Hamiltonian in magnetic field using tight binding model

TRẦN KHÔI NGUYÊN

VẬT LÝ LÝ THUYẾT

Ngày 30 tháng 11 năm 2024

d_z band

$$
\begin{aligned}
h_0 &= 2E_{11}^{11}\left(\mathbf{R_1}\right)\left(\cos 2\alpha + 2\cos\alpha\cos\beta\right) + \epsilon_1 \\
&= 2t_0\left[\cos(k_x a) + 2\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{\sqrt{3}k_y a}{2}\right)\right] + \epsilon_1 \\
&= 2t_0\left[\cos\left(\frac{\hbar k_x a}{\hbar}\right) + 2\cos\left(\frac{1}{2}\frac{\hbar k_x a}{\hbar}\right)\cos\left(\frac{\sqrt{3}}{2}\frac{\hbar k_y a}{\hbar}\right)\right] + \epsilon_1 \\
&= 2t_0\left[\cos\left(\frac{p_x - eA_x}{\hbar}a\right) + 2\cos\left(\frac{1}{2}\frac{p_x - eA_x}{\hbar}a\right)\cos\left(\frac{\sqrt{3}}{2}\frac{p_y - eA_y}{\hbar}a\right)\right] + \epsilon_1 \\
&= 2t_0\left[\cos\left(\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}a\right) + 2\cos\left(\frac{1}{2}\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}a\right)\cos\left(\frac{\sqrt{3}}{2}\frac{-i\hbar\frac{\partial}{\partial y} - eBx}{\hbar}a\right)\right] + \epsilon_1 \\
&= 2t_0\underbrace{\left[\frac{e^{\frac{\partial}{\partial x}a} + e^{-\frac{\partial}{\partial x}a}}{2} + \frac{1}{2}\left(e^{\frac{\partial}{\partial x}a\frac{1}{2}} + e^{-\frac{\partial}{\partial x}a\frac{1}{2}}\right)\left(e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}\right)\right]}_{\text{hopping terms}} + \epsilon_1
\end{aligned}
$$

Schrödinger's equation now becomes

$$
\begin{aligned}
&\varphi_0(x+a,y) + \varphi_0(x-a,y) + \varphi_0(x+\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \varphi_0(x+\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&+ \varphi_0(x-\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \varphi_0(x-\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} = \frac{E_0}{t_0}\varphi_0(x,y) \qquad (1)
\end{aligned}
$$

where $\varphi_0 = |d_z\rangle$.

Let:

$$
\begin{cases}
x = ma \\
y = na
\end{cases}
$$

We rewrite (1) in the form of index (m,n)

$$
\begin{aligned}
\frac{E_0}{t_0}\varphi_0(m,n) = {} & \varphi_0(m+2,n) + \varphi_0(m-2,n) \\
& + \varphi_0(m+1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \varphi_0(m-1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
& + \varphi_0(m+1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \varphi_0(m-1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \qquad (2)
\end{aligned}
$$

Seperate variables method : $\varphi_0(m,n) = e^{ik_y na}G_0(m)$.

Let $\frac{e}{\hbar}\frac{Bma^2\sqrt{3}}{2} = 2\pi\frac{\Phi}{\Phi_0}m = 2\pi m\frac{p}{q}$, $\gcd(p, q) = 1$, this lead to:

$$\begin{aligned}\frac{E_0}{t_0}G_0(m) &= G_0(m+2) + G_0(m-2) + \left[e^{i(2\pi m\alpha - k_y a)} + e^{-i(2\pi m\alpha - k_y a)}\right] G_0(m-1)\\ &+ \left[e^{i(2\pi m\alpha - k_y a)} + e^{-i(2\pi m\alpha - k_y a)}\right] G_0(m+1)\\ &= G_0(m+2) + G_0(m-2)\\ &+ \cos\left(2\pi m\alpha - k_y a\right) G_0(m-1) + \cos\left(2\pi m\alpha - k_y a\right) G_0(m+1) \qquad (3)\end{aligned}$$

where m is to be set go through q, $m = 1, 2, ...q$. This leads to set equations by index m. Since the set of equations are repeated for $m \geq q + 1$.

