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

Connection with Niklas/Siheeon paper on dressed Graphene

1.1 Lattice Structure

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

clear up NN 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

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

The vectors between the Graphene A atom and the six neighbours on the same sub lattice are: The primitive reciprocal lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$ fulfill

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{1.4}$$

$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{1.5}$$

(a) (b)

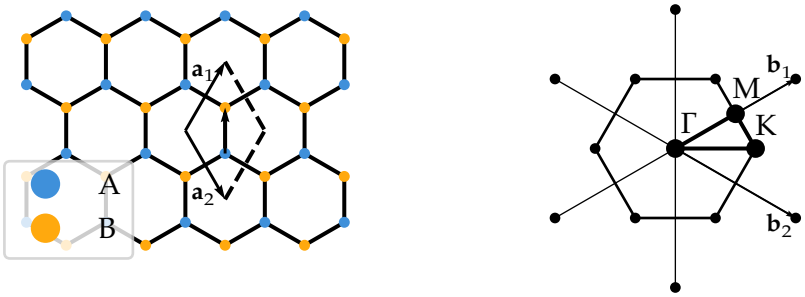

Figure 1.1 – (a) Graphene lattice structure and (b) Brilluoin zone created using lattpy [**Jones_lattpy_2022**]

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \ \mathbf{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{1.6}$$

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

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ \mathrm{M} = \frac{\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \ \mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix} 1 \\ 0 \end{pmatrix} . \tag{1.7}$$

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

$$H_0 = -t \sum_{\langle ij \rangle, \sigma} c^{(\mathrm{A}),\dagger}_{i,\sigma} c^{(\mathrm{B})}_{j,\sigma} + V \sum_{i,\sigma\sigma'} d^{\dagger}_{i,\sigma} c^{(\mathrm{A})}_{i,\sigma'} + \mathrm{h.c.} \tag{1.8}$$

with

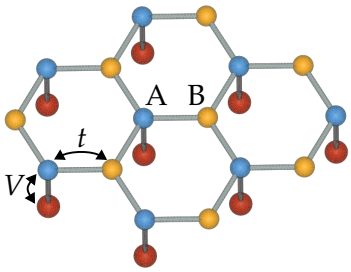

Figure 1.2 – Lattice structure of decorated graphene honeycomb lattice. with impurity X hybridized to sublattice site A. Only hopping t between sublattices A and B as well as V between X and A exist. Created using VESTA [2].

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

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

$$\alpha = 1, 2, 3 \tag{1.9}$$

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

$$H_0 = -t \sum_{\langle ij \rangle, \sigma} c^\dagger_{\alpha=1,i,\sigma} c_{\alpha=2,j,\sigma} + V \sum_{i,\sigma} c^\dagger_{\alpha=1,i,\sigma} c_{\alpha=3,i,\sigma} + \mathrm{h.c.} \tag{1.10}$$

The (attractive) Hubbard interaction has the following form:

$$H_{\mathrm{int}} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \, . \tag{1.11}$$

Fourier trafo :

Clean up the section from here

Fourier trafo with orbital positions

$$-t\sum_{\langle ij\rangle,\sigma} c_{i,\sigma}^{(\mathrm{A}),\dagger} c_{j,\sigma}^{(\mathrm{B})} = -t\sum_{i,\delta_{\mathrm{AB}},\sigma} c_{i,\sigma}^{(\mathrm{A})\dagger} c_{i+\delta_{\mathrm{AB}},\sigma}^{(\mathrm{B})} \tag{1.12}$$

$$= -\frac{t}{N^2}\sum_{i,\sigma}\sum_{\mathbf{k},\mathbf{k}',\delta_{\mathrm{AB}}} \left(e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k},\sigma}^{(\mathrm{A})\dagger}\right)\left(e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i+\delta_{AB}} c_{\mathbf{k}',\sigma}^{(B)}\right) \tag{1.13}$$

