1 Dressed Graphene Hamiltonian in Reciprocal Space

In this chapter, the Hamiltonian

$$H_0 = -t_\mathrm{X} \sum_{\langle ij \rangle, \sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_\mathrm{Gr} \sum_{\langle ij \rangle, \sigma} c^{(\mathrm{A}),\dagger}_{i,\sigma} c^{(\mathrm{B})}_{j,\sigma} + V \sum_{i,\sigma\sigma'} d^\dagger_{i,\sigma} c^{(\mathrm{A})}_{i,\sigma'} + \mathrm{h.c.} \tag{1.1}$$

from **??** will be treated to obtain the electronic band structure shown in the chapter. The first step is to write out the sums over nearest neighbors $\langle i, j \rangle$ explicitly, writing $\delta_\mathrm{X}, \delta_\epsilon$ ($\epsilon = A, B$) for the vectors to the nearest neighbors of the X atoms and Graphene A, B sites. For example, for the X atoms this gives:

$$-t_\mathrm{X} \sum_{\langle ij \rangle, \sigma} (d^\dagger_{i,\sigma} d_{j,\sigma} + d^\dagger_{j,\sigma} d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\delta_\mathrm{X},\sigma} d^\dagger_{i,\sigma} d_{i+\delta_\mathrm{X},\sigma} - \frac{t_X}{2} \sum_{j,\delta_\mathrm{X},\sigma} d^\dagger_{j,\sigma} d_{j+\delta_\mathrm{X},\sigma} \tag{1.2}$$

$$= -t_\mathrm{X} \sum_{i,\sigma} \sum_{\delta_\mathrm{X}} d^\dagger_{i,\sigma} d_{i+\delta_\mathrm{X},\sigma} \quad . \tag{1.3}$$

The factor $1/2$ in eq. (1.2) 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. (1.3) is obtained. Now, using the discrete Fourier transform

$$c_i = \frac{1}{\sqrt{N}} \sum_\mathbf{k} e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} c_\mathbf{k}, \; c^\dagger_i = \frac{1}{\sqrt{N}} \sum_\mathbf{k} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c^\dagger_\mathbf{k} \tag{1.4}$$

with the completeness relation

$$\sum_i e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\mathbf{r}_i} = N \delta_{\mathbf{k},\mathbf{k}'} \; , \tag{1.5}$$

eq. (1.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma} = -t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_X} \left(e^{-i\mathbf{k}\mathbf{r}_i} d^\dagger_{\mathbf{k},\sigma}\right) \left(e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma}\right) \tag{1.6}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\delta_X,\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} e^{i\mathbf{k}'\delta_X} \sum_{i} e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \tag{1.7}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k}',\sigma} \sum_{\delta_X} e^{i\mathbf{k}'\delta_X} \left(N \delta_{\mathbf{k},\mathbf{k}'}\right) \tag{1.8}$$

$$= -t_X \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \tag{1.9}$$

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

Clear up definition NN vectors and results

$$\mathbf{k} \cdot \delta_{\mathbf{AA},\mathbf{1}} = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = k_x + \sqrt{3} k_y \tag{1.10}$$

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \tag{1.11}$$

$$= -t_X \left[e^{ia(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right. \tag{1.12}$$

$$\left. + e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \tag{1.13}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \tag{1.14}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x) \cos(\sqrt{3}\frac{a}{2}k_y) \right) . \tag{1.15}$$

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

$$-t_{\mathrm{Gr}} \sum_{\langle ij \rangle,\sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_{\mathrm{Gr}} \sum_{i,\sigma\sigma'} \sum_{\delta_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\delta_{AB},\sigma'} \tag{1.16}$$

$$= -t_{\mathrm{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{1.17}$$

with again the sum over δ_{AB}

$$
\begin{aligned}
f_{\mathrm{Gr}}(\mathbf{k}) &= -t_{\mathrm{Gr}} \sum_{\delta_{AB}} e^{\mathrm{i}\mathbf{k}\delta_{AB}} && (1.18)\\
&= -t_{\mathrm{Gr}} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) && (1.19)\\
&= -t_{\mathrm{Gr}} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x} \right) \right) && (1.20)\\
&= -t_{\mathrm{Gr}} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) && (1.21)
\end{aligned}
$$

We note Show that!

$$
\sum_{\delta_{AB}} e^{\mathrm{i}\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{\mathrm{i}\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-\mathrm{i}\mathbf{k}\delta_{BA}} \tag{1.22}
$$

All in all:

$$
H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{\mathbf{k},\sigma} & c^{B,\dagger}_{\mathbf{k},\sigma} & d^{\dagger}_{\mathbf{k},\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{\mathbf{k},\sigma} \\ c^{B}_{\mathbf{k},\sigma} \\ d_{\mathbf{k},\sigma} \end{pmatrix} \tag{1.23}
$$