Equation (3) is Harper's equation for the hexagonal lattice with d_z band.

The next matrices element in Hamiltonian with d_z band is h_1 and h_2.

$\mathbf{h_1}$

$$
\begin{aligned}
h_1 &= -2\sqrt{3}t_2 \sin\alpha \sin\beta + 2it_1(\sin 2\alpha + \sin\alpha\cos\beta) \\
&= -2\sqrt{3}t_2 \sin\left(\frac{1}{2}\frac{\hbar k_x a}{\hbar}\right)\sin\left(\frac{\sqrt{3}}{2}\frac{\hbar k_y a}{\hbar}\right) + 2it_1\left[\sin\left(\frac{\hbar k_x a}{\hbar}\right) + \sin\left(\frac{1}{2}\frac{\hbar k_x a}{\hbar}\right)\cos\left(\frac{\sqrt{3}}{2}\frac{\hbar k_y a}{\hbar}\right)\right] \\
&= -2\sqrt{3}t_2 \sin\left(\frac{a}{2}\frac{p_x - eA_x}{\hbar}\right)\sin\left(\frac{\sqrt{3}a}{2}\frac{p_y - eA_y}{\hbar}\right) \\
&+ 2it_1\left[\sin\left(\frac{p_x - eA_x}{\hbar}a\right) + \sin\left(\frac{a}{2}\frac{p_x - eA_x}{\hbar}\right)\cos\left(\frac{\sqrt{3}a}{2}\frac{p_y - eA_y}{\hbar}\right)\right] \\
&= -2\sqrt{3}t_2 \sin\left(\frac{a}{2}\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}\right)\sin\left(\frac{\sqrt{3}a}{2}\frac{-i\hbar\frac{\partial}{\partial y} - eBx}{\hbar}\right) \\
&+ 2it_1\left[\sin\left(\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}a\right) + \sin\left(\frac{a}{2}\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}\right)\cos\left(\frac{\sqrt{3}a}{2}\frac{-i\hbar\frac{\partial}{\partial y} - eBx}{\hbar}\right)\right] \\
&= -2\sqrt{3}t_2\left(\frac{e^{\frac{\partial}{\partial x}\frac{a}{2}} - e^{-\frac{\partial}{\partial x}\frac{a}{2}}}{2i}\right)\left(\frac{e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}}{2i}\right) \\
&+ 2it_1\left[\left(\frac{e^{\frac{\partial}{\partial x}a} - e^{-\frac{\partial}{\partial x}a}}{2i}\right) + \left(\frac{e^{\frac{\partial}{\partial x}\frac{a}{2}} - e^{-\frac{\partial}{\partial x}\frac{a}{2}}}{2i}\right)\left(\frac{e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}}{2}\right)\right] \\
&= \frac{\sqrt{3}}{2}t_2\left(e^{\frac{\partial}{\partial x}\frac{a}{2}} - e^{-\frac{\partial}{\partial x}\frac{a}{2}}\right)\left(e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}\right) \\
&+ t_1\left[\left(e^{\frac{\partial}{\partial x}a} - e^{-\frac{\partial}{\partial x}a}\right) + \frac{1}{2}\left(e^{\frac{\partial}{\partial x}\frac{a}{2}} - e^{-\frac{\partial}{\partial x}\frac{a}{2}}\right)\left(e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}\right)\right]
\end{aligned}
$$

