Decorated Graphene Model 1

Following the 2018 discovery of superconductivity in twisted Bilayer Graphene [1], graphene-based systems gained a renewed interest as a platform for strongly correlated physics. Two methods to engineer strong electron correlations emerged: twisted multilayer systems [1–5] and multilayer systems without twisting, such as Bernal bilayer, ABC or ABCA layered systems [6]. Through different means, electrons in these systems become localized so that interaction effects get more strongly pronounced. Connecting both kind of systems is the strong quantum geometry coming from the Graphene Dirac cones [7], which plays a role in stabilizing superconducting [2, 8] and magnetic order [9, 10].

Witt et al. suggested another platform for strongly correlated physics based on Graphene with the same strong quantum geometry coming from the Graphene band structure [11]. It follows an earlier experiment [12] showing a flat band in a system of a SiC(0001) substrate with a single layer of Graphene on top and Sn as an intercalant[1]. By using different group-IV intercalants (C, Si, Ge, Sn, Pb) between the graphene sheet and the semiconducting SiC(0001) substrate, different distances to the Graphene sheet occur in the ground state. Band structures obtained from Density Functional Theory show a relatively flat band at the Fermi level from the intercalant's p_z orbitals hybridized to the Dirac bands of graphene for all intercalants, with the hybridization strength being tuned by the equilibrium distance of the Graphene sheet and the intercalants.

In this thesis I will be treating an elemental model introduced in the work by Witt et al. capturing the essential flat band character of the system. The lattice structure can be seen in fig. 1.1. It consists of the usual hexagonal Graphene lattice, with an additional atom at one of the sublattice sites providing the flat band. Here, the hopping V models the hybridization

This elemental model shows two symmetry distinct Mott states for the small and large V regimes: in the low V regime, development of local moments and Mottness is at the X sites, where in the high V limit, this occurs at the B sites. Between these Mott states emerges a metallic state, similar to the topological phase transition of non-interacting bands in the Su-Schrieffer-Heger model [14].

[1] An intercalant is an atom or molecule inserted between the layers of layered system.

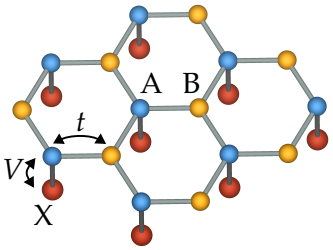

Figure 1.1 – Lattice structure of decorated graphene honeycomb lattice. with impurity X hybridized to sublattice site A. Only hopping t between sublattices A and B as well as V between X and A exist. Created using VESTA [13].

In contrast to the twisted or untwisted multilayer systems, the energy scale of emergence of flat bands in this model is set by the hopping t, i.e. in the range of eV for Graphene, so the correlated flat band physics might persist to higher temperatures.

1.1 Lattice Structure

Monolayer graphene forms a honeycomb lattice [15], which is a hexagonal Bravais lattice with a two atom basis, as can be seen in fig. 1.2a. 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

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

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

(a) (b)

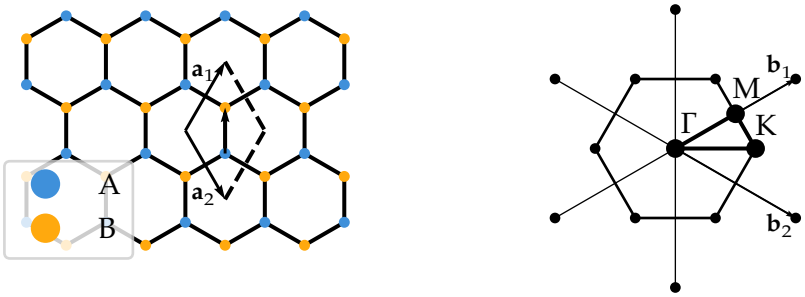

Figure 1.2 – (a) Graphene lattice structure and (b) Brilluoin zone created using lattpy [16]

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{1.4}$$
$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{1.5}$$

so that

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

The first Brilluoin zone of the hexagonal lattice is shown in fig. 1.2b, with the points of high symmetry

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

The elemental model as shown in fig. 1.1 has the following kinetic terms:

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

with

- 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.

Using the Fourier transformation

$$c_{i\alpha\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\mathbf{r}_{i\alpha}} c_{\mathbf{k}\alpha\sigma} \,, \tag{1.9}$$

the hopping term becomes

$$-t \sum_{\langle ij\rangle,\sigma} c^{(\mathrm{A}),\dagger}_{i,\sigma} c^{(\mathrm{B})}_{j,\sigma} \tag{1.10}$$

$$= -t \sum_{i,\delta_{\mathrm{AB}},\sigma} c^{(\mathrm{A})\dagger}_{i,\sigma} c^{(\mathrm{B})}_{i+\delta_{\mathrm{AB}},\sigma} \tag{1.11}$$

$$= -\frac{t}{N^2} \sum_{i,\sigma} \sum_{\mathbf{k},\mathbf{k}',\delta_{\mathrm{AB}}} \left(e^{-\mathrm{i}\mathbf{k}\mathbf{r}_{i\alpha}} c^{(\mathrm{A})\dagger}_{\mathbf{k},\sigma} \right) \left(e^{\mathrm{i}\mathbf{k}'\mathbf{r}_{i\alpha}+\delta_{AB}} c^{(B)}_{\mathbf{k}',\sigma} \right) \tag{1.12}$$

