Contents

I	Superconductivity	1
I.1	BCS Theory	1
I.2	Ginzburg-Landau theory of superconductivity,Phase transitions and broken symmetry	2
I.2.1	Order parameter concept	2
I.2.2	Landau theory	2
I.2.3	Ginzburg-Landau theory I: Ising order	4
I.2.4	Ginzburg-Landau theory II: complex order and superflow	4
I.3	Coherence length and penetration depth in strongly correlated superconductors	6
II	Green's Function Formalism	9
II.1	Perturbation theory, Dyson equation	11
II.2	Nambu-Gorkov GF	11
III	Dynamical Mean-Field Theory	13
IV	Quantum Metric	15
V	Noninteracting EG-X Model and structure	17
V.1	Lattice Structure of Graphene	17
V.2	EG-X Model	20
V.2.1	Review: Hubbard model on the honeycomb lattice	21
V.2.2	Band structure of the non-interacting EG-X model	21
VI	EG-X Model with interactions	25
VI.1	BdG	25
VI.1.1	BdG Hamiltonian	25
VI.1.2	BdG Hamiltonian in band basis	27
VI.2	Grand potential	29

Bibliography 31

List of Symbols 33

Todo list

More details on history . . . 1
Meissner effect, leads to supercurrent . . . 1
Some words: why is it interesting? . . . 1
Why supercurrent? . . . 1
BCS hamiltonian, pairing . . . 1
Mean-field . . . 1
Phonon interaction . . . 1
Mean field level can already explain a lot . . . 1
More recent developments: strongly correlated superconductors . . . 2
Could put a bit more into here about second order phase transition . . . 3
What is the h here? . . . 4
What is c? . . . 4
length scale/correlation length . . . 4
energy density of bosonic field? -> for comparison! . . . 5
Compare with Ising order, especially dependence on T . . . 6
Compare with Ising order. Is that derived or postulated? . . . 6
Here: particle-current operator, especially for coherent state, connection with phase twist . . . 6
Show GFs can be related to observables . . . 10
How to resolve ambiguity at borders of integral . . . 10
single-particle Matsubara GF . . . 11
equations of motion for Matsubara GF . . . 11
Short introduction to diagrams . . . 11

Self energy 11
Dyson equation 11
More general introduction into NG GFs, how they look like, what they describe etc. 11
Sources for these? 11
How to get quasiparticle weight? 11
See what is specific to this paper, see that I can derive that myself . . . 15
Dont get it here 15
Spin-orbit coupling, drop second spin index? 20
Write review for Hubbard model on the honeycomb lattice 21

I Superconductivity

This chapter gives an introduction to the phenomenology and theory of superconductivity. Superconductivity describes the phenomenon of the electrical resistance of a metal suddenly dropping to zero below a critical temperature.

At the beginning of the 20th century,

More details on history

Discovered in mercury in 1911 by Heike Onnes [1].

Meissner effect, leads to supercurrent

Some words: why is it interesting?

I.1 BCS Theory

Following [2, ch. 14].

Theoretical description of SC: 1956 by Bardeen, his postdoc Leon Cooper and the graduate in the group, J. Robert Schrieffer. Description is based on the fact, that the Fermi sea is unstable towards development of bound pairs under arbitrarily small attraction [3]. These bound electrons show bosonic behaviour and

Why supercurrent?

This model Hamiltonian

BCS hamiltonian, pairing

It can be connected to

The final element in this description was the origin of the attractive interaction between electrons, which Bardeen, Cooper and Schrieffer identified as a retarded electron-phonon interaction [4]. This so-called BCS-theory of superconductivity is very successful in explaining experimental results in many compounds, Surprisingly, it

Mean-field

Phonon interaction

Mean field level can already explain a lot

BCS-theory gave a microscopic explanation to a phenomenological description of superconductivity pioneered by Fritz London in 1937 [5]. This descriptions is based on a one-particle wavefunction $\phi(x)$

Later, this one-particle wa vefunction was identified as the order parameter in the developing GL-theory of phase transitions [6]. GL-theory is discussed in more detail in section I.2. This explains the Meissner effect and in turn the supercurrent.

More recent developments: strongly correlated superconductors

I.2 Ginzburg-Landau theory of superconductivity,Phase transitions and broken symmetry

Following [2, ch. 11].

I.2.1 Order parameter concept

Landau theory: phase transitions (e.g. iron becomes magnetic, water freezes, superfluidity/superconductivity) are associated with the development of an order parameter when the temperature drops below the transition temperature T_C.

$$|\psi| = \begin{cases} 0\ ,\ T > T_C \\ |\psi_0| > 0\ ,\ T < T_C \end{cases} \tag{I.1}$$

Landau theory does not need microscopic expression for order parameter, it provides corse-grained description of the properties of matter. The order parameter description is good at length scales above ξ_0, the coherence length (e.g. size of Cooper pairs for SC).