Schrödinger's equation now becomes

$$
\begin{aligned}
&t_1\varphi_1(x+a,y) - t_1\varphi_1(x-a,y) + \frac{t_1}{2}\varphi_1(x+\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&+ \frac{t_1}{2}\varphi_1(x+\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} - \frac{t_1}{2}\varphi_1(x-\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&- \frac{t_1}{2}\varphi_1(x-\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \frac{\sqrt{3}t_2}{2}\varphi_1(x+\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&+ \frac{\sqrt{3}t_2}{2}\varphi_1(x+\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} - \frac{\sqrt{3}t_2}{2}\varphi_1(x-\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&- \frac{\sqrt{3}t_2}{2}\varphi_1(x-\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} = E_1\varphi_1(x,y) \qquad (4)
\end{aligned}
$$

Simplify equation (4),this lead to

$$t_1\varphi_1(x+a,y)-t_1\varphi_1(x-a,y)+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(x+\frac{a}{2},y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(x+\frac{a}{2},y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(x-\frac{a}{2},y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(x-\frac{a}{2},y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}=E_1\varphi_1(x,y) \tag{5}$$

We write equation (5) in form of index (m,n)

$$t_1\varphi_1(m+2,n)-t_1\varphi_1(m-2,n)+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(m+1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(m+1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(m-1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\varphi_1(m-1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}=E\varphi_1(m,n) \tag{6}$$

And rewrite in form of $G_1(m)$

$$\begin{aligned}E_1G_1(m)&=t_1G_1(m+2)+t_1G_1(m-2)+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\left[e^{i(2\pi m\alpha-k_ya)}+e^{-i(2\pi m\alpha-k_ya)}\right]G_1(m+1)\\&-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\left[e^{i(2\pi m\alpha-k_ya)}+e^{-i(2\pi m\alpha-k_ya)}\right]G_1(m-1)\\&=t_1G_1(m+2)+t_1G_1(m-2)+\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\cos\big(2\pi m\alpha-k_ya\big)G_1(m+1)\\&-\left(\frac{t_1+\sqrt{3}t_2}{2}\right)\cos\big(2\pi m\alpha-k_ya\big)G_1(m-1)\end{aligned} \tag{7}$$

$\mathbf{h_2}$

$$
\begin{aligned}
h_2 &= 2t_2\left(\cos 2\alpha - \cos\alpha\cos\beta\right) + 2\sqrt{3}it_1\cos\alpha\sin\beta \\
&= 2t_2\left[\cos\left(\frac{\hbar k_x a}{\hbar}\right) - \cos\left(\frac{1}{2}\frac{\hbar k_x a}{\hbar}\right)\cos\left(\frac{\sqrt{3}}{2}\frac{\hbar k_y a}{\hbar}\right)\right] + 2\sqrt{3}it_1\cos\left(\frac{1}{2}\frac{\hbar k_x a}{\hbar}\right)\sin\left(\frac{\sqrt{3}}{2}\frac{\hbar k_y a}{\hbar}\right) \\
&= 2t_2\left[\cos\left(\frac{p_x - eA_x}{\hbar}a\right) - \cos\left(\frac{1}{2}\frac{p_x - eA_x}{\hbar}a\right)\cos\left(\frac{\sqrt{3}}{2}\frac{p_y - eA_y}{\hbar}a\right)\right] \\
&+ 2\sqrt{3}it_1\cos\left(\frac{1}{2}\frac{p_x - eA_x}{\hbar}a\right)\sin\left(\frac{\sqrt{3}}{2}\frac{p_y - eA_y}{\hbar}a\right) \\
&= 2t_2\left[\cos\left(\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}a\right) - \cos\left(\frac{a}{2}\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}\right)\cos\left(\frac{\sqrt{3}a}{2}\frac{-i\hbar\frac{\partial}{\partial x} - eBx}{\hbar}\right)\right] \\
&+ 2\sqrt{3}it_1\cos\left(\frac{a}{2}\frac{-i\hbar\frac{\partial}{\partial x}}{\hbar}\right)\sin\left(\frac{\sqrt{3}a}{2}\frac{-i\hbar\frac{\partial}{\partial y} - eBx}{\hbar}\right) \\
&= 2t_2\left[\frac{e^{\frac{\partial}{\partial x}a} + e^{-\frac{\partial}{\partial x}a}}{2} - \left(\frac{e^{\frac{\partial}{\partial x}\frac{a}{2}} + e^{-\frac{\partial}{\partial x}\frac{a}{2}}}{2}\right)\left(\frac{e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}}{2}\right)\right] \\
&+ 2\sqrt{3}it_1\left(\frac{e^{\frac{\partial}{\partial x}\frac{a}{2}} + e^{-\frac{\partial}{\partial x}\frac{a}{2}}}{2}\right)\left(\frac{e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}}{2i}\right) \\
&= t_2\left[\left(e^{\frac{\partial}{\partial x}a} + e^{-\frac{\partial}{\partial x}a}\right) - \frac{1}{2}\left(e^{\frac{\partial}{\partial x}\frac{a}{2}} + e^{-\frac{\partial}{\partial x}\frac{a}{2}}\right)\left(e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}\right)\right] \\
&+ \frac{\sqrt{3}}{2}t_1\left(e^{\frac{\partial}{\partial x}\frac{a}{2}} + e^{-\frac{\partial}{\partial x}\frac{a}{2}}\right)\left(e^{\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + e^{-\frac{\sqrt{3}}{2}\frac{\partial}{\partial y}a}e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}\right)
\end{aligned}
$$

