Derivation of Hofstadter's butterfly

Le Hoang Anh

ID 2018010903, Physics Department, Korea University, Seoul 136-713, Korea

We consider tight-binding model applied on a square lattice with lattice constant a whose sites are located at $(x, y) = (ma, na)$. We assume $0 \leq m, n < L$ so the system size is $N = L^2$. The system is subjected to an external magnetic field along z direction, and here we choose the Landau gauge $\vec{A} = (0, Bx, 0)$. In the presence of magnetic field, the hopping terms transform as

$$\begin{aligned} -te^{-i\frac{e}{\hbar c}\vec{A}\cdot(\vec{r}_1-\vec{r}_2)} &= -te^{-i\frac{2\pi}{\phi_0}Bx\vec{e}_y\cdot(\vec{r}_1-\vec{r}_2)} \\ &= \begin{cases} -t & \text{, hopping in } x \text{ direction} \\ -te^{i2\pi\frac{Ba^2}{\phi_0}m} = te^{i2\pi\frac{\phi}{\phi_0}m} = te^{i2\pi\alpha m} & \text{, hopping in } y \text{ direction} \end{cases} . \end{aligned} \tag{1}$$

We hence obtain the Hamiltonian for system as follows

$$H = \sum_{m,n}\left(-ta^\dagger_{m+1,n}a_{m,n} - te^{i2\pi\alpha m}a^\dagger_{m,n+1}a_{m,n}\right) + \text{h.c.} \tag{2}$$

We will perform the Fourier transformation to the field operators $a^\dagger$ and a

$$a_{m,n} = \frac{1}{N}\sum_{k_x,k_y} e^{ik_xma+ik_yna}b_{k_x,k_y}, \tag{3}$$

where $-\frac{\pi}{a} \leq k_x, k_y < \frac{\pi}{a}$. Because of the Landau gauge, the hopping term in the x-direction is not affected by the magnetic field. Its Fourier transformation is therefore straightforward as

$$-t\sum_{m,n} a^\dagger_{m+1,n}a_{m,n} + \text{h.c} = \sum_{m,n} -2t\cos(k_xa)b^\dagger_{k_x,k_y}b_{k_x,k_y} \tag{4}$$

On the other hand, the hopping term in y direction is affected by the magnetic field, it transforms as follow

$$\begin{aligned} \sum_{m,n} -te^{i2\pi\alpha m}a^\dagger_{m,n+1}a_{m,n} + \text{h.c} &= \frac{-te^{i2\pi\alpha m}}{N^2}\sum_{k_x,k_y,k'_x,k'_y} e^{-ik_xma-ik_y(n+1)a}b^\dagger_{k_x,k_y}e^{ik'_xma+ik'_yna}b_{k'_x,k'_y} + \text{h.c} \\ &= \frac{-t}{N^2}\sum_{k_x,k_y,k'_x,k'_y} e^{i\left(k'_x-k_x+\frac{2\pi\alpha m}{a}\right)ma}e^{i\left(k'_y-k_y\right)na}e^{-ik_ya}b^\dagger_{k_x,k_y}b_{k'_x,k'_y} + \text{h.c} \\ &= \sum_{k_x,k_y} -te^{-ik_ya}b^\dagger_{k_x-\frac{2\pi\alpha}{a},k_y}b_{k_x,k_y} - te^{ik_ya}b^\dagger_{k_x+\frac{2\pi\alpha}{a},k_y}b_{k_x,k_y}. \end{aligned} \tag{5}$$

The total Hamiltonian now takes the following form

$$H = \sum_{k_x,k_y} -2t\cos(k_xa)b^\dagger_{k_x,k_y}b_{k_x,k_y} - te^{-ik_ya}b^\dagger_{k_x-\frac{2\pi\alpha}{a},k_y}b_{k_x,k_y} - te^{ik_ya}b^\dagger_{k_x+\frac{2\pi\alpha}{a},k_y}b_{k_x,k_y}. \tag{6}$$

