

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

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

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

$$\psi_{\alpha, n}(\bar{\mathbf{k}}) = \frac{1}{\sqrt{N_m N_a}} \sum_{\mathbf{I}, i} e^{i(\bar{\mathbf{k}} + \mathbf{G}_n) \cdot \mathbf{R}_{Ii\alpha}}, \quad (2)$$

And

$$\mathbf{R}_{Ii\alpha} = \mathbf{L}_I + \boldsymbol{\tau}_{i\alpha}. \quad (3)$$

The matrix element of the Hamiltonian should be written as:

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

$N_a = N_{\text{atom}}/4$ Tricky here, we write down the matrix form of the Hamiltonian,

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

The above equation describes a block matrix multiplication. α, β runs in $[A_1, B_1, A_2, B_2]$

The matrix element:

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