I EG-X model

Test

Test source

The tight-binding Hamiltonian for the model reads

$$\begin{aligned} H_0 = &- t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma} d^{\dagger}_{i,\sigma} d_{j,\sigma} - t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma} \left(c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma} + c^{(B),\dagger}_{j,\sigma'} c^{(A)}_{i,\sigma} \right) \\ &+ V \sum_{i,\sigma} d^{\dagger}_{i,\sigma} c^{(A)}_{i,\sigma} + \mathrm{h.c.} \end{aligned} \tag{I.1}$$

with:

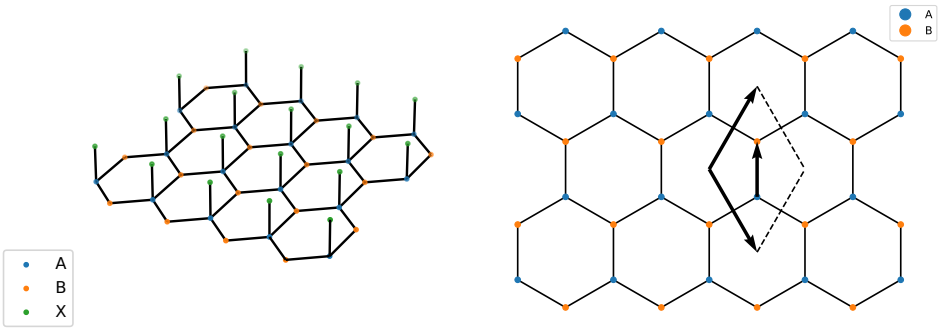
- d operators on the X atom
- $c^{(\epsilon)}$ operators on the Graphene site ($\epsilon = A, B$)
- t_X next-nearest hopping for the X atoms
- t_{Gr} next-nearest hopping on the Graphene
- V hopping between X and Graphene B sites

This describes the

In material terms, this can be thought of as a sheet of graphene on top of another material, providing the additional X atoms, but in this thesis the model will be taken as a toy model, providing certain favorable aspects.

I.1 Lattice Structure of Graphene

This section reviews the lattice structure of graphene and by extension also of the flat-band model, following the review [**yangStructureGrapheneIts2018**].



(a) *EG-X model* **(b)** *Graphene lattice structure*

Figure I.1: *EG-X model and Hexagonal lattice structure*

Monolayer graphene forms a hexagonal lattice as seen in fig. I.1b. This is formed by two triangular sub lattices, so the unit cell of the hexagonal lattice has two atoms. The primitive vectors of the hexagonal lattice are

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

with lattice constant $a \approx 2.46\,\text{Å}$ for graphene. The distance between nearest neighbor is

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

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

$$\begin{aligned}\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \text{ and}\\ \mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0 \, ,\end{aligned} \tag{I.4}$$

so

$$\mathbf{b}_1 = \frac{2\pi}{a}\begin{pmatrix}1\\\frac{1}{\sqrt{3}}\end{pmatrix}, \ \mathbf{b}_2 = \frac{2\pi}{a}\begin{pmatrix}1\\-\frac{1}{\sqrt{3}}\end{pmatrix} \, . \tag{I.5}$$

Graphic for primitive BZ

Explain primitive BZ

Explain: what symmetries does EG-X break? How does that influence BZ?

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix}0\\0\end{pmatrix}, \ \mathrm{M} = \frac{\pi}{a}\begin{pmatrix}1\\\frac{1}{\sqrt{3}}\end{pmatrix}, \ \mathrm{K} = \frac{4\pi}{3a}\begin{pmatrix}1\\0\end{pmatrix} \, . \tag{I.6}$$

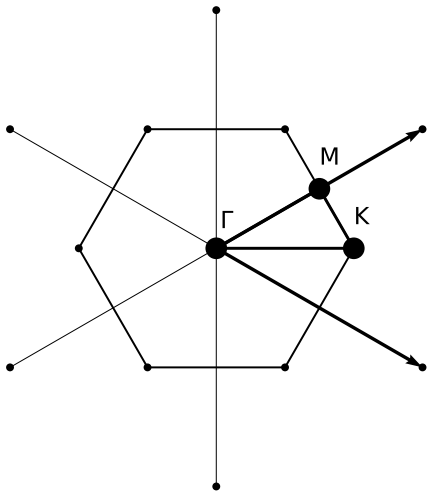


Figure I.2: *Graphene Brillouin Zone*

I.2 Band structure

aka why is the model interesting?
The detailed derivation can be found in **??**.

$$H_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^{*}_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{I.7}$$