I.2.2 Landau theory

Basic idea of Landau theory: write free energy as function $F[\psi]$ of the order parameter. Region of small ψ, expand free energy of many-body system as simple polynomial:

$$f_L = \frac{1}{V}F[\psi] = \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 \tag{I.2}$$

Provided r and u are greater that 0: minimum of $f_L[\psi]$) lies at $\psi = 0$. Landau theory assumes: at phase transition temperature r changes sign, so:

$$r = a(T - T_C) \tag{I.3}$$

Minimum of free energy occurs for:

$$\psi = \begin{cases} 0 \\ \pm\sqrt{\frac{a(T_C - T)}{u}} \end{cases} \tag{I.4}$$

Two minima for free energy function for $T < T_C$. With this, we can extract T_C from the knowledge of the dependence of $|\psi|^2$ on T via a linear fit. This is only valid for an area near T_C (where Landau theory holds), but can be used to get T_C from microscopic theories.

Could put a bit more into here about second order phase transition

Going from a one to a n-component order parameters, OP acquires directions and magnitude. Particularly important example: complex or two component order parameter in superfluids and superconductors:

$$\psi = \psi_1 + \mathrm{i}\psi_2 = |\psi| e^{\mathrm{i}\phi} \tag{I.5}$$

The Landau free energy takes the form:

$$f[\psi] = r(\psi^*\psi) + \frac{u}{2}(\psi^*\psi)^2 \tag{I.6}$$

As before:

$$r = a(T - T_C) \tag{I.7}$$

Figure I.1 shows the Landau free energy as function of ψ.

Rotational symmetry, because free energy is independent of the global phase of the OP:

$$f[\psi] = f[e^{\mathrm{i}a}\psi] \tag{I.8}$$

In this 'Mexican hat' potential: order parameter can be rotated continuously from one broken-symmetry state to another. If we want the phase to be rigid, we need to introduce an There is a topological argument for the fact that the phase is rigid. This leads to Ginzburg-Landau theory. Will see later: well-defined phase is associated with persistent currents or superflow.

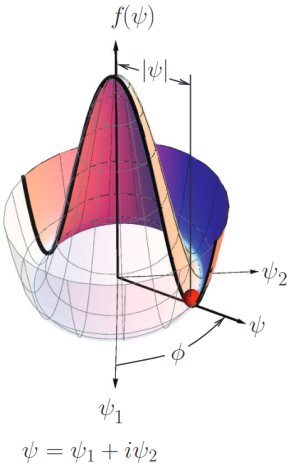

Figure I.1: *Mexican hat potential*

I.2.3 Ginzburg-Landau theory I: Ising order

Landau theory: energy cost of a uniform order parameter, more general theory needs to account for inhomogenous order parameters, in which the amplitude varies or direction of order parameter is twisted -> GL theory. First: one-component, 'Ising' order parameter. GL introduces additional energy $\delta f \propto |\Delta\psi|^2, f_{GL}[\psi, \Delta\psi] = \frac{s}{2}|\Delta\psi|^2 + f_L[\psi(s)]$, or in full:

$$f_{GL}[\psi, \Delta\psi, h] = \frac{s}{2}(\Delta\psi)^2 + \frac{r}{2}\psi^2 + \frac{u}{4}\psi^4 - h\psi \tag{I.9}$$

What is the h here?

What is c?

length scale/correlation length

GL theory is only valid near critical point, where OP is small enough to permit leading-order expansion. Dimensional analysis shows: $\frac{c}{r} = L^2$ has dimension of length squared. Length scale introduced by

I.2.4 Ginzburg-Landau theory II: complex order and superflow

Now: GL theory of complex or two-component order parameters, so superfluids and superconductors. Heart of discussion: emergence of a 'macroscopic wavefunction', where the microscopic field operators $\hat{\psi}(x)$ acquire an expectation value:

$$\langle\hat{\psi}(x)\rangle = \psi(x) = |\psi(x)|e^{i\theta(x)} \tag{I.10}$$

Reminder: Field operators are the real space representations of creation/annihilation operators. They can be thought of the super position of all ways of creating a particle at position x via the basis coefficients.

Magnitude determines density of particles in the superfluid:

$$|\psi(x)|^2 = n_s(x) \tag{I.11}$$

Density operator is

$$\hat{\rho} = \hat{\psi}(x)\hat{\psi^\dagger}(x) \tag{I.12}$$

so expectation value of that is the formula above.

