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 language 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:

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

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:

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

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

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

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:

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