Schrödinger's equation now becomes

$$
\begin{aligned}
&t_2\varphi_2(x+a,y) + t_2\varphi_2(x-a,y) - \frac{t_2}{2}\varphi_2(x+\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&- \frac{t_2}{2}\varphi_2(x+\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} - \frac{t_2}{2}\varphi_2(x-\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&- \frac{t_2}{2}\varphi_2(x-\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \frac{\sqrt{3}}{2}t_1\varphi_2(x+\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&+ \frac{\sqrt{3}}{2}t_1\varphi_2(x+\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} + \frac{\sqrt{3}}{2}t_1\varphi_2(x-\frac{a}{2}, y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} \\
&+ \frac{\sqrt{3}}{2}t_1\varphi_2(x-\frac{a}{2}, y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}} = E_2\varphi_2(x,y) \qquad (8)
\end{aligned}
$$

Symplify equation (8) , leads to

$$t_2\varphi_2(x+a,y)+t_2\varphi_2(x-a,y)+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(x+\frac{a}{2},y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(x+\frac{a}{2},y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(x-\frac{a}{2},y+\frac{a\sqrt{3}}{2})e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(x-\frac{a}{2},y-\frac{a\sqrt{3}}{2})e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}=E_2\varphi_2(x,y)$$

And rewrite it in form index (m,n)

$$t_2\varphi_2(m+2,n)+t_2\varphi_2(m-2,n)+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(m+1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(m+1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(m-1,n+1)e^{-\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}$$
$$+\left(\frac{\sqrt{3}}{2}t_1-\frac{t_2}{2}\right)\varphi_2(m-1,n-1)e^{\frac{ie}{\hbar}Bxa\frac{\sqrt{3}}{2}}=E_2\varphi_2(m,n)$$

Use variables seperation method, give

$$E_1G_2(m)=t_2G_2(m+2)+t_2G_2(m-2)+\left(\frac{\sqrt{3}t_1-t_2}{2}\right)\left[e^{i(2\pi m\alpha-k_ya)}+e^{-i(2\pi m\alpha-k_ya)}\right]G_2(m+1)$$
$$+\left(\frac{\sqrt{3}t_1-t_2}{2}\right)\left[e^{i(2\pi m\alpha-k_ya)}+e^{-i(2\pi m\alpha-k_ya)}\right]G_2(m-1) \tag{9}$$