Twist/gradient of phase determines superfluid velocity:

$$\mathbf{v}_s(x) = \frac{\hbar}{m}\Delta\phi(x) \tag{I.13}$$

We will derive this later in the chapter. Counterintuitive from quantum mechanics: GL suggested that $\Phi(x)$ is a macroscopic manifestation of a macroscopic number of particles condensed into precisely the same quantum state. Emergent phenomenon, collective properties of mater not a-priori self-evident from microscopic physics.

GL free energy density for superfluid (with one added term in comparison to Landau energy):

$$f_{GL}[\psi, \Delta\psi] = \frac{\hbar^2}{2m}|\Delta\psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 \tag{I.14}$$

Interpreted as energy density of a condensate of bosons in which the field operator behaves as a complex order parameter. Gives interpretation of gradient term as kinetic energy:

energy density of bosonic field? -> for comparison!

$$s|\Delta\psi|^2 = \frac{\hbar^2}{2m}\langle\Delta\hat{\psi}^\dagger\Delta\hat{\psi}\rangle \implies s = \frac{\hbar^2}{2m} \tag{I.15}$$

As in Ising order: correlation length/GL-coherence length governs characteristic range of amplitude fluctuations of the order parameter:

$$\xi = \sqrt{\frac{s}{|r|}} = \sqrt{\frac{\hbar^2}{2m|r|}} = \xi_0(1 - \frac{T}{T_C})^{-\frac{1}{2}} \tag{I.16}$$

where $\xi_0 = \xi(T=0) = \sqrt{\frac{\hbar^2}{2maT_c}}$ is the coherence length. Beyond this length: only phase fluctuations survive. Freeze out fluctuations in amplitude (no x-dependence in amplitude) $\psi(x) = \sqrt{n_s}e^{i\phi(x)}$, then $\Delta\psi = i\Delta\phi\psi$ and $|\Delta\psi|^2 = n_s(\Delta\phi)^2$, dependency of kinetic energy on the phase twist is (bringing it into the form $\frac{m}{2}v^2$):

$$\frac{\hbar^2 n_s}{2m}(\Delta\phi)^2 = \frac{mn_s}{2}(\frac{\hbar}{m}\Delta\phi)^2 \tag{I.17}$$

Compare with order, especiall dependence or

Compare with order. Is that d rived or postul

So twist of phase results in increase in kinetic energy, associated with a superfluid velocity:

$$\mathbf{v}_s = \frac{\hbar}{m}\Delta\phi \tag{I.18}$$

For interpretation of superfluid states: coherent states. These are eigenstates of the field operator

$$\hat{\psi}(x)\,|\psi\rangle = \psi(x)\,|\psi\rangle \tag{I.19}$$

and don't have a definite particle number. Importantly, this small uncertainty in particle number enables a high degree of precision in phase (which is the property of a condensate).

Phase rigidity and superflow: in GL theory, energy is sensitive to a twist of the phase. Substitute $\psi = |\psi|e^{i\phi}$ into GL free energy, gradient term is:

$$\Delta\psi = (\Delta|\psi| + i\Delta\phi|\psi|)e^{i\phi} \tag{I.20}$$

So:

$$f_{GL} = \frac{\hbar}{2m}|\psi|^2(\Delta\phi)^2 + \left[\frac{\hbar}{2m}(\Delta|\psi|)^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4\right] \tag{I.21}$$

The second term resembles GL functional for an Ising order parameter, describes energy cost of variations in the magnitude of the order parameter.

Here: particle-current operator, especially for coherent state, connection with phase twist

I.3 Coherence length and penetration depth in strongly correlated superconductors

From [7].

In most materials: Cooper pairs do not carry finite center-of-mass momentum. In presence of e.g. external fields or magnetism: SC states with FMP might arise.

Theory/procedure in the paper: enforce FMP states via constraints on pair-center-of-mass momentum $\mathbf{q}$, access characteristic lenght scales ξ_0, λ_L through analysis of the momentum and temperature-dependent OP. Constrain for FF-type pairing:

$$\psi_{\mathbf{q}}(\mathbf{r}) = |\psi_{\mathbf{q}}| e^{i\mathbf{q}\mathbf{r}} \tag{I.22}$$

II Green's Function Formalism

Following [8]

Green's functions: method to encode influence of many-body effects on propagation of particles in a system.

