

I DRESSED GRAPHENE MODEL

I.1 LATTICE STRUCTURE

Structure of honeycomb lattice following [1].

Monolayer graphene forms a honeycomb lattice, which is a hexagonal Bravais lattice with a two atom basis.

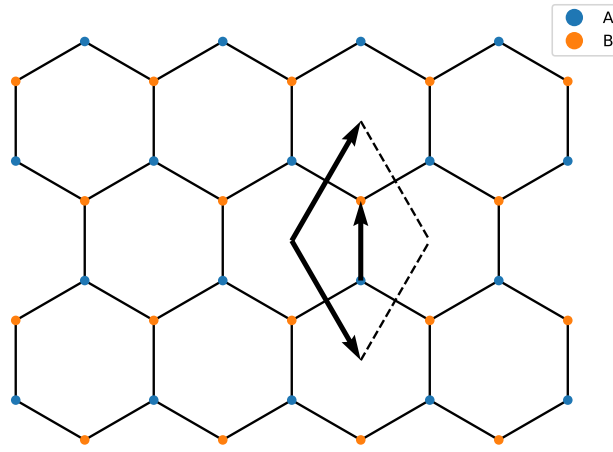


Figure I.1: *Graphene lattice structure*

Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \quad (\text{I.1})$$

$$\mathbf{a}_2 = \frac{a}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \quad (\text{I.2})$$

with lattice constant $a \approx 2.46 \text{ \AA}$ (distance between unit cells). Have

$$a = \sqrt{3}a_0 \quad (\text{I.3})$$

with the nearest-neighbour distance a_0 .

Vectors to the nearest-neighbor B_i ($i = 1, 2, 3$) atoms from atom A :

$$\delta_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \quad (\text{I.4})$$

Vectors to the nearest-neighbor A_i ($i = 1, 2, 3$) atoms from atom B :

$$\delta_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix} \quad (\text{I.5})$$

The vectors between the Graphene A atom and the six neighbours on the same sub lattice can be found by rotating \mathbf{a}_1 six times by $1/6 * 2\pi = \pi/3$:

$$\delta_{AA,1} = \mathbf{a}_1 = \frac{a}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = a \begin{pmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} = a \begin{pmatrix} \sin(\frac{\pi}{6}) \\ \cos(\frac{\pi}{6}) \end{pmatrix} \quad (\text{I.6})$$

$$\delta_{AA,2} = a \begin{pmatrix} \sin(\frac{3\pi}{6}) \\ \cos(\frac{3\pi}{6}) \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{I.7})$$

$$\delta_{AA,3} = a \begin{pmatrix} \sin(\frac{5\pi}{6}) \\ \cos(\frac{5\pi}{6}) \end{pmatrix} = a \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{I.8})$$

$$\delta_{AA,4} = a \begin{pmatrix} \sin(\frac{7\pi}{6}) \\ \cos(\frac{7\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{I.9})$$

$$\delta_{AA,5} = a \begin{pmatrix} \sin(\frac{9\pi}{6}) \\ \cos(\frac{9\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -1 \\ 0 \end{pmatrix} \quad (\text{I.10})$$

$$\delta_{AA,6} = a \begin{pmatrix} \sin(\frac{11\pi}{6}) \\ \cos(\frac{11\pi}{6}) \end{pmatrix} = a \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \quad (\text{I.11})$$

The primitive reciprocal lattice vectors $\mathbf{b}_1, \mathbf{b}_2$ fulfill

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \quad (\text{I.12})$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0, \quad (\text{I.13})$$

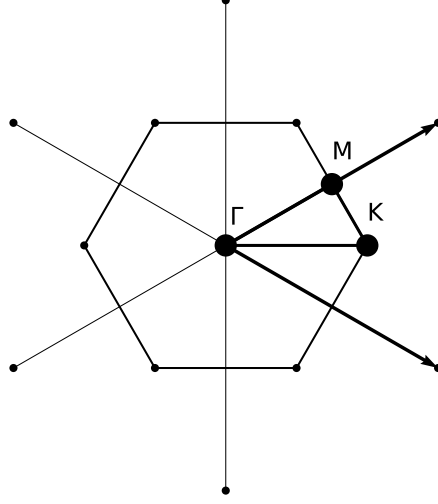


Figure I.2: *Graphene Brillouin Zone*

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{I.14})$$

$$\mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{I.15})$$

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (\text{I.16})$$

$$\mathbf{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \quad (\text{I.17})$$

$$\mathbf{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (\text{I.18})$$

I.2 EG-X MODEL

Graphene lattice and a site X.

