Master thesis

# Title

May 2025

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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
"Remembrance of Superconductivity Past", BCS: 50 Years [1].

Typeset with LaTeX in TeX Gyre Pagella, TeX Gyre Heros, and `TeX Gyre Cursor`.

## Kurzzusammenfassung

## Abstract

# Contents


I Introduction 1

II Superconductivity 3

III Quantum Geometry, normal state something? 5
- III.1 EG-X model . . . . . . . . . . . . . . . . . . . . . . . . . . . 5
- III.2 Lattice Structure of Graphene . . . . . . . . . . . . . . . . . . . 5
- III.3 Band structure . . . . . . . . . . . . . . . . . . . . . . . . . . . 7
- III.4 Quantum Metric normal state? . . . . . . . . . . . . . . . . . . . 8

IV Mean field treatment, multi-band BCS theory 9
- IV.1 BdG Hamiltonian . . . . . . . . . . . . . . . . . . . . . . . . . . 9
  - IV.1.1 BdG Hamiltonian in band basis . . . . . . . . . . . . . . . 11
- IV.2 Grand potential . . . . . . . . . . . . . . . . . . . . . . . . . . 13

V Conclusion and Outlook 15

A EG-X Hamiltonian in Reciprocal Space 17

Bibliography 21

Acknowledgement 25

# I Introduction

# II Superconductivity

# III Quantum Geometry, normal state something?

## III.1 EG-X model

The tight-binding Hamiltonian for the model reads

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

with:

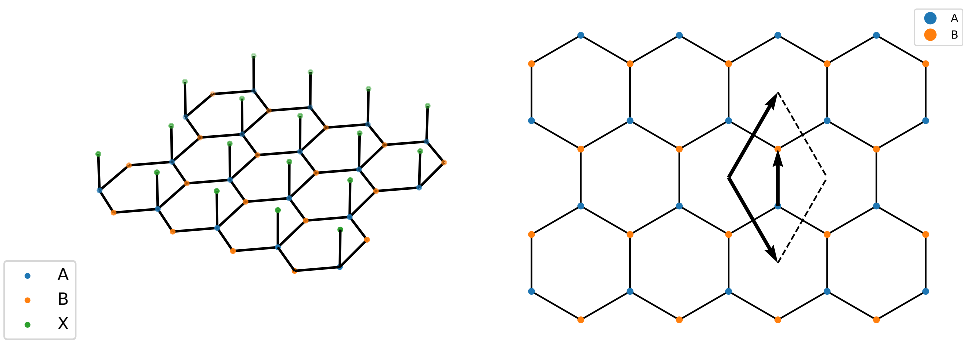
- $d$ operators on the X atom
- $c^{(\epsilon)}$ operators on the Graphene site ($\epsilon = A, B$)
- $t_X$ next-nearest hopping for the X atoms
- $t_{Gr}$ next-nearest hopping on the Graphene
- $V$ hopping between X and Graphene B sites

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.

## III.2 Lattice Structure of Graphene

This section reviews the lattice structure of graphene and by extension also of the flat-band model, following the review [2].




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

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

Monolayer graphene forms a hexagonal lattice as seen in fig. III.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

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

Te with lattice constant $a \approx 2.46$ Å for graphene. The distance between nearest neighbor is

$$a = \sqrt{3}a_0 . \tag{III.3}$$

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

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

so

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

Graphic for primitive BZ

Explain primitive BZ

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

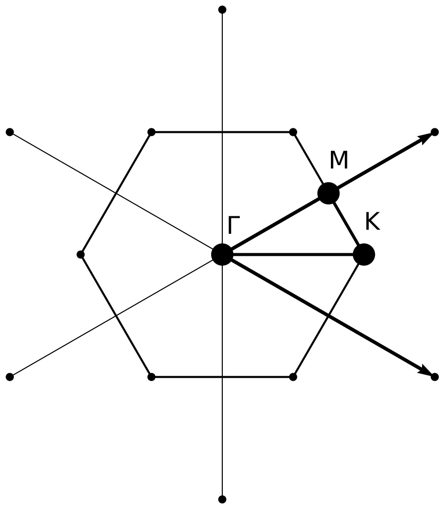



**Figure III.2:** *Graphene Brillouin Zone*

Points of high symmetry in the Brillouin zone are:

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

## III.3 Band structure

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

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

## III.4 Quantum Metric normal state?

# IV Mean field treatment, multi-band BCS theory

Introduced BCS theory in chapter II, but EG-X has multiple band, this is the important factor for having quantum geometry.

## IV.1 BdG Hamiltonian

Define sublattice index

$$\alpha = 1, 2, 3 \tag{IV.1}$$

with $1 \mathrel{\widehat{=}} \mathrm{Gr}_1, 2 \mathrel{\widehat{=}} \mathrm{Gr}_2, 3 \mathrel{\widehat{=}} \mathrm{X}$. Then we can write the non-interacting term as

$$H_0 = -\sum_{\langle i,j\rangle,\alpha,\beta,\sigma} [\mathbf{t}]_{i\alpha,j\beta}\, c^\dagger_{i\alpha} c_{j\beta} \tag{IV.2}$$

with the matrix

$$\mathbf{t} = \begin{pmatrix} 0 & t_{\mathrm{Gr}} & 0 \\ t_{\mathrm{Gr}} & 0 & -V\delta_{ij} \\ 0 & -V\delta_{ij} & t_{\mathrm{X}} \end{pmatrix} \tag{IV.3}$$

Add chemical potential:

$$-\mu \sum_{i\alpha\sigma} n_{i\alpha\sigma} \tag{IV.4}$$

Also write the interaction part with $\alpha$ (with changed signs compared to Niklas, to keep in line with papers about the attractive Hubbard model):

$$H_{int} = -\sum_{i\alpha} U_\alpha c^\dagger_{i\alpha\uparrow} c^\dagger_{i\alpha\downarrow} c_{i\alpha\downarrow} c_{i\alpha\uparrow} \tag{IV.5}$$

Fourier transformation:

$$H_{int} = -\frac{1}{N^2} \sum_{\alpha, \mathbf{k}_{1,2,3,4}} U_\alpha e^{\mathrm{i}(\mathbf{k}_1 + \mathbf{k}_4 - \mathbf{k}_1 - \mathbf{k}_3) r_{i\alpha}} c^\dagger_{\mathbf{k}_1 \alpha \uparrow} c^\dagger_{\mathbf{k}_3 \alpha \downarrow} c_{\mathbf{k}_2 \alpha \downarrow} c_{\mathbf{k}_4 \alpha \uparrow} \tag{IV.6}$$

Impose zero-momentum pairing: $\mathbf{k}_1 + \mathbf{k}_3 = 0$ and $\mathbf{k}_2 + \mathbf{k}_4 = 0$:

$$H_{int} = - \sum_{\alpha, \mathbf{k}, \mathbf{k}'} U_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \tag{IV.7}$$

Mean-field approximation:

$$H_{int} \approx \sum_{\alpha, \mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{IV.8}$$

with

$$\Delta_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \tag{IV.9}$$

$$\Delta^*_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\alpha\uparrow} c^\dagger_{-\mathbf{k}'\alpha\downarrow} \rangle \tag{IV.10}$$