We notice that k_x is being shifted by an amount of $\frac{2\pi\alpha}{a}$. Let us apply the following variable change, $k_x \to k_x + \frac{2\pi\alpha}{a}m$ with $0 \leq m < L$, as a result the first BZ along k_x is changed as $-\frac{\pi}{aL} \leq k_x < \frac{\pi}{aL}$. One should notice that with such variable change, if the ratio of unit-cell flux is a rational number, i.e $\alpha = p/q$, k_x is periodic with period q. The Hamiltonian is rewritten as

$$\begin{aligned} H = \sum_{k_x,k_y} &- 2t\cos(k_xa + \frac{2\pi\alpha m}{a})b^\dagger_{k_x+\frac{2\pi\alpha m}{a},k_y}b_{k_x+\frac{2\pi\alpha m}{a},k_y} \\ &- te^{-ik_ya}b^\dagger_{k_x+\frac{2\pi\alpha(m-1)}{a},k_y}b_{k_x+\frac{2\pi\alpha m}{a},k_y} - te^{ik_ya}b^\dagger_{k_x+\frac{2\pi\alpha(m+1)}{a},k_y}b_{k_x+\frac{2\pi\alpha m}{a},k_y}. \end{aligned} \tag{7}$$

Assume the eigenstates can be written in the form of

$$|\psi\rangle_{k_x,k_y} = \sum_{m=0}^{L-1} A_m b^\dagger_{k_x+\frac{2\pi\alpha m}{a},k_y} |0\rangle\,, \tag{8}$$

one can derive a system of L equations, in which the m^{th} equation is written as

$$-2\cos(k_x + 2\pi\alpha m)A_m - e^{-ik_y}A_{m-1} - e^{ik_y}A_{m+1} = \epsilon A_m, \tag{9}$$

here $\epsilon = E/t$ and $a = 1$ for simplicity. Before constructing the matrix for general q, we first examine several small-q cases which can be solved analytically. In the case $q = 1$ (or $\alpha = \phi/\phi_0 = 1$ equivalently), according to the periodic condition we have $A_0 = A_{0+1} = A_{0-1}$, the solution of energy is straightforwardly computed as

$$\epsilon = -2\cos k_x - e^{-ik_y} - e^{ik_y} = -2\cos k_x - 2\cos k_y \tag{10}$$

In the case $q = 2$ (or $\alpha = \phi/\phi_0 = 1/2$), there are 2 energy bands corresponding to the eigenvalues of the following 2×2 matrix

$$\begin{pmatrix} -2\cos(2\pi\alpha\cdot 0 + k_x) & -e^{-ik_y} - e^{ik_y} \\ -e^{-ik_y} - e^{ik_y} & -2\cos(2\pi\alpha\cdot 1 + k_x) \end{pmatrix} \rightarrow \epsilon = \pm 2\sqrt{\cos^2 k_x + \cos^2 k_y}. \tag{11}$$

In the case of general q, there exists exactly q energy bands as they are the eigenvalues of a $q\times q$ matrix

$$\begin{pmatrix} -2\cos(2\pi\alpha\cdot 0 + k_x) & -e^{ik_y} & 0 & \cdots & e^{-ik_y} \\ -e^{-ik_y} & -2\cos(2\pi\alpha\cdot 1 + k_x) & -e^{ik_y} & \cdots & 0 \\ 0 & -e^{-ik_y} & -2\cos(2\pi\alpha\cdot 2 + k_x) & \cdots & 0 \\ \vdots & & & & \vdots \\ e^{ik_y} & & & \cdots & -2\cos(2\pi\alpha\cdot(q-1) + k_x) \end{pmatrix}. \tag{12}$$

Notice that the periodic boundary condition is encoded by position of e^{ik_y} at the bottom left of the matrix and its conjugated element.

I numerically solved the above matrix for various data points of k_x and k_y to obtain such Hofstadter's butterfly.