d_{xy} **band**

d_{z^2} **band**

Recurrence

Assume $p=1,q=3$, we write Harper's equation (3) as,

$$m=1:G_0(3)+G(-1)+\cos\left(2\pi.1.\frac{1}{3}-k_ya\right)G_0(0)+\cos\left(2\pi.1.\frac{1}{3}-k_ya\right)G_0(2)=\frac{E_0}{t_0}G_0(1)$$
$$m=2:G_0(4)+G_0(0)+\cos\left(2\pi.2.\frac{1}{3}-k_ya\right)G_0(1)+\cos\left(2\pi.2.\frac{1}{3}-k_ya\right)G_0(3)=\frac{E_0}{t_0}G_0(2)$$
$$m=3:G_0(5)+G_0(1)+\cos\left(2\pi.3.\frac{1}{3}-k_ya\right)G_0(2)+\cos\left(2\pi.3.\frac{1}{3}-k_ya\right)G_0(4)=\frac{E_0}{t_0}G_0(3)$$

As we can see, $G(-1),G_0(0),G_0(4),G_0(5)$ are unknow points, so we need initial condition for those points, which we will use is the Bloch condition and take(Gumps, et al, 1997)

$$G(-1) = e^{-ik_xqa}G(q-1) \quad ; \quad G(0) = e^{-ik_xqa}G(q)$$
$$G(q+1) = e^{ik_xqa}G(1) \quad ; \quad G(q+2) = e^{ik_xqa}G(2)$$

We apply Bloch condition on $G(-1), G_0(0), G_0(4), G_0(5)$ wave function in the set m of Harper equations, this leads to

$$\begin{cases} G_0(3) + e^{-3ik_xa}G_0(2) + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right)e^{-3ik_xa}G_0(3) + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right)G_0(2) & = \dfrac{E_0}{t_0}G_0(1) \\ e^{3ik_xa}G_0(1) + e^{-3ik_xa}G_0(3) + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right)G_0(1) + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right)G_0(3) & = \dfrac{E_0}{t_0}G_0(2) \\ e^{3ik_xa}G_0(2) + G_0(1) + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right)G_0(2) + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right)e^{3ik_xa}G_0(1) & = \dfrac{E_0}{t_0}G_0(3) \end{cases}$$

$$\begin{cases} -\dfrac{E_0}{t_0}G_0(1) + \left[e^{-3ik_xa} + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right)\right]G_0(2) + \left[1 + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right)e^{-3ik_xa}\right]G_0(3) & = 0 \\ \left[e^{3ik_xa} + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right)\right]G_0(1) - \dfrac{E_0}{t_0}G_0(2) + \left[e^{-3ik_xa} + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right)\right]G_0(3) & = 0 \\ \left[1 + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right)e^{3ik_xa}\right]G_0(1) + \left[e^{3ik_xa} + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right)\right]G_0(2) - \dfrac{E_0}{t_0}G_0(3) & = 0 \end{cases}$$

These three independent equations rewrite in a charaterisc equation:

$$\begin{pmatrix} -\frac{E_0}{t_0} & e^{-3ik_xa} + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right) & 1 + \cos\left(2\pi.1.\frac{1}{3} - k_ya\right)e^{-3ik_xa} \\ e^{3ik_xa} + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right) & -\frac{E_0}{t_0} & e^{-3ik_xa} + \cos\left(2\pi.2.\frac{1}{3} - k_ya\right) \\ 1 + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right)e^{3ik_xa} & e^{3ik_xa} + \cos\left(2\pi.3.\frac{1}{3} - k_ya\right) & -\frac{E_0}{t_0} \end{pmatrix}$$
$$\times \begin{pmatrix} G_0(1) \\ G_0(2) \\ G_0(3) \end{pmatrix} = 0$$

which, E_0 is on-site energy, t_0 is hopping energy.

