) \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.239}$$

where $\mathcal{H}$ is a 2×2 Hermitian matrix as a function of k. It is called the kernel of the Hamiltonian. It contains all the useful information of a Hamiltonian but it is NOT the Hamiltonian, although in literature, it is usually called a Hamiltonian.

For the model considered here,

$$\mathcal{H}(k) = \begin{pmatrix} V_a & -2\,t\,\cos\left(\frac{k\,a}{2}\right) \\ -2\,t\cos\left(\frac{k\,a}{2}\right) & V_b \end{pmatrix} \tag{3.240}$$

For more generic cases, if one have m quantum state per unit cell, this $\mathcal{H}$(k) will become a m×m Hermitian matrix. It captures all the information about the system, including the topological nature.

The bottom line: for any tight-binding models, at the end of the day, one will get a n×n matrix $\mathcal{H}$(k) which contains all the information of the Hamiltonian.

When we have a matrix, we know what to do to get eigenvalue and eigenfunctions of the Hamiltonian: we diagonalize the matrix.

At each k point, one can define a unitary transformation

$$\begin{pmatrix} c_k \\ d_k \end{pmatrix} = U_k^{-1} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.241}$$

$$\begin{pmatrix} c_k^\dagger & d_k^\dagger \end{pmatrix} = \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} U_k \tag{3.242}$$

where $U_k^{-1} = U_k^\dagger$

$$H = \sum_k \left(c_k^\dagger,\ d_k^\dagger\right) U_k^+ \mathcal{H}\, U_k \begin{pmatrix} c_k \\ d_k \end{pmatrix} \tag{3.243}$$

If we choose U_k such that $\mathrm{U_k}^+\ \mathcal{H}\ \mathrm{U_k}$ is a diagonal matrix,

$$U_k\, \mathcal{H}\, U_k^{-1} = \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix} \tag{3.244}$$

(assume $\epsilon_c < \epsilon_d$)

$$H = \sum_k \left(c_k^\dagger,\ d_k^\dagger\right) \begin{pmatrix} \epsilon_c & 0 \\ 0 & \epsilon_d \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix} = \sum_k \epsilon_c(k)\, c_k^\dagger\, c_k + \sum_k \epsilon_d(k)\, d_k^\dagger\, d_k \tag{3.245}$$

We know that using Bloch waves (which are eigenstates of the Hamiltonian), the total energy is

$$E = \sum_{k,n} \epsilon_n(k)\, n_n(k) = \sum_k \epsilon_1\, n_1(k) + \sum_k \epsilon_2\, n_2(k) + \sum_k \epsilon_3\, n_3(k) + \ldots \tag{3.246}$$

Therefore, in terms of Bloch waves, the Hamiltonian should take the form:

$$H = \sum_k \epsilon_1(k)\, \gamma_{1,k}^\dagger\, \gamma_{1,k} + \sum_k \epsilon_2(k)\, \gamma_{2,k}^\dagger\, \gamma_{2,k} + \sum_k \epsilon_3(k)\, \gamma_{3,k}^\dagger\, \gamma_{3,k} + \ldots \tag{3.247}$$

where $\gamma_{n,k}^\dagger$ is the creation operator for a bloch wave in band n at momentum k.

Compare with Eq. 245, we find that in this model we get a two energy bands (c and d). The dispersions are $\epsilon_c(k)$ and $\epsilon_d(k)$ respectively. $c^\dagger$ creates a Bloch wave with momentum k in the lower band. $d_k^\dagger$ creates a Bloch wave with momentum k in the upper bands.

For the problem we considered here, the dispersions are

$$\epsilon_c = \frac{V_a + V_b}{2} - \sqrt{\left[2\,t\cos\left(\frac{k\,a}{2}\right)\right]^2 + \left(\frac{V_a - V_b}{2}\right)^2} \tag{3.248}$$

$$\epsilon_d = \frac{V_a + V_b}{2} + \sqrt{\left[2\,t\cos\left(\frac{k\,a}{2}\right)\right]^2 + \left(\frac{V_a - V_b}{2}\right)^2} \tag{3.249}$$

Q: What determines the number of bands n?

