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Master thesis

Title

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Conventions

Throughout the text of this thesis scalars are written in italic s, vectors in bold italic $*s$ and matrices in bold $\mathbf{M}$ fonts. A matrix element is denoted as $[\mathbf{M}]_{\alpha,\beta}$. The summation/multiplication over nearest neighbour sites i and j is $\langle ij \rangle$ as a subscript to $\sum/\prod$. Furthermore, Hartree atomic units are used in general and only in selected instances it is deviated from this: $\hbar = m_\mathrm{e} = \mathrm{e} = {}^{4\pi}/_{\varepsilon_0} = 1$.

I EG-X model

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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:

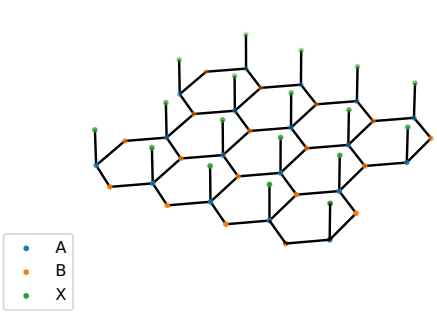
- d operators on the X atom
- $c^{(\epsilon)}$ operators on the Graphene site ($\epsilon = A, B$)
- t_X next-nearest hopping for the X atoms
- t_{Gr} next-nearest hopping on the Graphene
- V hopping between X and Graphene B sites

This describes the

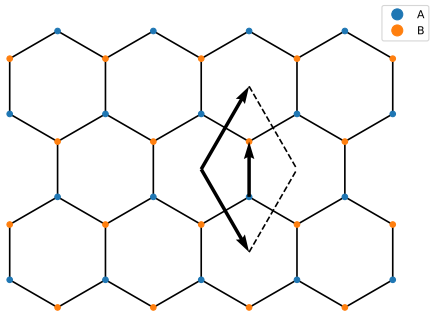
In material terms, this can be thought of as a sheet of graphene on top of another material, providing the additional X atoms, but in this thesis the model will be taken as a toy model, providing certain favorable aspects.

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 [1].



(a) *EG-X model*



(b) *Graphene 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

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

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

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

so

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

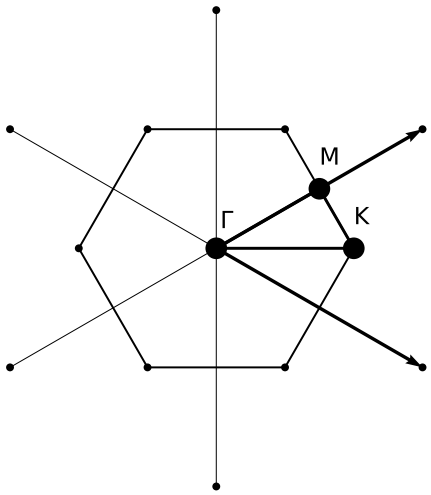


Figure I.2: *Graphene Brillouin Zone*

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Z

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in: what sym-
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? How does
nfluence BZ?

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{I.6}$$

$$\mathrm{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{I.7}$$

$$\mathrm{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} . \tag{I.8}$$

I.2 Band structure

aka why is the model interesting?

The detailed derivation can be found in appendix A.

$$H_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^{*}_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{I.9}$$

II Conclusion

A EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

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

will be treated via Fourier transform.

