I Dressed Graphene Model

Write introduction to the model and what is done in this chapter

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.

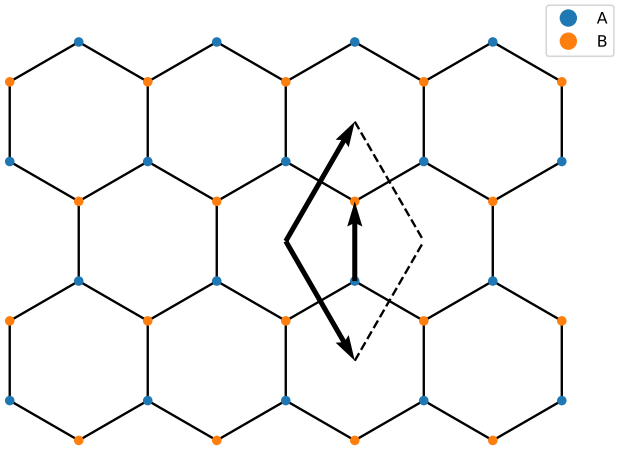

Figure I.1: *Graphene lattice structure*

Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \tag{I.1}$$

$$\mathbf{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \tag{I.2}$$

with lattice constant $a \approx 2.46$ Å (distance between unit cells). Have

$$a = \sqrt{3}a_0 \tag{I.3}$$

with the nearest-neighbour distance a_0.

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

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

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

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

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 $1/6 * 2\pi = \pi/3$:

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

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

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

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

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

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

First BZ vs this Gamma centered one

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

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{I.12}$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{I.13}$$

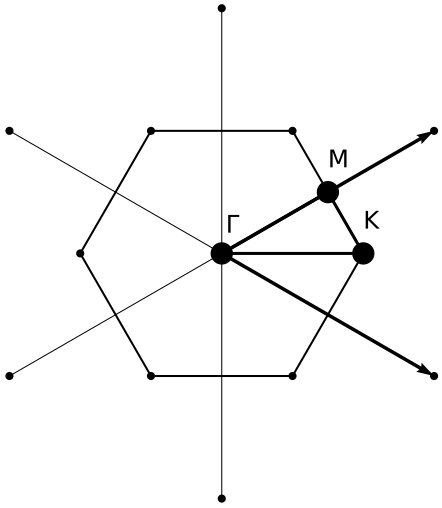

Figure I.2: *Graphene Brillouin Zone*

so we have:

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

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

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{I.16}$$

$$\mathrm{M} = \frac{\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.17}$$

$$\mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{I.18}$$

I.2 EG-X Model

Graphene lattice and a site X.

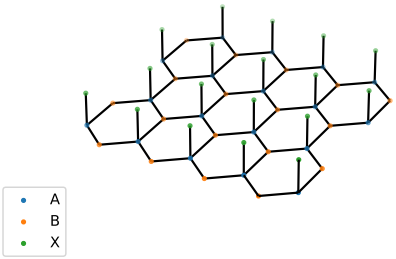

Figure I.3: *EG-X model*

Without interaction:

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

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:

$$H_{\mathrm{int}} = U_X \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{\mathrm{Gr}} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{I.20}$$

Hamilto-
n orbital

Define sublattice index

$$\alpha = 1, 2, 3 \tag{I.21}$$

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

$$H_0 = -\sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{I.22}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{I.23}$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{I.24}$$

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

$$H_{int} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{I.25}$$

I.2.1 Band structure of the non-interacting EG-X model