A: Number of allowed quantum states in a unit cells.

In general, if each unit cell contains m quantum states described by the fermion operators c_1, c_2… c_m, the tight-binding model will contains m energy bands and the kernel $\mathcal{H}_k$ will be a m×m matrix.

Q: What can we learn from the eigenvectors of $\mathcal{H}$(k).

A: $u_{n,k}$, the coeffiicent for the Bloch waves.

We know that a Bloch wave in a continous space is:

$$\psi_{n,k}(x) = u_{n,\,k}(x)\,\frac{e^{i\,k\,x}}{\sqrt{N}} \tag{3.250}$$

For tight-binding models, $u_{n,k}(x)$ is now a discrete function in the real space. Due to the periodic structure, we only need to know the value $u_{n,k}(x)$ in one unit cell. In other works, we just need to know the value of this function at site a and b for the two band model we considered here (only two values). Therefore, $u_{n,k}$ is now a two component vector:

$$u_{n,k}(x) = (u_{i,a}(k),\ u_{i,b}(k)) \tag{3.251}$$

The eignevectors of $\mathcal{H}$(k) are also a 2-component vector:

$$\mathcal{H}\begin{pmatrix} v^{(-)}{}_a(k) \\ v^{(-)}{}_b(k) \end{pmatrix} = \epsilon_c \begin{pmatrix} v^{(-)}{}_a(k) \\ v^{(-)}{}_b(k) \end{pmatrix} \tag{3.252}$$

$$\mathcal{H}\begin{pmatrix} v^{(+)}{}_a(k) \\ v^{(+)}{}_b(k) \end{pmatrix} = \epsilon_d \begin{pmatrix} v^{(+)}{}_a(k) \\ v^{(+)}{}_b(k) \end{pmatrix} \tag{3.253}$$

And in fact, these eigenvectors are percisely the coefficent of the Bloch waves ($u_{n,k}$).

$$c_k{}^\dagger = v^{(-)}{}_a(k)\,a_k{}^\dagger + v^{(-)}{}_b(k)\,b_k{}^\dagger \tag{3.254}$$

$$d_k{}^\dagger = v^{(+)}{}_a(k)\,a_k{}^\dagger + v^{(+)}{}_b(k)\,b_k{}^\dagger \tag{3.255}$$

For more generic cases, for a m-band model, there are m eigenvectors $u_{n,\alpha}(k)$ with n=1,2,…m, where n is the band index. For each band n, the eignevector is precisely the coeffiecient $u_{n,k}$ of the Bloch wave for this band.

In the continoum we have $u_{n,k}(x)$. For tight-binding models, we have $u_n(k) = (u_{n,1}(k),\ u_{n,2}(k)\ \ldots\ u_{n,m}(k))$.

For each bands, we can define $\mathcal{A}$

For the continous case, we have

$$\mathcal{A}_n = -i\,\langle u_n(k)\,|\,\partial_k\,|\,u_n(k)\rangle = -i\int d\vec{r}\,u_n(k,\,r)^*\,\partial_k\,u_n(k,\,r) \tag{3.256}$$

For tight-binding models, we have

$$\mathcal{A}_n = -i\,\langle u_n(k)\,|\,\partial_k\,|\,u_n(k)\rangle = -i\sum_\alpha u_{n,\alpha}(k)^*\,\partial_k\,u_{n,\alpha}(k) \tag{3.257}$$

3.12.4. Summary

- Tight-Binding model: a discrete version of Bloch waves
- The key properties of a tight-binding model is coded in $\mathcal{H}_k$, which is a m×m Hermitian matrix. Each component is a function of k. (In other words, $\mathcal{H}_k$ is a matrix function of k.)
- The eigenvalues if $\mathcal{H}$ (as a function of k) gives the band structure (the dispersion relation) for each bands $\epsilon_n(k)$ with $n = 1,\ 2,\ \ldots$m
- The eigenvectors as a function of k gives the Bloch wave: $u_{n,\alpha}(k)$, where n=1,2,…, m is the band index and α=1,2…m marks different site in a unit cell.