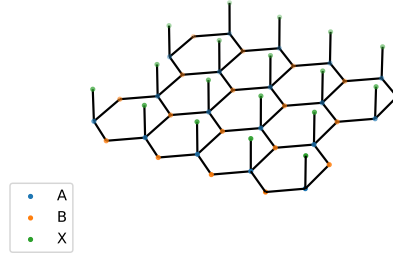


Figure I.3: EG-X model

Without interaction:

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma} d_{i, \sigma}^\dagger d_{j, \sigma} - t_{Gr} \sum_{\langle ij \rangle, \sigma} c_{i, \sigma}^{(A), \dagger} c_{j, \sigma}^{(B)} + V \sum_{i, \sigma \sigma'} d_{i, \sigma}^\dagger c_{i, \sigma'}^{(A)} + \text{h.c.} \quad (\text{I.19})$$

with:

- d operators on the X atom
- $c^{(\epsilon)}$ operators on the graphene site ($\epsilon = A, B$)
- t_X NN hopping for X
- t_{Gr} NN hopping of Gr
- V hybridization between X and Graphene B sites

We can also introduce an onsite Hubbard interaction:

$$H_{\text{int}} = U_X \sum_i d_{i, \uparrow}^\dagger d_{i, \downarrow}^\dagger d_{i, \downarrow} d_{i, \uparrow} + U_{Gr} \sum_{i, \epsilon=A, B} c_{i, \uparrow}^{(\epsilon), \dagger} c_{i, \downarrow}^{(\epsilon), \dagger} c_{i, \downarrow}^\epsilon c_{i, \uparrow}^\epsilon \quad (\text{I.20})$$

Write the Hamiltonian with orbital indices

Define sublattice index

$$\alpha = 1, 2, 3 \quad (\text{I.21})$$

with $1 \cong \text{Gr}_1, 2 \cong \text{Gr}_2, 3 \cong \text{X}$. Then we can write the non-interacting term as

$$H_0 = - \sum_{\langle i,j \rangle, \alpha, \beta, \sigma} [\mathbf{t}]_{i\alpha, j\beta} c_{i\alpha}^\dagger c_{j\beta} \quad (\text{I.22})$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\text{Gr}} & 0 \\ t_{\text{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\text{X}} \end{pmatrix} \quad (\text{I.23})$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \quad (\text{I.24})$$

Also write the interaction part with α (with changed signs compared to Niklas, to keep in line with papers about the attractive Hubbard model):

$$H_{\text{int}} = - \sum_{i\alpha} U_\alpha c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\alpha\downarrow} c_{i\alpha\uparrow} \quad (\text{I.25})$$

I.2.1 REVIEW: HUBBARD MODEL ON THE HONEYCOMB LATTICE

Write review for Hubbard model on the honeycomb lattice

I.2.2 BAND STRUCTURE OF THE NON-INTERACTING EG-X MODEL

To treat eq. I.19, we first write out the sums over nearest neighbours $\langle i, j \rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) for the connections to the nearest neighbours of the X atoms and Graphene A, B sites. Doing the calculation for the example of the X atoms:

$$-t_X \sum_{\langle ij \rangle, \sigma\sigma'} (d_{i,\sigma}^\dagger d_{j,\sigma'} + d_{j,\sigma}^\dagger d_{i,\sigma'}) \quad (\text{I.26})$$

$$= -\frac{t_X}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} - \frac{t_X}{2} \sum_{j,\sigma,\sigma'} \sum_{\delta_X} d_{j,\sigma}^\dagger d_{j+\delta_X,\sigma'} \quad (\text{I.27})$$

$$= -t_X \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} \quad (\text{I.28})$$

(The factor $1/2$ is to account for double counting when going to the sum over all lattice sites i)

