I EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

$$H_0 = -\,t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + V \sum_{i,\sigma} d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma} + \text{h.c.} \tag{I.1}$$

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 $\boldsymbol{\delta}_{\mathrm{X}}, \boldsymbol{\delta}_\epsilon$ $(\epsilon = A, B)$ 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:

$$-t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma} (d^\dagger_{i,\sigma} d_{j,\sigma} + d^\dagger_{j,\sigma} d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_{\mathrm{X}},\sigma} - \frac{t_X}{2} \sum_{j,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{j,\sigma} d_{j+\boldsymbol{\delta}_{\mathrm{X}},\sigma} \tag{I.2}$$

$$= -t_X \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_{\mathrm{X}},\sigma} \tag{I.3}$$

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 $j \to i$ in the second sum, the two sum are the same and eq. (I.3) is obtained. Using now the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}, \;\; c^\dagger_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c^\dagger_{\mathbf{k}} \tag{I.4}$$

with the completeness relation

$$\sum_i e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'}\;, \tag{I.5}$$

eq. (I.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_{\mathrm{X}},\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\boldsymbol{\delta}_{\mathrm{X}}} \left(e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} d^\dagger_{\mathbf{k},\sigma}\right) \left(e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_{\mathrm{X}}} d_{\mathbf{k}',\sigma}\right) \tag{I.6}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\boldsymbol{\delta}_{\mathrm{X}},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_{\mathrm{X}}} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \tag{I.7}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_{\mathrm{X}}} \left(N \delta_{\mathbf{k},\mathbf{k}'}\right) \tag{I.8}$$

$$= -t_X \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{\mathrm{X}}} \,. \tag{I.9}$$

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

Correct exp expressions

Example for a vector product

$$f_{\mathrm{X}}(\mathbf{k}) = -t_X \sum_{\boldsymbol{\delta}_{\mathrm{X}}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{\mathrm{X}}} \tag{I.10}$$

$$= -t_X \left[\exp\left(\mathrm{i}a\left(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2}\right)\right) + e^{\mathrm{i}ak_x} + e^{\mathrm{i}a(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})}\right. \tag{I.11}$$

$$\left. + \, e^{\mathrm{i}a(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-\mathrm{i}ak_x} + e^{\mathrm{i}a(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})}\right] \tag{I.12}$$

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

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

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

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

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

We note

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

and calculate

$$\begin{aligned} f_{Gr} &= -t_{Gr} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} && \text{(I.18)} \\ &= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) && \text{(I.19)} \\ &= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x} \right) \right) && \text{(I.20)} \\ &= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) && \text{(I.21)} \end{aligned}$$

All together, we get:

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