This gives the BCS mean field Hamiltonian:

$$H_{BCS} = \sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} c^\dagger_{\mathbf{k}\alpha\sigma} c_{\mathbf{k}\beta\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{\mathbf{k}\alpha\sigma} + \sum_{\alpha, \mathbf{k}} (\Delta_\alpha c^\dagger_{\mathbf{k}\alpha\uparrow} c^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta^*_\alpha c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \tag{IV.11}$$

with Nambu spinor

$$\Psi_\mathbf{k} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c^\dagger_{1,-\mathbf{k}\downarrow} \\ c^\dagger_{2,-\mathbf{k}\downarrow} \\ c^\dagger_{3,-\mathbf{k}\downarrow} \end{pmatrix} \tag{IV.12}$$

we have:

$$H_{MF} = \sum_\mathbf{k} \Psi^\dagger_\mathbf{k} \mathcal{H}(\mathbf{k}) \Psi_\mathbf{k} \tag{IV.13}$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^\dagger & -H^*_{0,\downarrow}(-\mathbf{k}) + \mu \end{pmatrix} \tag{IV.14}$$

with $H_{0,\sigma}$ being the F.T. of the kinetic term and $\Delta = diag(\Delta_1, \Delta_2, \Delta_3)$.

### IV.1.1 BdG Hamiltonian in band basis

Use transformation

$$c^{\dagger}_{\mathbf{k}\alpha\sigma} = \sum_{n} [\mathbf{G}]^{*}_{\alpha n} d^{\dagger}_{n\mathbf{k}\sigma} \tag{IV.15}$$

where the columns are made up of the eigenvectors of $\mathbf{H}_{0,\sigma}$ for a given $\mathbf{k}$:

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_1 & \mathbf{G}_2 & \mathbf{G}_3 \end{pmatrix} \tag{IV.16}$$

with that:

$$\mathbf{G}^{\dagger}_{\sigma}(\mathbf{k})\mathbf{H}_{0,\sigma}(\mathbf{k})\mathbf{G}_{\sigma}(\mathbf{k}) = \begin{pmatrix} \epsilon_1 & 0 & 0 \\ 0 & \epsilon_2 & 0 \\ 0 & 0 & \epsilon_3 \end{pmatrix} \tag{IV.17}$$

So the kinetic part of the BdG Hamiltonian becomes:

$$\sum_{\mathbf{k}\alpha\beta\sigma} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} \sum_{n} [\mathbf{G}(\mathbf{k})]^{*}_{\alpha n} d^{\dagger}_{n\mathbf{k}\sigma} \sum_{m} [\mathbf{G}(\mathbf{k})]_{\beta m} d_{m\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{IV.18}$$

$$= \sum_{mn\mathbf{k}\sigma} d^{\dagger}_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \sum_{\alpha\beta} [\mathbf{G}(\mathbf{k})]^{*}_{\alpha n} [H_{0,\sigma}(\mathbf{k})]_{\alpha\beta} [\mathbf{G}(\mathbf{k})]_{\beta m} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{IV.19}$$

$$= \sum_{mn\mathbf{k}\sigma} d^{\dagger}_{n\mathbf{k}\sigma} d_{m\mathbf{k}\sigma} \epsilon_n \delta_{nm} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{IV.20}$$

$$= \sum_{n\mathbf{k}\sigma} \epsilon_n d^{\dagger}_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} - \mu \sum_{\mathbf{k}\alpha\sigma} n_{n\mathbf{k}\sigma} \tag{IV.21}$$

$$=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^{\dagger}_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} \tag{IV.22}$$

with $\xi_{\mathbf{k}} := \epsilon_{\mathbf{k}} - \mu$. The pairing terms become:

$$\sum_{\mathbf{k}\alpha} \Delta_{\alpha} c^{\dagger}_{\mathbf{k}\alpha\uparrow} c^{\dagger}_{-\mathbf{k}\alpha\downarrow} = \sum_{\mathbf{k}\alpha} \Delta_{\alpha} \sum_{n} [\mathbf{G}_{\uparrow}(\mathbf{k})]^{*}_{\alpha n} d^{\dagger}_{n\mathbf{k}\uparrow} \sum_{m} [\mathbf{G}_{\downarrow}(-\mathbf{k})]^{*}_{\beta m} d^{\dagger}_{m-\mathbf{k}\downarrow} \tag{IV.23}$$

$$= \tag{IV.24}$$

So that:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & G^{\dagger}\Delta G \\ G^{\dagger}\Delta^{\dagger}G & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix} \tag{IV.25}$$

with

$$\epsilon_{\mathbf{k}} = \begin{pmatrix} \epsilon_1(\mathbf{k}) & 0 & 0 \\ 0 & \epsilon_2(\mathbf{k}) & 0 \\ 0 & 0 & \epsilon_3(\mathbf{k}) \end{pmatrix} \tag{IV.26}$$