Have different kinds of Green's functions, for example the retarded Green's function:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(t')\}\rangle \tag{II.1}$$

They give the amplitude of a particle inserted at point $\mathbf{r}'$ at time t' to propagate to position $\mathbf{r}$ at time t. For time-independent Hamiltonians and systems in equilibrium, the GFs only depend on time differences:

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t-t') \tag{II.2}$$

So we can take $t' = 0$ and consider t as the only free variable:

$$G^R(\mathbf{r}\sigma, \mathbf{r}'\sigma', t) = -\mathrm{i}\Theta(t)\,\langle\{c_{\mathbf{r}\sigma}(t), c^\dagger_{\mathbf{r}\sigma}(0)\}\rangle \tag{II.3}$$

In a translation invariant system: can use $\mathbf{k}$ as a natural basis set:

$$G^R(\mathbf{k}, \sigma, \sigma' t) = -\mathrm{i}\Theta(t-t')\,\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma'}(0)\}\rangle \tag{II.4}$$

Define Fourier-transform:

$$G^R(\mathbf{k}, \sigma, \sigma', \omega) = \int_{-\infty}^{\infty} \mathrm{d}t G^R(\mathbf{k}, \sigma, \sigma' t) \tag{II.5}$$

Can define the spectral function from this:

$$A(\mathbf{k}\sigma, \omega) = -2\Im G^R(\mathbf{k}\sigma, \omega) \tag{II.6}$$

Looking at the diagonal elements of G^R here. The spectral function can be thought of as the energy resolution of a particle with energy ω. This mean,

for non-interacting systems, the spectral function is a delta-function around the single-particle energies:

$$A_0(\mathbf{k}\sigma, \omega) = 2\pi\delta(\omega - \epsilon_{\mathbf{k}\sigma}) \tag{II.7}$$

For interacting systems this is not true, but A can still be peaked.

Show GFs can related to obse ables

Mathematical technique to calculate retarded GFs involves defining GFs on imaginary times τ:

$$t \to -\mathrm{i}\tau \tag{II.8}$$

where τ is real and has the dimension time. This enables the simultaneous expansion of exponential $e^{-\beta H}$ coming from the thermodynamic average and $e^{-\mathrm{i}Ht}$ coming from the time evolution of operators.

Define imaginary time/Matsubara GF $C_{AB}(\tau, 0)$:

$$C_{AB}(\tau, 0) = -\left\langle T_\tau(A(\tau)B(0))\right\rangle \tag{II.9}$$

with time-ordering operator in imaginary time:

$$T_\tau(A(\tau)B(\tau')) = \Theta(\tau - \tau')A(\tau)B(\tau') \pm \Theta(\tau' - \tau)B(\tau')A(\tau) \tag{II.10}$$

so that operators with later 'times' go to the left.

Can prove from properties of Matsubara GF, that they are only defined for

$$-\beta < \tau < \beta \tag{II.11}$$

Due to this, the Fourier transform of the Matsubara GF is defined on discrete values:

$$C_{AB}(\mathrm{i}\omega_n) = \int_0^\beta \mathrm{d}\tau \tag{II.12}$$

with fermionic/bosonic Matsubara frequencies

$$\omega_n = \begin{cases} \frac{2n\pi}{\beta} \text{ for bosons} \\ \frac{(2n+1)\pi}{\beta} \text{ for fermions} \end{cases} \tag{II.13}$$

How to resolve ambiguity at borders of integral

It turns out that Matsubara GFs and retarded GFs can be generated from a common function $C_{AB}(z)$ that is defined on the entire complex plane except

for the real axis. So we can get the retarded GF $C^R_{AB}(\omega)$ by analytic continuation:

$$C^R_{AB}(\omega) = C_{AB}(\mathrm{i}\omega_n \to \omega + \mathrm{i}\eta) \tag{II.14}$$

So in particular the extrapolation of the Matsubara GF to zero is proportional to the density of states at the chemical potential. Gapped: density is zero (Matsubara GF goes to 0), metal: density is finite (Matsubara GF goes to finite value) [8, p. 8.3.4].

single-particle Matsubara GF

equations of motion for Matsubara GF

II.1 Perturbation theory, Dyson equation

Short introduction to diagrams

Dyson equation:

$$\mathcal{G}_\sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}{1 - \mathcal{G}^0_\sigma(\mathbf{k}, \mathrm{i}\omega_n)\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)} = \frac{1}{\mathrm{i}\omega_n - \tilde{\xi}_{\mathbf{k}-\Sigma_\sigma(\mathbf{k}, \mathrm{i}\omega_n)}} \tag{II.15}$$

Self energy

Dyson equation

II.2 Nambu-Gorkov GF

Introduction following [2, ch. 14.7]

More general introduction into NG GFs, how they look like, what they describe etc.

Order parameter can be chosen as the anomalous GF:

$$\Psi = F^{\mathrm{loc}}(\tau = 0^-) \tag{II.16}$$

or the superconducting gap

$$\Delta = Z\Sigma^{\mathrm{AN}} \tag{II.17}$$

that can be calculated from the anomalous self-energy Σ^{AN} and quasiparticle weight Z

Sources for these?

