I EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma} d_{i,\sigma}^\dagger d_{j,\sigma} - t_{Gr} \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^{(A),\dagger} c_{j,\sigma}^{(B)} + V \sum_{i,\sigma} d_{i,\sigma}^\dagger c_{i,\sigma}^{(A)} + \text{h.c.} \qquad (I.1)$$

will be treated to obtain the band structure. The first step is to write out the sums over nearest neighbors $\langle i, j \rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) for the vectors to the nearest neighbors of the X atoms and Graphene A, B sites. Doing the calculation for example of the X atoms:

$$-t_X \sum_{\langle ij \rangle, \sigma} (d_{i,\sigma}^\dagger d_{j,\sigma} + d_{j,\sigma}^\dagger d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\sigma} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma} - \frac{t_X}{2} \sum_{j,\sigma} \sum_{\delta_X} d_{j,\sigma}^\dagger d_{j+\delta_X,\sigma}$$
$$(I.2)$$

$$= -t_X \sum_{i,\sigma} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma} \qquad (I.3)$$

The factor $1/2$ in eq. (I.2) is to account for double counting when going to the sum over all lattice sites i. By relabeling $j \rightarrow i$ in the second sum, the two sum are the same and eq. (I.3) is obtained. Using now the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}, \; c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \qquad (I.4)$$

with the completeness relation

$$\sum_i e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} , \qquad (I.5)$$

eq. (I.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_X} \left(e^{-i\mathbf{k}\mathbf{r}_i} d^\dagger_{\mathbf{k},\sigma} \right) \left(e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma} \right) \quad \text{(I.6)}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\delta_X,\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} e^{i\mathbf{k}'\delta_X} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \quad \text{(I.7)}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} \sum_{\delta_X} e^{i\mathbf{k}'\delta_X} \left(N\delta_{\mathbf{k},\mathbf{k}'} \right) \quad \text{(I.8)}$$

$$= -t_X \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} . \quad \text{(I.9)}$$

This part is now diagonal in $\mathbf{k}$ space. The nearest neighbours vectors δ_X for the X atoms are the vectors $\delta_{AA,i}$ from **??**. With that, the sum over δ_X can be explicitly calculated:

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad \text{(I.10)}$$

$$= -t_X \left[\exp\left(ia \left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} \right) \right) + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right. \quad \text{(I.11)}$$

$$\left. + e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \quad \text{(I.12)}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \quad \text{(I.13)}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x) \cos(\sqrt{3}\frac{a}{2}k_y) \right) . \quad \text{(I.14)}$$

The same can be done for the hopping between Graphene sites, for example :

$$-t_{Gr} \sum_{\langle ij \rangle, \sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_{Gr} \sum_{i,\sigma\sigma'} \sum_{\delta_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\delta_{AB},\sigma'} \quad \text{(I.15)}$$

$$= -t_{Gr} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad \text{(I.16)}$$

We note

Correct exp expressions

Example for a vector product

Show that!

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^{*} = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \tag{I.17}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{I.18}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{i\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{i\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{I.19}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{-i\frac{a}{2\sqrt{3}}k_y} \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x} \right) \right) \tag{I.20}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + 2e^{-i\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) \tag{I.21}$$

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c_{k,\sigma}^{A,\dagger} & c_{k,\sigma}^{B,\dagger} & d_{k,\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^{*} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{k,\sigma}^{A} \\ c_{k,\sigma}^{B} \\ d_{k,\sigma} \end{pmatrix} \tag{I.22}$$