$$= -\frac{t}{N^2}\sum_{\mathbf{k},\mathbf{k}',\delta_{\mathrm{AB}},\sigma} c_{\mathbf{k},\sigma}^{(\mathrm{A})\dagger} c_{\mathbf{k}',\sigma}^{(\mathrm{B})} e^{\mathrm{i}\mathbf{k}'\delta_{\mathrm{AB}}} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \tag{1.14}$$

$$= -\frac{t}{N^2}\sum_{\mathbf{k},\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}^{(\mathrm{A})\dagger} c_{\mathbf{k}',\sigma}^{(\mathrm{B})} \sum_{\delta_{\mathrm{AB}}} e^{\mathrm{i}\mathbf{k}'\delta_{\mathrm{AB}}} \left(N^2\delta_{\mathbf{k},\mathbf{k}'}\right) \tag{1.15}$$

$$= -t\sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^{(\mathrm{A})\dagger} c_{\mathbf{k},\sigma}^{(\mathrm{B})} \sum_{\delta_{\mathrm{AB}}} e^{\mathrm{i}\mathbf{k}\delta_{AB}} = \sum_{\mathbf{k},\sigma} f_{\mathbf{k}} c_{\mathbf{k},\sigma}^{(\mathrm{A})\dagger} c_{\mathbf{k},\sigma}^{(\mathrm{B})} \tag{1.16}$$

Clear up definition NN vectors and results

$$\mathbf{k}\cdot\delta_{\mathbf{AA},\mathbf{1}} = \begin{pmatrix} k_x \\ k_y \end{pmatrix}\cdot\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} = k_x + \sqrt{3}k_y \tag{1.17}$$

$$f_{\mathbf{k}} = -t\sum_{\delta_{AB}} e^{\mathrm{i}\mathbf{k}\delta_{AB}} \tag{1.18}$$

$$= -t_{\mathrm{Gr}}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x-k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x-k_y)}\right) \tag{1.19}$$

$$= -t_{\mathrm{Gr}}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y}\left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x}\right)\right) \tag{1.20}$$

$$= -t_{\mathrm{Gr}}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y}\cos\left(\frac{a}{2}k_x\right)\right) \tag{1.21}$$

We have $\delta_{\mathrm{BA},i} = -\delta_{\mathrm{AB},i}$, so

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

which then gives

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c_{k,\sigma}^{A,\dagger} & c_{k,\sigma}^{B,\dagger} & d_{k,\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} 0 & f_{\mathbf{k}} & V \\ f_{\mathbf{k}}^* & 0 & 0 \\ V & 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k,\sigma}^{A} \\ c_{k,\sigma}^{B} \\ d_{k,\sigma} \end{pmatrix} \tag{1.23}$$

The band structure for the non-interacting dressed graphene model is easily obtained by diagonalising the matrix in eq. (1.23). This was done in fig. 1.3.

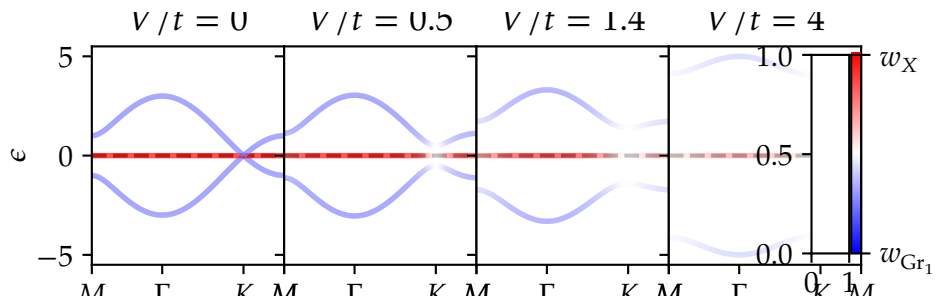

Figure 1.3 – Bands of the non-interacting dressed Graphene model