How to get quasiparticle weight?

III Dynamical Mean-Field Theory

Following [9].

Most general non-interacting electronic Hamiltonian in second quantization:

$$H_0 = \sum_{i,j,\sigma} \tag{III.1}$$

with lattice coordinates i, j and spin σ.

One particle Green's function (many-body object, coming from the Hubbard model):

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{\mathrm{i}\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)} \tag{III.2}$$

with the self energy $\Sigma(\mathrm{i}\omega_n)$ coming from the solution of the effect on-site problem:

The Dyson equation

$$G(\mathbf{k}, \mathrm{i}\omega_n) = \left(G_0(\mathbf{k}, \mathrm{i}\omega_n) - \Sigma(\mathbf{k}, \mathrm{i}\omega_n)\right)^{-1} \tag{III.3}$$

relates the non-interacting Greens function $G_0(\mathbf{k}, \mathrm{i}\omega_n)$ and the fully-interacting Greens function $G(\mathbf{k}, \mathrm{i}\omega_n)$ (inversion of a matrix!).

IV Quantum Metric

First formulated in [10]

Following Cheng - a pedagogical Introduction

See what is specific to this paper, see that I can derive that myself

Parameter dependent Hamiltonian $\{H(\lambda)\}$, smooth dependence on parameter $\lambda = (\lambda_1, \lambda_2, ...) \in \mathcal{M}$ (base manifold)

Hamiltonian acts on parametrized Hilbert space $\mathcal{H}(\lambda)$

Eigenenergies $E_n(\lambda)$, eigenstates $|\phi_n(\lambda)\rangle$

System state $|\psi(\lambda)\rangle$ is linear combination of $|\psi_n(\lambda)\rangle$ at every point in $\mathcal{M}$

Infinitesimal variation of the parameter $\mathrm{d}\lambda$:

Dont get it here

$$\mathrm{d}s^2 = \||\psi(\lambda+\mathrm{d}\lambda)-(\lambda)\|^2 = \langle\delta\psi|\,\delta\psi\rangle = \langle\partial_\mu\psi|\,\partial_\nu\psi\rangle\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu = (\gamma_{\mu\nu}+\mathrm{i}\sigma_{\mu\nu})\,\mathrm{d}\lambda^\mu\,\mathrm{d}\lambda^\nu \tag{IV.1}$$

Last part is splitting up into real and imaginary part

V Noninteracting EG-X Model and structure

V.1 Lattice Structure of Graphene

Structure of honeycomb lattice following [11].
Monolayer graphene forms a hexagonal lattice.
Primitive lattice vectors of the hexagonal lattice:

$$\mathbf{a}_1 = \frac{a}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix} \tag{V.1}$$

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

with lattice constant $a \approx 2.46\,\text{Å}$ (distance between unit cells). Have

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

with the nearest-neighbour distance a_0.
Vectors to the nearest-neighbor B_i $(i = 1, 2, 3,)$ atoms from atom A:

$$\delta_{AB,1} = \begin{pmatrix} 0 \\ \frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{AB,2} = \begin{pmatrix} \frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{AB,3} = \begin{pmatrix} -\frac{a}{2} \\ -\frac{a}{2\sqrt{3}} \end{pmatrix} \tag{V.4}$$

Vectors to the nearest-neighbor A_i $(i = 1, 2, 3,)$ atoms from atom B:

$$\delta_{BA,1} = \begin{pmatrix} 0 \\ -\frac{a}{\sqrt{3}} \end{pmatrix}, \delta_{BA,2} = \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix}, \delta_{BA,3} = \begin{pmatrix} -\frac{a}{2} \\ \frac{a}{2\sqrt{3}} \end{pmatrix} \tag{V.5}$$

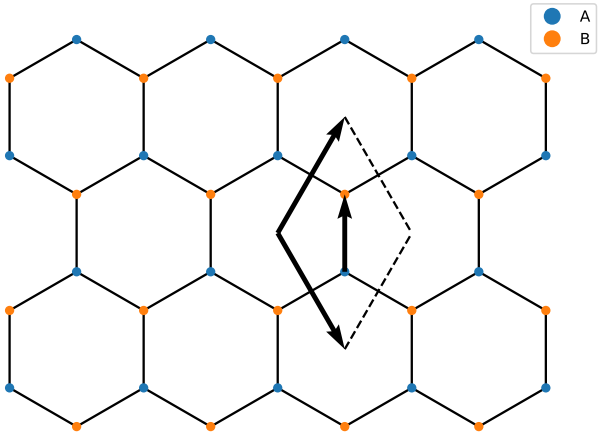

Figure V.1: *Graphene lattice structure*

The vectors between the Graphene A atom and the six neighbours on the same sub lattice can be found by rotating $\mathbf{a}_1$ six times by $1/6 * 2\pi = \pi/3$:

$$\delta_{AA,1} = \mathbf{a}_1 = \frac{a}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} = a\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} = a\begin{pmatrix}\sin(\frac{\pi}{6})\\ \cos(\frac{\pi}{6})\end{pmatrix} \tag{V.6}$$

$$\delta_{AA,2} = a\begin{pmatrix}\sin(\frac{3\pi}{6})\\ \cos(\frac{3\pi}{6})\end{pmatrix} = a\begin{pmatrix}1\\ 0\end{pmatrix} \tag{V.7}$$

$$\delta_{AA,3} = a\begin{pmatrix}\sin(\frac{5\pi}{6})\\ \cos(\frac{5\pi}{6})\end{pmatrix} = a\begin{pmatrix}\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} \tag{V.8}$$

$$\delta_{AA,4} = a\begin{pmatrix}\sin(\frac{7\pi}{6})\\ \cos(\frac{7\pi}{6})\end{pmatrix} = a\begin{pmatrix}-\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix} \tag{V.9}$$

$$\delta_{AA,5} = a\begin{pmatrix}\sin(\frac{9\pi}{6})\\ \cos(\frac{9\pi}{6})\end{pmatrix} = a\begin{pmatrix}-1\\ 0\end{pmatrix} \tag{V.10}$$

$$\delta_{AA,6} = a\begin{pmatrix}\sin(\frac{11\pi}{6})\\ \cos(\frac{11\pi}{6})\end{pmatrix} = a\begin{pmatrix}-\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix} \tag{V.11}$$

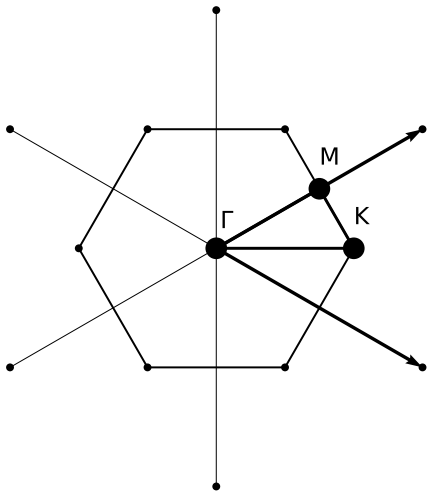

Figure V.2: *Graphene Brillouin Zone*

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

$$\mathbf{a}_1 \cdot \mathbf{b}_1 = \mathbf{a}_2 \cdot \mathbf{b}_2 = 2\pi \tag{V.12}$$
$$\mathbf{a}_1 \cdot \mathbf{b}_2 = \mathbf{a}_2 \cdot \mathbf{b}_1 = 0\,, \tag{V.13}$$

so we have:

$$\mathbf{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{V.14}$$
$$\mathbf{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -\frac{1}{\sqrt{3}} \end{pmatrix} \tag{V.15}$$

Points of high symmetry in the Brillouin zone are:

$$\Gamma = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{V.16}$$

$$\mathrm{M} = \frac{\pi}{a} \begin{pmatrix} 1 \\ \frac{1}{\sqrt{3}} \end{pmatrix} \tag{V.17}$$

$$\mathrm{K} = \frac{4\pi}{3a} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{V.18}$$

V.2 EG-X Model

Graphene lattice and a site X. Real-life motivation: layer of graphene on top

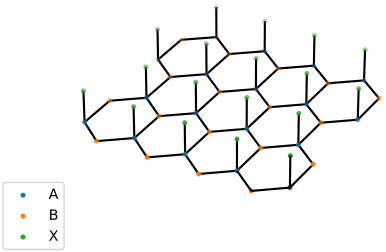

Figure V.3: *EG-X model*

of a substrate of another material (which provides the additional X atoms). There is no spin-orbit coupling considered in the model (but when according to Niklas: when mapping to substrates Sn or Pb, it could be necessary (but does not the qualitative result?)).

Spin-orbit coupling, drop second spin index?

