Tight Binding Model for Twist Bilayer Graphene*

Wangqian Miao

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* A footnote to the article title

I. SYMBOL CONVENTION

II. THE TIGHT BINDING HAMILTONIAN FOR TWIST BILAYER GRAPHENE

The tight binding Hamiltonian written in the second quantization langauge is

$$\hat{H} = \sum_{\bar{\mathbf{k}}} \sum_{\alpha n, \beta m} H_{\alpha n, \beta m} C^{\dagger}_{\alpha}(\bar{\mathbf{k}} + \mathbf{G}_n) C_{\beta}(\bar{\mathbf{k}} + \mathbf{G}_m). \tag{1}$$

The basis wave function can be expressed as a summation of planewave:

$$\psi_{\alpha,n}(\bar{\mathbf{k}}) = \frac{1}{\sqrt{N_{\mathrm{m}} N_{\mathrm{a}}}} \sum_{\mathrm{I},i} \mathrm{e}^{\mathrm{i}(\bar{\mathbf{k}}+\mathbf{G}_n)\mathbf{R}_{\mathrm{I}i\alpha}} \left|\phi_{p_z}\right\rangle, \tag{2}$$

$N_{\mathrm{a}} = N_{\mathrm{atom}}/4$, And

$$\mathbf{R}_{\mathrm{I}i\alpha} = \mathbf{L}_{\mathrm{I}} + \boldsymbol{\tau}_{i\alpha}. \tag{3}$$

The matrix element of the Hamiltonian should be written as:

$$\begin{aligned}
H_{\alpha n,\beta m} &= \frac{1}{N_{\mathrm{m}} N_{\mathrm{a}}} \sum_{\mathrm{IJ},ij} t(\mathbf{R}_{\mathrm{I}i\alpha} - \mathbf{R}_{\mathrm{J}j\beta}) \mathrm{e}^{-\mathrm{i}(\bar{\mathbf{k}}+\mathbf{G}_n)\mathbf{R}_{\mathrm{I}i\alpha}} \mathrm{e}^{\mathrm{i}(\bar{\mathbf{k}}+\mathbf{G}_m)\mathbf{R}_{\mathrm{J}j\beta}} \\
&= \frac{1}{N_{\mathrm{m}} N_{\mathrm{a}}} \sum_{\mathrm{IJ},ij} t(\mathbf{R}_{\mathrm{I}i\alpha} - \mathbf{R}_{\mathrm{J}j\beta}) \mathrm{e}^{-\mathrm{i}(\bar{\mathbf{k}}+\mathbf{G}_n)\cdot(\mathbf{L}_{\mathrm{I}}+\boldsymbol{\tau}_{i\alpha})} \mathrm{e}^{\mathrm{i}(\bar{\mathbf{k}}+\mathbf{G}_m)\cdot(\mathbf{L}_{\mathrm{J}}+\boldsymbol{\tau}_{j\beta})} \\
&= \frac{1}{N_{\mathrm{m}} N_{\mathrm{a}}} \sum_{\mathrm{IJ},ij} \mathrm{e}^{-\mathrm{i}\mathbf{G}_n\boldsymbol{\tau}_{i\alpha}} \mathrm{e}^{-\mathrm{i}\bar{\mathbf{k}}(\mathbf{L}_{\mathrm{I}}-\mathbf{L}_{\mathrm{J}}+\boldsymbol{\tau}_{i\alpha}-\boldsymbol{\tau}_{j\beta})} t(\mathbf{L}_{\mathrm{I}} - \mathbf{L}_{\mathrm{J}} + \boldsymbol{\tau}_{i\alpha} - \boldsymbol{\tau}_{j\beta}) \mathrm{e}^{\mathrm{i}\mathbf{G}_m\boldsymbol{\tau}_{j\beta}} \\
\text{cutoff: } \langle \mathrm{I}, \mathrm{J}\rangle, \quad &= \frac{1}{N_{\mathrm{m}} N_{\mathrm{a}}} \sum_{\mathrm{I},ij} \mathrm{e}^{-\mathrm{i}\mathbf{G}_n\boldsymbol{\tau}_{i\alpha}} \mathrm{e}^{-\mathrm{i}\bar{\mathbf{k}}(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta})} t(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta}) \mathrm{e}^{\mathrm{i}\mathbf{G}_m\boldsymbol{\tau}_{j\beta}} \\
\frac{1}{N_{\mathrm{m}}} \sum_{\mathrm{I}} = 1, \quad &= \frac{1}{N_{\mathrm{a}}} \sum_{ij} \mathrm{e}^{-\mathrm{i}\mathbf{G}_n\boldsymbol{\tau}_{i\alpha}} \mathrm{e}^{-\mathrm{i}\bar{\mathbf{k}}(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta})} t(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta}) \mathrm{e}^{\mathrm{i}\mathbf{G}_m\boldsymbol{\tau}_{j\beta}}.
\end{aligned} \tag{4}$$

Tricky here, we write down the matrix form of the Hamiltonian,

$$\begin{aligned}
\mathbf{H}_{\alpha\beta} &= \mathbf{X}^{\dagger}_{\alpha} \mathbf{T}_{\alpha\beta} \mathbf{X}_{\beta} \\
\mathbf{H} &= \oplus_{\alpha\beta} \mathbf{H}_{\alpha\beta}
\end{aligned} \tag{5}$$