The first step is to write out the sums over nearest neighbors $\langle i, j\rangle$ explicitly, writing $\boldsymbol{\delta}_{\mathrm{X}}, \boldsymbol{\delta}_\epsilon$ ($\epsilon = A, B$) for the vectors to the nearest neighbors of the X atoms and Graphene A, B sites. Doing the calculation for example of the X atoms:

$$-t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma} (d^\dagger_{i,\sigma} d_{j,\sigma} + d^\dagger_{j,\sigma} d_{i,\sigma}) = -\frac{t_X}{2} \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_{\mathrm{X}},\sigma} - \frac{t_X}{2} \sum_{j,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{j,\sigma} d_{j+\boldsymbol{\delta}_{\mathrm{X}},\sigma} \tag{A.2}$$

$$= -t_X \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_{\mathrm{X}}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_{\mathrm{X}},\sigma} \tag{A.3}$$

The factor $1/2$ in eq. (A.2) is to account for double counting when going to the sum over all lattice sites i. By relabeling $j \to i$ in the second sum, we then get eq. (A.3). Using now the discrete Fourier transform

$$\begin{aligned} c_i &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}} \\ c^\dagger_i &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c^\dagger_{\mathbf{k}} \end{aligned} \tag{A.4}$$

with the completeness relation:

$$\sum_i e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} \ , \tag{A.5}$$

eq. (A.3) reads:

$$-t_X \frac{1}{N} \sum_{i,\sigma} \sum_{\boldsymbol{\delta}_\mathrm{X}} d^\dagger_{i,\sigma} d_{i+\boldsymbol{\delta}_\mathrm{X},\sigma'} = -t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} \sum_{\mathbf{k},\mathbf{k}'} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} d^\dagger_{\mathbf{k},\sigma} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} \tag{A.6}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} d^\dagger_{\mathbf{k},\sigma} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \tag{A.7}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} d^\dagger_{\mathbf{k},\sigma} e^{\mathrm{i}\mathbf{k}'\boldsymbol{\delta}_\mathrm{X}} d_{\mathbf{k}',\sigma'} N\delta_{\mathbf{k},\mathbf{k}'} \tag{A.8}$$

$$= -t_X \sum_{\mathbf{k},\sigma,\sigma'} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma'} \sum_{\boldsymbol{\delta}_\mathrm{X}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_\mathrm{X}} \tag{A.9}$$

The nearest neighbours for X atoms are the vectors $\boldsymbol{\delta}_{AA,i}$ from section I.1. With that, we can calculate:

$$f_\mathrm{X}(\mathbf{k}) = -t_X \sum_{\boldsymbol{\delta}_\mathrm{X}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_\mathrm{X}} \tag{A.10}$$

$$= -t_X \left(e^{\mathrm{i}a(\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} + e^{\mathrm{i}ak_x} + e^{\mathrm{i}a(\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} \right. \tag{A.11}$$

$$\left. + \ e^{\mathrm{i}a(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-\mathrm{i}ak_x} + e^{\mathrm{i}a(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right) \tag{A.12}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{\mathrm{i}a\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-\mathrm{i}a\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \tag{A.13}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x)\cos(\sqrt{3}\frac{a}{2}k_y) \right) \tag{A.14}$$

We can do the same for the hopping between Graphene sites, for example :

$$-t_\mathrm{Gr} \sum_{\langle ij\rangle,\sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_\mathrm{Gr} \sum_{i,\sigma\sigma'} \sum_{\boldsymbol{\delta}_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\boldsymbol{\delta}_{AB},\sigma'} \tag{A.15}$$

$$= -t_\mathrm{Gr} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} \tag{A.16}$$

We note

$$\sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} = \left(\sum_{\boldsymbol{\delta}_{BA}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}}\right)^* = \sum_{\boldsymbol{\delta}_{BA}} e^{-\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{BA}} \tag{A.17}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\boldsymbol{\delta}_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} \tag{A.18}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{A.19}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x} \right) \right) \tag{A.20}$$

$$= -t_{Gr} \left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y} \cos\left(\frac{a}{2}k_x\right) \right) \tag{A.21}$$

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^*_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{A.22}$$

Bibliography

[1] G. Yang et al. “Structure of Graphene and Its Disorders: A Review”. In: *Science and Technology of Advanced Materials* 19.1 (Aug. 2018), pp. 613–648. ISSN: 1468-6996. DOI: 10.1080/14686996.2018.1494493.

List of Symbols

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