Equation (7)

$$m = 1: t_1G_1(3) + t_1G_1(-1) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.1.\alpha - k_ya\right)G_1(2)$$
$$-\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.1.\alpha - k_ya\right)G_1(0) = E_1G_1(1)$$
$$m = 2: t_1G_1(4) + t_1G_1(0) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.2.\alpha - k_ya\right)G_1(3)$$
$$-\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.2.\alpha - k_ya\right)G_1(1) = E_1G_1(2)$$
$$m = 3: t_1G_1(5) + t_1G_1(1) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.3.\alpha - k_ya\right)G_1(4)$$
$$-\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.3.\alpha - k_ya\right)G_1(2) = E_1G_1(3)$$

Apply Bloch condition on $G_1(-1), G_1(0), G_1(4), G_1(5)$, give

$$\begin{cases} t_1G_1(3) + t_1e^{-3ik_xa}G_1(2) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.1.\alpha - k_ya\right)G_1(2) \\ -\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.1.\alpha - k_ya\right)e^{-3ik_xa}G_1(3) = E_1G_1(1) \\ t_1e^{3ik_xa}G_1(1) + t_1e^{-3ik_xa}G_1(3) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.2.\alpha - k_ya\right)G_1(3) \\ -\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.2.\alpha - k_ya\right)G_1(1) = E_1G_1(2) \\ t_1e^{3ik_xa}G_1(2) + t_1G_1(1) + \left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.3.\alpha - k_ya\right)e^{3ik_xa}G_1(1) \\ -\left(\frac{t_1 + \sqrt{3}t_2}{2}\right)\cos\left(2\pi.3.\alpha - k_ya\right)G_1(2) = E_1G_1(3) \end{cases}$$

$$
\begin{cases}
-E_1 G_1(1) + \left[t_1 e^{-3ik_x a} + \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.1.\alpha - k_y a\right) \right] G_1(2) \\
+ \left[t_1 - \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.1.\alpha - k_y a\right) e^{-3ik_x a} \right] G_1(3) = 0, \\
\left[t_1 e^{3ik_x a} - \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.2.\alpha - k_y a\right) \right] G_1(1) - E_1 G_1(2) \\
+ \left[t_1 e^{-3ik_x a} + \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.2.\alpha - k_y a\right) \right] G_1(3) = 0, \\
\left[t_1 + \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.3.\alpha - k_y a\right) e^{3ik_x a} \right] G_1(1) \\
\left[t_1 e^{3ik_x a} - \left(\dfrac{t_1 + \sqrt{3} t_2}{2} \right) \cos\left(2\pi.3.\alpha - k_y a\right) \right] G_1(2) - E_1 G_1(3) = 0
\end{cases}
$$

These three independent equations rewrite in a charaterisc equation:

$$
\left(\begin{array}{c|c|c}
-E_1 & \begin{array}{c} t_1 e^{-3ik_x a} \\ + \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.1.\alpha - k_y a\right) \end{array} & \begin{array}{c} t_1 \\ - \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.1.\alpha - k_y a\right) e^{-3ik_x a} \end{array} \\
\hline
\begin{array}{c} t_1 e^{3ik_x a} \\ - \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.2.\alpha - k_y a\right) \end{array} & -E_1 & \begin{array}{c} t_1 e^{-3ik_x a} \\ + \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.2.\alpha - k_y a\right) \end{array} \\
\hline
\begin{array}{c} t_1 \\ + \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.3.\alpha - k_y a\right) e^{3ik_x a} \end{array} & \begin{array}{c} t_1 e^{3ik_x a} \\ - \left(\frac{t_1 + \sqrt{3} t_2}{2} \right) \\ \times \cos\left(2\pi.3.\alpha - k_y a\right) \end{array} & -E_1
\end{array}\right)
$$

$$
\times \begin{pmatrix} G_1(1) \\ G_1(2) \\ G_1(3) \end{pmatrix} = 0
$$

Equation (9)

$$m = 1 : t_2G_2(3) + t_2G_2(-1) + \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)G_2(2)$$
$$+ \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)G_2(0) = E_2G_2(1)$$
$$m = 2 : t_2G_2(4) + t_2G_2(0) + \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)G_2(3)$$
$$+ \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)G_2(1) = E_2G_2(2)$$
$$m = 3 : t_2G_2(5) + t_2G_2(1) + \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)G_2(4)$$
$$+ \left(\frac{\sqrt{3}t_1 - t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)G_2(2) = E_2G_2(3)$$