$$= -\frac{t}{N^2} \sum_{\mathbf{k},\mathbf{k}',\delta_{\mathrm{AB}},\sigma} c^{(\mathrm{A})\dagger}_{\mathbf{k},\sigma} c^{(\mathrm{B})}_{\mathbf{k}',\sigma} e^{\mathrm{i}\mathbf{k}'\delta_{\mathrm{AB}}} e^{\mathrm{i}(\mathbf{k}(\delta_A-\delta_B)+\mathbf{k}'(\delta_A-\delta_B))} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{R}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{R}_i} \tag{1.13}$$

$$= -\frac{t}{N^2} \sum_{\mathbf{k},\mathbf{k}',\sigma} c^{(\mathrm{A})\dagger}_{\mathbf{k},\sigma} c^{(\mathrm{B})}_{\mathbf{k}',\sigma} \sum_{\delta_{\mathrm{AB}}} e^{\mathrm{i}\mathbf{k}'\delta_{\mathrm{AB}}} e^{\mathrm{i}(\mathbf{k}(\delta_A-\delta_B)+\mathbf{k}'(\delta_A-\delta_B))} \left(N^2 \delta_{\mathbf{k},\mathbf{k}'} \right) \tag{1.14}$$

$$= -t \sum_{\mathbf{k},\sigma} c^{(\mathrm{A})\dagger}_{\mathbf{k},\sigma} c^{(\mathrm{B})}_{\mathbf{k},\sigma} \sum_{\delta_{\mathrm{AB}}} e^{\mathrm{i}(\mathbf{k}\delta_{AB}+2k_y a)} = \sum_{\mathbf{k},\sigma} f_{\mathbf{k}} c^{(\mathrm{A})\dagger}_{\mathbf{k},\sigma} c^{(\mathrm{B})}_{\mathbf{k},\sigma} \,. \tag{1.15}$$

The factor $f_{\mathbf{k}}$ can be written out explicitly using the nearest-neighbor vectors, for example

$$\mathbf{k} \cdot \delta_{\mathbf{AB},1} = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix} = \frac{1}{\sqrt{3}} k_y \,. \tag{1.16}$$

This gives:

$$f_{\mathbf{k}} = -t \sum_{\delta_{AB}} e^{\mathrm{i}(\mathbf{k}\delta_{AB}+2k_y a)} \tag{1.17}$$

$$= -t_{\mathrm{Gr}} e^{2\mathrm{i}k_y a} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{1.18}$$

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

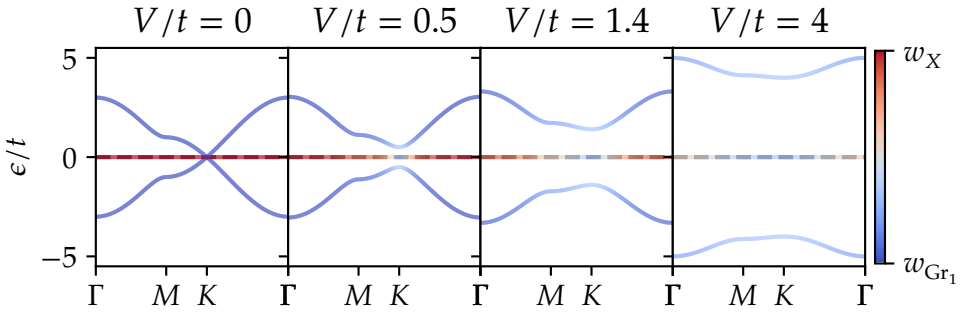

Figure 1.3 – Bands of the non-interacting decorated Graphene model

Using the fact that $\delta_{\mathrm{BA},i} = -\delta_{\mathrm{AB},i}$, it follows

$$-t\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} = -t\sum_{\delta_{AB}} e^{-i\mathbf{k}\delta_{AB}} = \left(-t\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}}\right)^* = f_{\mathbf{k}}^* \,, \tag{1.20}$$

which then gives

$$H_0 = \sum_{\mathbf{k},\sigma} C_{\mathbf{k},\sigma}^\dagger \begin{pmatrix} 0 & f_{\mathbf{k}} & V \\ f_{\mathbf{k}}^* & 0 & 0 \\ V & 0 & 0 \end{pmatrix} C_{\mathbf{k},\sigma} \tag{1.21}$$

$$C_{\mathbf{k},\sigma} = \begin{pmatrix} c_{\mathbf{k},\sigma}^{A,\dagger} & c_{\mathbf{k},\sigma}^{B,\dagger} & d_{\mathbf{k},\sigma}^\dagger \end{pmatrix}^T \tag{1.22}$$

The band structure for the non-interacting decorated graphene model is obtained by diagonalizing the matrix in eq. (1.21). This was done in fig. 1.3.

1.2 Quantum Geometry

Section about quantum geometry, maybe with lattice site local quantum metric?