Without interaction :

$$H_0 = -t_X \sum_{\langle ij\rangle,\sigma\sigma'} d^\dagger_{i,\sigma} d_{j,\sigma'} + \text{h.c.} - t_{Gr} \sum_{\langle ij\rangle,\sigma\sigma'} \left(c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} + c^{(B),\dagger}_{j,\sigma'} c^{(A)}_{i,\sigma} + \text{h.c.} \right) \tag{V.19}$$

$$+ V \sum_{i,\sigma\sigma'} \left(d^\dagger_{i,\sigma} c^{(A)}_{i,\sigma'} + c^{(A),\dagger}_{i,\sigma} d_{i,\sigma'} \right) \tag{V.20}$$

with:

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

We can also introduce an onsite Hubbard interaction:

$$H_{\text{int}} = U_X \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{Gr} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{V.21}$$

V.2.1 Review: Hubbard model on the honeycomb lattice

Write review for Hubbard model on the honeycomb lattice

V.2.2 Band structure of the non-interacting EG-X model

To treat eq. V.20, we first write out the sums over nearest neighbours $\langle i, j\rangle$ explicitly, writing $\delta_X, \delta_\epsilon$ ($\epsilon = A, B$) for the connections to the nearest neighbours of the X atoms and Graphene A, B sites. Doing the calculation for the example of the X atoms:

$$- t_X \sum_{\langle ij\rangle,\sigma\sigma'} (d^\dagger_{i,\sigma} d_{j,\sigma'} + d^\dagger_{j,\sigma} d_{i,\sigma'}) \tag{V.22}$$

$$= -\frac{t_X}{2} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma'} - \frac{t_X}{2} \sum_{j,\sigma,\sigma'} \sum_{\delta_X} d^\dagger_{j,\sigma} d_{j+\delta_X,\sigma'} \tag{V.23}$$

$$= -t_X \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d^\dagger_{i,\sigma} d_{i+\delta_X,\sigma'} \tag{V.24}$$

(The factor $1/2$ is to account for double counting when going to the sum over all lattice sites i)

Now we can input the discrete Fourier transform (for both graphene and X operators) into eq. V.24

$$c_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}} \tag{V.25}$$

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} c_{\mathbf{k}}^\dagger \tag{V.26}$$

with the completeness relation:

$$\sum_i e^{\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\mathbf{r}_i} = N\delta_{\mathbf{k},\mathbf{k}'} \ . \tag{V.27}$$

We get:

$$-t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} d_{i,\sigma}^\dagger d_{i+\delta_X,\sigma'} = -t_X \frac{1}{N} \sum_{i,\sigma,\sigma'} \sum_{\delta_X} \sum_{\mathbf{k},\mathbf{k}'} e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \tag{V.28}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} \sum_i e^{-\mathrm{i}\mathbf{k}\mathbf{r}_i} e^{\mathrm{i}\mathbf{k}'\mathbf{r}_i} \tag{V.29}$$

$$= -t_X \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} \sum_{\delta_X} d_{\mathbf{k},\sigma}^\dagger e^{\mathrm{i}\mathbf{k}'\delta_X} d_{\mathbf{k}',\sigma'} N\delta_{\mathbf{k},\mathbf{k}'} \tag{V.30}$$

$$= -t_X \sum_{\mathbf{k},\sigma,\sigma'} d_{\mathbf{k},\sigma}^\dagger d_{\mathbf{k},\sigma'} \sum_{\delta_X} e^{\mathrm{i}\mathbf{k}\delta_X} \tag{V.31}$$

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

$$f_X(\mathbf{k}) = -t_X \sum_{\delta_X} e^{i\mathbf{k}\delta_X} \tag{V.32}$$

$$= -t_X \left(e^{ia(\frac{k_x}{2}+\frac{\sqrt{3}k_y}{2})} + e^{iak_x} + e^{ia(\frac{k_x}{2}-\frac{\sqrt{3}k_y}{2})} \right. \tag{V.33}$$

$$\left. + e^{ia(-\frac{k_x}{2}-\frac{\sqrt{3}k_y}{2})} + e^{-iak_x} + e^{ia(-\frac{k_x}{2}+\frac{\sqrt{3}k_y}{2})} \right) \tag{V.34}$$

$$= -t_X \left(2\cos(ak_x) + 2e^{ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) + 2e^{-ia\frac{\sqrt{3}k_y}{2}} \cos(\frac{a}{2}k_x) \right) \tag{V.35}$$

$$= -2t_X \left(\cos(ak_x) + 2\cos(\frac{a}{2}k_x)\cos(\sqrt{3}\frac{a}{2}k_y) \right) \tag{V.36}$$

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

$$-t_{\mathrm{Gr}} \sum_{\langle ij\rangle,\sigma\sigma'} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{j,\sigma'} = -t_{\mathrm{Gr}} \sum_{i,\sigma\sigma'} \sum_{\delta_{AB}} c^{(A),\dagger}_{i,\sigma} c^{(B)}_{i+\delta_{AB},\sigma'} \tag{V.37}$$

$$= -t_{\mathrm{Gr}} \sum_{\mathbf{k},\sigma,\sigma'} c^{(A)\dagger}_{\mathbf{k},\sigma} c^{(B)}_{\mathbf{k},\sigma'} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{V.38}$$