Concrete example for transformation of gaps from orbital to band basis at K = $\frac{4\pi}{3a}\begin{pmatrix}1\\0\end{pmatrix}$. There, the non-interacting part becomes simply:

$$\mathcal{H}_0 = \begin{pmatrix} 0 & 0 & V \\ 0 & 0 & 0 \\ V & 0 & 3t_X \end{pmatrix} \tag{IV.27}$$

The eigenvalue problem can be solved e.g. via sympy:

$$G = \begin{pmatrix} \frac{-3t_X - \sqrt{4V^2+9t_X^2}}{\sqrt{4V^2+\left(3t_X+\sqrt{4V^2+9t_X^2}\right)^2}} & 0 & \frac{-3t_X + \sqrt{4V^2+9t_X^2}}{\sqrt{4V^2+\left(3t_X-\sqrt{4V^2+9t_X^2}\right)^2}} \\ 0 & 1 & 0 \\ \frac{2V}{\sqrt{4V^2+\left(3t_X+\sqrt{4V^2+9t_X^2}\right)^2}} & 0 & \frac{2V}{\sqrt{4V^2+\left(3t_X-\sqrt{4V^2+9t_X^2}\right)^2}} \end{pmatrix} \tag{IV.28}$$

So for $V \to 0$:

$$G = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{IV.29}$$

but for $V > 0$, there are off-diagonal elements, e.g. $V = 0.1$:

$$G = \begin{pmatrix} -0.7578 & 0 & 0.6526 \\ 0 & 1 & 0 \\ 0.6526 & 0 & 0.7578 \end{pmatrix} \tag{IV.30}$$

So the transformation of the gap from orbital to band space reads:

$$G^\dagger \Delta G = \begin{pmatrix} \frac{3\Delta_1 t_X - 3\Delta_3 t_X + (\Delta_1+\Delta_3)\sqrt{4V^2+9t_X^2}}{2\sqrt{4V^2+9t_X^2}} & 0 & \frac{V(-\Delta_1+\Delta_3)}{\sqrt{4V^2+9t_X^2}} \\ 0 & \Delta_2 & 0 \\ \frac{V(-\Delta_1+\Delta_3)}{\sqrt{4V^2+9t_X^2}} & 0 & \frac{-3\Delta_1 t_X + 3\Delta_3 t_X + (\Delta_1+\Delta_3)\sqrt{4V^2+9t_X^2}}{2\sqrt{4V^2+9t_X^2}} \end{pmatrix} \tag{IV.31}$$

So in particular there is no interband pairing for $V \to 0$:

$$G^\dagger \Delta G = \begin{pmatrix} \Delta_1 & 0 & 0 \\ 0 & \Delta_2 & 0 \\ 0 & 0 & \Delta_3 \end{pmatrix} \tag{IV.32}$$

But for $V > 0$, there is interband pairing (e.g. $V = 0.1$):

$$G^\dagger \Delta G = \begin{pmatrix} 0.5742\Delta_1 + 0.4258\Delta_3 & 0 & -0.4945\Delta_1 + 0.4945\Delta_3 \\ 0 & \Delta_2 & 0 \\ -0.4945\Delta_1 + 0.4945\Delta_3 & 0 & 0.4258\Delta_1 + 0.5742\Delta_3 \end{pmatrix} \tag{IV.33}$$

## IV.2 Grand potential

See [**peottaSuperfluidityTopologicallyNontrivial2015**], especially supplementary material, notes 1 and 3.