Now we can input the discrete Fourier transform (for both graphene and X operators) into eq. [I.28](#)

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}} \quad (\text{I.29})$$

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \quad (\text{I.30})$$

with the completeness relation:

$$\sum_i e^{i\mathbf{k}\mathbf{r}_i} e^{-i\mathbf{k}'\mathbf{r}_i} = N \delta_{\mathbf{k},\mathbf{k}'} . \quad (\text{I.31})$$

We get:

$$-t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} = -t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} \sum_{\mathbf{k},\mathbf{k}'} e^{-i\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\mathbf{r}_i} e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \quad (\text{I.32})$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \sum_i e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}'\mathbf{r}_i} \quad (\text{I.33})$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{i\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} N \delta_{\mathbf{k},\mathbf{k}'} \quad (\text{I.34})$$

$$= -t_X \sum_{\mathbf{k},\sigma,\sigma'} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma'} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad (\text{I.35})$$

The nearest neighbours for X atoms are the vectors $\delta_{AA,i}$ from section I.1. With that, we can calculate:

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \quad (\text{I.36})$$

$$= -t_X \left(e^{ia(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} + e^{iak_x} + e^{ia(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right) \quad (\text{I.37})$$

$$+ e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right) \quad (\text{I.38})$$

$$= -t_X \left(2 \cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \quad (\text{I.39})$$

$$= -2t_X \left(\cos(ak_x) + 2 \cos(\frac{a}{2}k_x) \cos(\sqrt{3}\frac{a}{2}k_y) \right) \quad (\text{I.40})$$

We can do the same for the hopping between Graphene sites, for example :

$$-t_{Gr} \sum_{\langle ij \rangle, \sigma \sigma'} c_{i,\sigma}^{(A)\dagger} c_{j,\sigma'}^{(B)} = -t_{Gr} \sum_{i,\sigma \sigma'} \sum_{\delta_{AB}} c_{i,\sigma}^{(A)\dagger} c_{i+\delta_{AB},\sigma'}^{(B)} \quad (\text{I.41})$$

$$= -t_{Gr} \sum_{\mathbf{k}, \sigma, \sigma'} c_{\mathbf{k},\sigma}^{(A)\dagger} c_{\mathbf{k},\sigma'}^{(B)} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{I.42})$$

We note

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \quad (\text{I.43})$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \quad (\text{I.44})$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{i\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{i\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \quad (\text{I.45})$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{-i\frac{a}{2\sqrt{3}}k_y} \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x} \right) \right) \quad (\text{I.46})$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + 2e^{-i\frac{a}{2\sqrt{3}}k_y} \cos(\frac{a}{2}k_x) \right) \quad (\text{I.47})$$

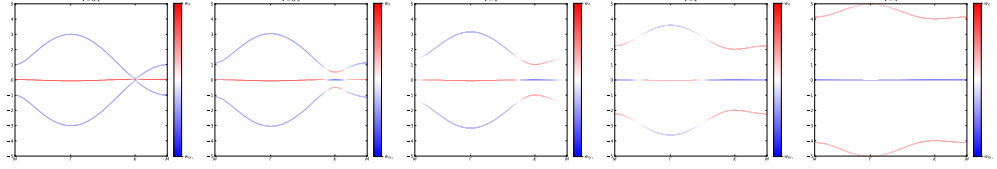


Figure I.4: Bands of the non-interacting EG-X model. All the bands are spin-degenerate.

All together, we get:

$$H_0 = \sum_{\mathbf{k}, \sigma} \begin{pmatrix} c_{\mathbf{k}, \sigma}^{A, \dagger} & c_{\mathbf{k}, \sigma}^{B, \dagger} & d_{\mathbf{k}, \sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f_{Gr}^* & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}, \sigma}^A \\ c_{\mathbf{k}, \sigma}^B \\ d_{\mathbf{k}, \sigma} \end{pmatrix} \quad (\text{I.48})$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. I.48. This was done in fig. I.4.

Values used for calculation:

- $a_0 = 1$
- $t_{Gr} = 1$
- $t_X = 0.01$

V is the control parameter. A range from $V = 0.1$ to $V = 2$ can be mapped onto materials in experiment.