Dressed Graphene Model 1

This thesis concerned with a specific model. Idea: Graphene with an added orbital on one of the lattice site with a low hopping, as to provide a flat band. I will call this model dressed Graphene from here on. This chapter reviews the lattice structure in section 1.1.

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

1.1 Lattice Structure

There exist a few different ways to define the lattice structure of Graphene which are all equivalent, but intermediate steps in calculating tight-binding models look different depending on the definition. This review on follows ref. [1].

Connection with Niklas/Siheeon paper on dressed Graphene

Monolayer graphene forms a honeycomb lattice, which is a hexagonal Bravais lattice with a two atom basis, as can be seen in fig. 1.1a. The primitive lattice vectors of the hexagonal lattice are:

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \ \mathbf{a}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \tag{1.1}$$

with lattice constant $a = \sqrt{3}a_0 \approx 2.46$ Å, using the nearest-neighbour distance a_0. The vectors to the nearest-neighbor atoms B_i $(i = 1, 2, 3,)$ from atom A are

Labels on vectors

$$\delta_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \ \delta_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \ \delta_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \tag{1.2}$$

and the vectors to the nearest-neighbor atoms A_i $(i = 1, 2, 3,)$ from atom B are

$$\delta_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \ \delta_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \ \delta_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}. \tag{1.3}$$

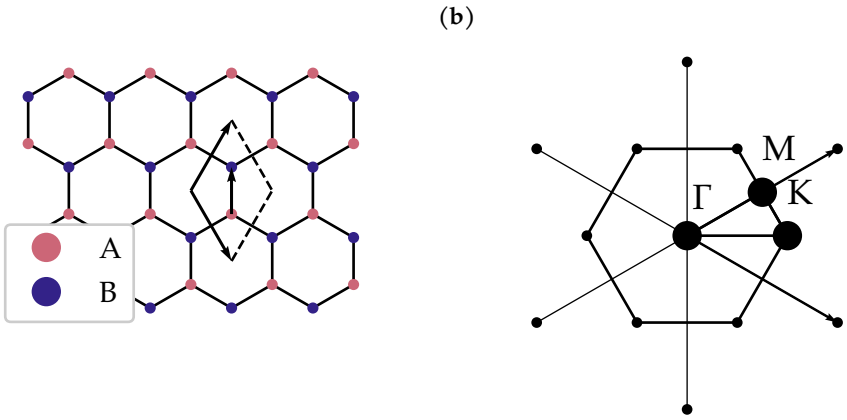

Figure 1.1: *(a) Graphene lattice structure and (b) Brilluoin zone*

The vectors between the Graphene A atom and the six neighbours on the same sub lattice are:

$$\delta_{AA,1} = \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad \delta_{AA,2} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \delta_{AA,3} = a \begin{pmatrix} \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \tag{1.4}$$

$$\delta_{AA,4} = a \begin{pmatrix} -\frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix}, \delta_{AA,5} = a \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \delta_{AA,6} = a \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} \tag{1.5}$$

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

labels on vectors

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{1.6}$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{1.7}$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \ \mathbf{b}_2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{1.8}$$

The first Brilluoin zone of the hexagonal lattice is shown in fig. 1.1b, with the points of high symmetry

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ \mathrm{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \ \mathrm{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix}\,. \tag{1.9}$$

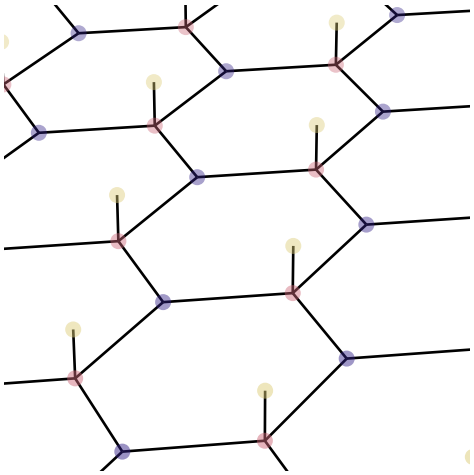

Figure 1.2: *Dressed Graphene model*

1.2 Dressed Graphene Model

The model I am concerned with in this thesis consists of a Hubbard Hamiltonian (as introduced in **??**) on a Graphene lattice, with one additional atom at one of the two sites in a unit cell, which I will call X. This is shown in fig. 1.2. The kinetic term is

Work over image for dressed graphene lattice

$$H_0 = -t_X \sum_{\langle ij\rangle,\sigma} d^\dagger_{i,\sigma} d_{j,\sigma} - t_{Gr} \sum_{\langle ij\rangle,\sigma} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + V \sum_{i,\sigma\sigma'} d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma'} + \text{h.c.} \tag{1.10}$$

with

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

The (attractive) Hubbard interaction has the following form:

$$H_{\text{int}} = -U_{\text{X}} \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} - U_{\text{Gr}} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{1.11}$$

The notation using different letters for the sites connects intuitively to the physical picture, but it is more economical and in line with the notation for mean field-theory established in **??** to write the Hamiltonian using a sublattice index

$$\alpha = 1, 2, 3 \tag{1.12}$$

with $1 \mathrel{\widehat{=}} \text{Gr}_\text{A}$, $2 \mathrel{\widehat{=}} \text{Gr}_\text{B}$, $3 \mathrel{\widehat{=}} \text{X}$. Then we can write the non-interacting term as

$$H_0 = \sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{1.13}$$

with the matrix in the sublattice indices

$$\mathbf{t} = \begin{pmatrix} 0 & -t_{\text{Gr}} & V\delta_{ij} \\ -t_{\text{Gr}} & 0 & 0 \\ V\delta_{ij} & 0 & -t_{\text{X}} \end{pmatrix} \tag{1.14}$$

Also write the interaction part as

$$H_{\text{int}} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \,. \tag{1.15}$$

Using the Fourier transformation **??**

Clean up the section from here

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^\dagger_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_{\text{X}} \end{pmatrix} \begin{pmatrix} c^A_{k,\sigma} \\ c^B_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{1.16}$$

The band structure for the non-interacting dressed graphene model is easily obtained by diagonalising the matrix in eq. (1.16). This was done in fig. 1.3.

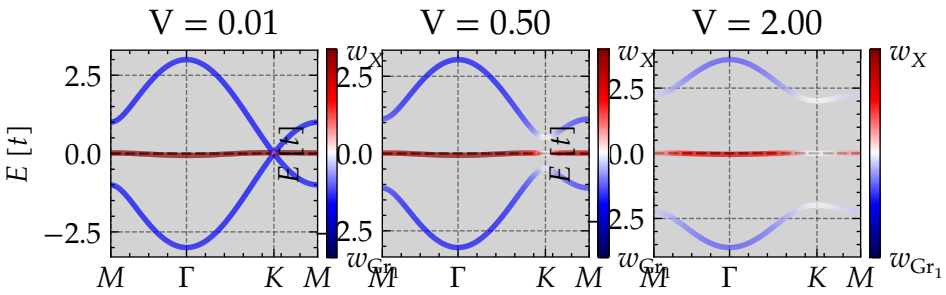

Figure 1.3: *Bands of the non-interacting dressed Graphene model, with parameters* $t_X = 0 \cdot t_{Gr}$