Mean-Field Hamiltonian (with the last two terms due to exchange of anticommuting fermion operators and the term quadratic in the expectation value from the mean-field decoupling respectively):

$$H_{MF} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} + \sum_{\mathbf{k}} \mathrm{Tr}(H^\downarrow_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} \tag{IV.34}$$

The second term is the trace of the non-interacting Hamiltonian.

Thermodynamic grand potential (which at zero temperature is equivalent to the mean-field energy):

$$\Omega(T, \Delta) = -\frac{1}{\beta} \ln Z_\Omega = -\frac{1}{\beta} \ln \mathrm{Tr}(e^{-\beta H_{MF}}) \tag{IV.35}$$

$$= \sum_{\mathbf{k}} \mathrm{Tr}(H^\downarrow_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{\beta} \ln \mathrm{Tr}(e^{-\beta \Psi^\dagger_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}}) \tag{IV.36}$$

Zero temperature limit:

$$\Omega(\Delta) = \sum_{\mathbf{k}} \mathrm{Tr}(H^\downarrow_{\mathbf{k}}) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{2} \sum_{\mathbf{k}} \mathrm{Tr}([|\mathcal{H}_{\mathbf{k}}|]) \tag{IV.37}$$

where a function of a matrix $H$ (such as taking the absolute value of the BdG Hamiltonian $\mathcal{H}_{\mathbf{k}}$) is defined for the diagonal matrix of eigenvalues $D$ and the unitary matrix $U$ that diagonalizes $H$:

$$f(H) = U f(D) U^\dagger \tag{IV.38}$$

The route to finding the value of the order parameter for a fixed interaction $U$ is minimizing the grand potential with respect to $\Delta$.

# V Conclusion and Outlook

# A EG-X Hamiltonian in Reciprocal Space

In the following chapter, the model Hamiltonian

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

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 $\delta_{\mathrm{X}}, \delta_\epsilon$ $(\epsilon = A, B)$ 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:

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

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

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

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

Correct exp expressions

Example for a vector product

eq. (A.3) reads:

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

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

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

$$= -t_X \sum_{\mathbf{k},\sigma} d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \,. \tag{A.9}$$

This part is now diagonal in $\mathbf{k}$ space. The nearest neighbours vectors $\delta_X$ for the X atoms are the vectors $\delta_{AA,i}$ from section III.2. With that, the sum over $\delta_X$ can be explicitly calculated:

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \tag{A.10}$$

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

$$\left. + e^{ia(-\frac{k_x}{2} - \frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2})} \right] \tag{A.12}$$

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

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

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

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

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

Show that!

We note

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

and calculate

$$\begin{aligned}
f_{Gr} &= -t_{Gr} \sum_{\delta_{AB}} e^{\mathrm{i}\mathbf{k}\boldsymbol{\delta}_{AB}} && \text{(A.18)}\\
&= -t_{Gr}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{\mathrm{i}\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)}\right) && \text{(A.19)}\\
&= -t_{Gr}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y}\left(e^{\mathrm{i}\frac{a}{2}k_x} + e^{-\mathrm{i}\frac{a}{2}k_x}\right)\right) && \text{(A.20)}\\
&= -t_{Gr}\left(e^{\mathrm{i}\frac{a}{\sqrt{3}}k_y} + 2e^{-\mathrm{i}\frac{a}{2\sqrt{3}}k_y}\cos\left(\frac{a}{2}k_x\right)\right) && \text{(A.21)}
\end{aligned}$$

All together, we get:

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

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# Listings

## List of Figures

III.1 EG-X model and Hexagonal lattice structure . . . . . . . . . . . . 6
III.2 Graphene Brillouin Zone . . . . . . . . . . . . . . . . . . . . . . . . . 7

## List of Tables

# Acknowledgement