We note

$$\sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} = \left(\sum_{\delta_{BA}} e^{i\mathbf{k}\delta_{BA}} \right)^* = \sum_{\delta_{BA}} e^{-i\mathbf{k}\delta_{BA}} \tag{V.39}$$

and calculate

$$f_{Gr} = -t_{Gr} \sum_{\delta_{AB}} e^{i\mathbf{k}\delta_{AB}} \tag{V.40}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{i\frac{a}{2\sqrt{3}}(\sqrt{3}k_x - k_y)} + e^{i\frac{a}{2\sqrt{3}}(-\sqrt{3}k_x - k_y)} \right) \tag{V.41}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + e^{-i\frac{a}{2\sqrt{3}}k_y} \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x} \right) \right) \tag{V.42}$$

$$= -t_{Gr} \left(e^{i\frac{a}{\sqrt{3}}k_y} + 2e^{-i\frac{a}{2\sqrt{3}}k_y} \cos(\frac{a}{2}k_x) \right) \tag{V.43}$$

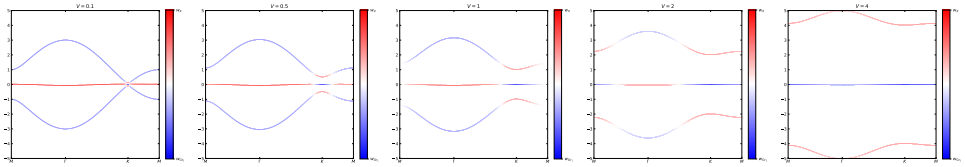

Figure V.4: *Bands of the non-interacting EG-X model. All the bands are spin-degenerate.*

All together, we get:

$$H_0 = \sum_{\mathbf{k},\sigma,\sigma'} \begin{pmatrix} c^{A,\dagger}_{k,\sigma} & c^{B,\dagger}_{k,\sigma} & d^{\dagger}_{k,\sigma} \end{pmatrix} \begin{pmatrix} 0 & f_{Gr} & V \\ f^{*}_{Gr} & 0 & 0 \\ V & 0 & f_X \end{pmatrix} \begin{pmatrix} c^{A}_{k,\sigma} \\ c^{B}_{k,\sigma} \\ d_{k,\sigma} \end{pmatrix} \tag{V.44}$$

The band structure for the non-interacting EG-X model is easily obtained by diagonalising the matrix in eq. V.44. This was done in fig. V.4.

Values used for calculation:

- $a_0 = 1$
- $t_{\mathrm{Gr}} = 1$
- $t_{\mathrm{X}} = 0.01$

V is the control parameter. (According to Niklas), a range from $V = 0.1$ to $V = 2$ can be mapped onto materials in experiment.

VI EG-X Model with interactions

VI.1 BdG

VI.1.1 BdG Hamiltonian

Define sublattice index

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

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

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

with the matrix

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

Add chemical potential:

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

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

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

Fourier transformation:

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

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

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

Mean-field approximation:

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

with

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

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

This gives the BCS mean field Hamiltonian:

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

with Nambu spinor

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

we have:

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

with

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

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

VI.1.2 BdG Hamiltonian in band basis

Use transformation

$$c^\dagger_{\mathbf{k}\alpha\sigma} = \sum_n [\mathbf{G}]^*_{\alpha n} d^\dagger_{n\mathbf{k}\sigma} \tag{VI.15}$$

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

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

with that:

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

So the kinetic part of the BdG Hamiltonian becomes:

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

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

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

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

$$=: \sum_{n\mathbf{k}\sigma} \xi_{\mathbf{k}} d^\dagger_{n\mathbf{k}\sigma} d_{n\mathbf{k}\sigma} \tag{VI.22}$$

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

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

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

So that:

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

with

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

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

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

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

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

So for $V \to 0$:

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

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

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

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

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

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

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

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

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

VI.2 Grand potential

See [12], 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):

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

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):

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

$$= \sum_{\mathbf{k}} \mathrm{Tr}(H_{\mathbf{k}}^\downarrow) + \sum_{\mathbf{k}\alpha} \frac{|\Delta_\alpha|^2}{U} - \frac{1}{\beta} \ln \mathrm{Tr}(e^{-\beta \Psi_{\mathbf{k}}^\dagger \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}}}) \tag{VI.36}$$

Zero temperature limit:

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

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:

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

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

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List of Symbols

Symbol	Meaning	Definition
τ	general imaginary time variable	10
$C_{AB}(\tau, 0)$	Correlation function in imaginary time	10