The above equation describes a block matrix multiplication. α, β runs in $[\mathrm{A}_1, \mathrm{B}_1, \mathrm{A}_2, \mathrm{B}_2]$

The matrix element:

$$\begin{aligned}
(\mathbf{X}_{\alpha}{}^{\dagger})_{n,i} &= \mathrm{e}^{\mathrm{i}\mathbf{G}_n\boldsymbol{\tau}_{i\alpha}}, \\
(\mathbf{T}_{\alpha\beta})_{i,j} &= \mathrm{e}^{-\mathrm{i}\bar{\mathbf{k}}(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta})} t(\bar{\boldsymbol{\tau}}_{i\alpha,j\beta}).
\end{aligned} \tag{6}$$

III. TBG UNDER MAGNETIC FIELD

A. Magnetic Translation Operator

The original lattice translation symmetry is broken by the vector potential:

$$\hat{T}_{\mathbf{L}_{\mathrm{I}}} \hat{T}_{\mathbf{L}_{\mathrm{J}}} = \hat{T}_{\mathbf{L}_{\mathrm{J}}} \hat{T}_{\mathbf{L}_{\mathrm{I}}} \exp\left(\mathrm{i}\frac{e}{\hbar} \oint \mathbf{A} \mathrm{d}\mathbf{r}\right) \tag{7}$$

which gives us the form of AB effect in lattice:

$$\hat{T}_{\mathbf{L}_\mathrm{I}}^{-1}\hat{T}_{\mathbf{L}_\mathrm{J}}^{-1}\hat{T}_{\mathbf{L}_\mathrm{I}}\hat{T}_{\mathbf{L}_\mathrm{J}} = \exp\left(\mathrm{i}\frac{e}{\hbar}\oint_S \mathbf{A}\mathrm{d}\mathbf{r}\right) \tag{8}$$

S is the cell size spaned by $\mathbf{L}_\mathrm{I}, \mathbf{L}_\mathrm{J}$. Cosider a specific case:

$$\begin{aligned}\mathbf{L}_\mathrm{I} &= \mathbf{L}_1\\ \mathbf{L}_\mathrm{J} &= q\mathbf{L}_2\\ \Phi &= B\mathcal{S} = \frac{p}{q}\Phi_0\end{aligned} \tag{9}$$

where p, q are relatively prime, $\mathcal{S}$ is the moire unit lattice size. $\Phi_0 = h/e$. When B is uniform,

$$\begin{aligned}S &= q\mathcal{S}\\ \exp\left(\mathrm{i}\frac{e}{\hbar}\oint_S \mathbf{A}\mathrm{d}\mathbf{r}\right) &= \exp\left(\mathrm{i}\frac{e}{\hbar}\int_{\partial S} B\mathrm{d}S\right)\\ &= \exp(2\pi\mathrm{i}p)\\ &= 1\end{aligned} \tag{10}$$

Subsequently, we have the commutation relationship:

$$\hat{T}_{\mathbf{L}_1}\hat{T}_{q\mathbf{L}_2} = \hat{T}_{q\mathbf{L}_2}\hat{T}_{\mathbf{L}_1} \tag{11}$$

It suggests that we should adopt a magnetic lattice unit cell q times lager than the original one.

B. Tight Binding Hopping term

By using Peierls substitution, the hopping term should be written as

$$\begin{aligned}\tilde{t}(\mathbf{R}_{\mathrm{I}i\alpha} - \mathbf{R}_{\mathrm{J}j\beta}) &= t(\mathbf{R}_{\mathrm{I}i\alpha} - \mathbf{R}_{\mathrm{J}j\beta})\exp\left(\mathrm{i}\frac{e}{\hbar}\int_{\mathbf{R}_{\mathrm{I}i\alpha}}^{\mathbf{R}_{\mathrm{J}j\beta}} \mathbf{A}\mathrm{d}\mathbf{r}\right)\\ &= t(\mathbf{R}_{\mathrm{I}i\alpha} - \mathbf{R}_{\mathrm{J}j\beta})\exp\left(2\pi\mathrm{i}\frac{1}{\Phi_0}\int_{\mathbf{R}_{\mathrm{I}i\alpha}}^{\mathbf{R}_{\mathrm{J}j\beta}} \mathbf{A}\mathrm{d}\mathbf{r}\right)\end{aligned} \tag{12}$$

Here we use the Landau gauge, $\mathbf{A} = (0, Bx, 0)$, the corresponding phase factor can be calculated in the following way:

$$\begin{aligned}\int_{\mathbf{R}_1}^{\mathbf{R}_2} \mathbf{A}\,\mathrm{d}\mathbf{r} &= \int_{\mathbf{R}_1}^{\mathbf{R}_2} Bx\,\mathrm{d}y\\ &= B\frac{y_2 - y_1}{x_2 - x_1}\int_{x_1}^{x_2} x\,\mathrm{d}x\\ &= \frac{B(x_2 + x_1)(y_2 - y_1)}{2}\end{aligned} \tag{13}$$