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UNIVERSITET

Master thesis

Title

Title Deutsch

vorgelegt von
Tjark Sievers

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Erstgutachterin: Prof. Dr. Annica Black-Schaffer (Uppsala University)
Zweitgutachter: Prof. Dr. Tim Wehling

Even Einstein [...] had attempted to construct a theory of superconductivity. Fortunately, I was unaware of these many unsuccessful attempts. So when John invited me to join him (he, somehow, neglected to mention these previous efforts), I decided to take the plunge.

Leon Cooper, BCS: 50 Years

Kurzzusammenfassung

Abstract

Contents

Motivation

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 $\sum/\prod$.

I Superconductivity

II EG-X model

Test

Test source

The tight-binding Hamiltonian for the model reads

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

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

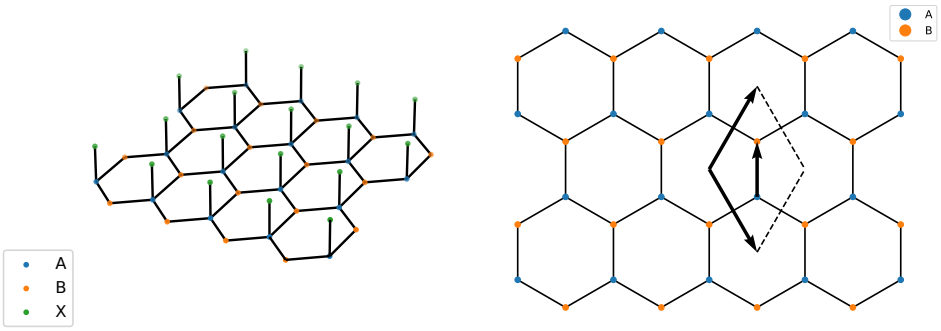
This describes the

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.

II.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].

Monolayer graphene forms a hexagonal lattice as seen in fig. II.1b. This is formed by two triangular sub lattices, so the unit cell of the hexagonal lattice



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

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

has two atoms. The primitive vectors of the hexagonal lattice are

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

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

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

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

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

so

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

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:

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

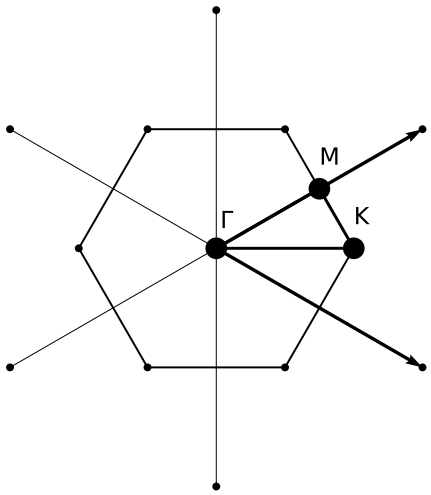


Figure II.2: *Graphene Brillouin Zone*

II.2 Band structure

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

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

III Conclusion

A EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

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

will be treated to obtain the band structure. 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, the two sum are the same and eq. (A.3) is obtained. Using now the discrete Fourier transform

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

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:

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

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

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

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

This part is now diagonal in $\mathbf{k}$ space. The nearest neighbours vectors $\boldsymbol{\delta}_\mathrm{X}$ for the X atoms are the vectors $\boldsymbol{\delta}_{AA,i}$ from section II.1. With that, the sum over $\boldsymbol{\delta}_\mathrm{X}$ can be explicitly calculated:

Correct exp expressions

Example for a vector product

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

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

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

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

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

The same can be done for the hopping between Graphene sites, for example :

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

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

Show that!

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.

Listings

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