Apply Bloch condition on $G(-1), G_0(0), G_0(4), G_0(5)$, leads to

$$\begin{cases} t_2G_2(3) + t_2e^{-3ik_xa}G_2(2) + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)G_2(2) \\ + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)e^{-3ik_xa}G_2(3) = E_2G_2(1) \\ t_2e^{3ik_xa}G_2(1) + t_2e^{-3ik_xa}G_2(3) + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)G_2(3) \\ + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)G_2(1) = E_2G_2(2) \\ t_2e^{3ik_xa}G_2(2) + t_2G_2(1) + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)e^{3ik_xa}G_2(1) \\ + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)G_2(2) = E_2G_2(3) \end{cases}$$

Rearrange these three equations

$$\begin{cases} -E_2G_2(1) + \left[t_2e^{-3ik_xa} + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)\right]G_2(2) \\ + \left[t_2 + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.1.\alpha - k_ya\big)e^{-3ik_xa}\right]G_2(3) = 0 \\ \left[t_2e^{3ik_xa} + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)\right]G_2(1) - E_2G_2(2) \\ + \left[t_2e^{-3ik_xa} + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.2.\alpha - k_ya\big)\right]G_2(3) = 0 \\ \left[t_2 + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)e^{3ik_xa}\right]G_2(1) \\ + \left[t_2e^{3ik_xa} + \left(\frac{\sqrt{3}t_1-t_2}{2}\right)\cos\big(2\pi.3.\alpha - k_ya\big)\right]G_2(2) - E_2G_2(3) = 0 \end{cases}$$

These three independent equations rewrite in a charaterisc equation:

$$\begin{pmatrix} -E_2 & \begin{array}{c} t_2 e^{-3ik_x a} \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.1.\alpha - k_y a\big) \end{array} & \begin{array}{c} t_2 \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.1.\alpha - k_y a\big) e^{-3ik_x a} \end{array} \\ \hline \begin{array}{c} t_2 e^{3ik_x a} \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.2.\alpha - k_y a\big) \end{array} & -E_2 & \begin{array}{c} t_2 e^{-3ik_x a} \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.2.\alpha - k_y a\big) \end{array} \\ \hline \begin{array}{c} \big[t_2 \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.3.\alpha - k_y a\big) e^{3ik_x a} \end{array} & \begin{array}{c} t_2 e^{3ik_x a} \\ +\left(\frac{\sqrt{3}t_1 - t_2}{2}\right) \\ \times\cos\big(2\pi.3.\alpha - k_y a\big) \end{array} & -E_2 \end{pmatrix}$$

$$\times \begin{pmatrix} G_2(1) \\ G_2(2) \\ G_2(3) \end{pmatrix} = 0$$

Summary

So the NN Hamiltonian has the form

$$H_{3q\times 3q} = \begin{pmatrix} h_{0_{3\times 3}} & h_{1_{3\times 3}} & h_{2_{3\times 3}} \\ h^*_{1_{3\times 3}} & h_{11_{3\times 3}} & h_{12_{3\times 3}} \\ h^*_{2_{3\times 3}} & h^*_{12_{3\times 3}} & h_{22_{3\times 3}} \end{pmatrix}$$

where the single block matrix elements is

$$h_{0_{3\times 3}} = \begin{pmatrix} -\frac{E_0}{t_0} & e^{-3ik_x a} + \cos\left(2\pi.1.\frac{1}{3} - k_y a\right) & 1 + \cos\left(2\pi.1.\frac{1}{3} - k_y a\right) e^{-3ik_x a} \\ e^{3ik_x a} + \cos\left(2\pi.2.\frac{1}{3} - k_y a\right) & -\frac{E_0}{t_0} & e^{-3ik_x a} + \cos\left(2\pi.2.\frac{1}{3} - k_y a\right) \\ 1 + \cos\left(2\pi.3.\frac{1}{3} - k_y a\right) e^{3ik_x a} & e^{3ik_x a} + \cos\left(2\pi.3.\frac{1}{3} - k_y a\right) & -\frac{E_0}{t_0} \end{pmatrix}$$

$$
h_{0_{3\times3}} = \left(\begin{array}{c|c|c}
-\frac{E_0}{t_0} & \begin{array}{c} e^{-3ik_xa} \\ +\cos\left(2\pi.1.\frac{1}{3}-k_ya\right)\end{array} & 1+\cos\left(2\pi.1.\frac{1}{3}-k_ya\right)e^{-3ik_xa} \\
\hline
\begin{array}{c} e^{3ik_xa} \\ +\cos\left(2\pi.2.\frac{1}{3}-k_ya\right)\end{array} & -\frac{E_0}{t_0} & \begin{array}{c} e^{-3ik_xa} \\ +\cos\left(2\pi.2.\frac{1}{3}-k_ya\right)\end{array} \\
\hline
1+\cos\left(2\pi.3.\frac{1}{3}-k_ya\right)e^{3ik_xa} & \begin{array}{c} e^{3ik_xa} \\ +\cos\left(2\pi.3.\frac{1}{3}-k_ya\right)\end{array} & -\frac{E_0}{t_0}
\end{array}\right)
$$

$$
h_{1_{3\times3}} = \left(\begin{array}{c|c|c}
-E_1 & \begin{array}{c} t_1e^{-3ik_xa} \\ +\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.1.\alpha-k_ya\right)\end{array} & \begin{array}{c} t_1 \\ -\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.1.\alpha-k_ya\right)e^{-3ik_xa}\end{array} \\
\hline
\begin{array}{c} t_1e^{3ik_xa} \\ -\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.2.\alpha-k_ya\right)\end{array} & -E_1 & \begin{array}{c} t_1e^{-3ik_xa} \\ +\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.2.\alpha-k_ya\right)\end{array} \\
\hline
\begin{array}{c} t_1 \\ +\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.3.\alpha-k_ya\right)e^{3ik_xa}\end{array} & \begin{array}{c} t_1e^{3ik_xa} \\ -\left(\frac{t_1+\sqrt{3}t_2}{2}\right) \\ \times\cos\left(2\pi.3.\alpha-k_ya\right)\end{array} & -E_1
\end{array}\right)
$$

$$
h_{2_{3\times3}} = \left(\begin{array}{c|c|c}
-E_2 & \begin{array}{c} t_2e^{-3ik_xa} \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.1.\alpha-k_ya\big)\end{array} & \begin{array}{c} t_2 \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.1.\alpha-k_ya\big)e^{-3ik_xa}\end{array} \\
\hline
\begin{array}{c} t_2e^{3ik_xa} \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.2.\alpha-k_ya\big)\end{array} & -E_2 & \begin{array}{c} t_2e^{-3ik_xa} \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.2.\alpha-k_ya\big)\end{array} \\
\hline
\begin{array}{c} [t_2 \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.3.\alpha-k_ya\big)e^{3ik_xa}\end{array} & \begin{array}{c} t_2e^{3ik_xa} \\ +\left(\frac{\sqrt{3}t_1-t_2}{2}\right) \\ \times\cos\big(2\pi.3.\alpha-k_ya\big)\end{array} & -E_2
\end{array}\right)
$$