Numerical analysis of superconducting phases in the extended Hubbard model with non-local pairing

University of Pisa, a.y. 2025-2026

Alessandro Gori*

Thesis for the Master's degree in Physics

Abstract

[To be continued...]

Contents

Draft: August 28, 2025

*a.gori23@studenti.unipi.it / nepero27178@github.com

Chapter 1

Mean-field theory solution

This chapter is devoted to develop a rough mean field approximation of the Extended Hubbard model of Eq. (**??**),

$$\hat{H} = \underbrace{-t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma}}_{\hat{H}_t} + \underbrace{U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}_{\hat{H}_U} \underbrace{- V \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'}}_{-\hat{H}_V}$$

Mean Field Theory (MFT) is a widely used and simple theoretical tool, often sufficient to describe the leading orders in phase transition phenomena of Many-Body Physics. Here MFT is employed following the path of Bardeen-Cooper-Schrieffer (BCS) theory in describing conventional s-wave superconductivity. As will be thoroughly described, the lattice spatial structure directly influences the topology of the gap function, giving rise to anisotropic pairing. Sec. 1.1 studies the non-local attraction in real-space, while Sec. 1.2 moves to reciprocal space and gives a self-consistent MFT solution. Finally, numerical results are exposed in Sec. 1.3.

1.1 Mean-Field theory real space description

In this section, an analytic discussion of the real-space hamiltonian of Eq. (**??**) is given. The first part focuses on the non-local interaction V, expected to be source of superconductivity; the second part on the local interaction U, known to be source of Slater-like anti-ferromagnetism, as described in App. **??**.

1.1.1 Mean-field treatment of the non-local term

Consider the non-local term,

$$\hat{H}_V \equiv -V \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \tag{1.1}$$

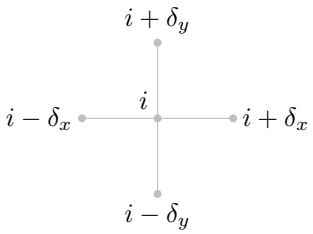


Figure 1.1 | Schematic representation of the four NNs of a given site i for a planar square lattice.

Evidently the hamiltonian can be decomposed in various spin terms,

$$\begin{aligned}\hat{H}_V &= \sum_{\sigma\sigma'} \hat{H}_V^{\sigma\sigma'} \\ &= \underbrace{\hat{H}_V^{\uparrow\uparrow} + \hat{H}_V^{\downarrow\downarrow}}_{\text{Ferromagnetic}} + \underbrace{\hat{H}_V^{\uparrow\downarrow} + \hat{H}_V^{\downarrow\uparrow}}_{\text{Anti-ferromagnetic}}\end{aligned}$$

Evidently, to carry out a summation over nearest neighbors $\langle ij \rangle$ of a square lattice means precisely to sum over all links of the lattice. Then we can identify the generic AF term $\hat{H}_V^{\sigma\overline{\sigma}}$ as the one collecting the σ operators of sublattice $\mathcal{S}_a$ and $\overline{\sigma}$ operators of sublattice $\mathcal{S}_b$. At half-filling, as described in Sec. **??**, the ground-state leading contribution will be the antiferromagnetic state, with the square lattice decomposed in two oppositely polarized square lattices with spacing increased by a factor $\sqrt{2}$. Then, it is to be expected that on this configuration the ferromagnetic contributions are suppressed[1]. Anyways, the calculation will be carried out considering both terms. The AF non-local interactions can be written as a sum of terms over just one of the two sublattices $\mathcal{S}_a$ and $\mathcal{S}_b$, oppositely polarized in the AF configuration (see Fig. **??**)

$$\begin{aligned}\hat{H}_V^{(\mathrm{AF})} &= \overbrace{\sum_{i\in\mathcal{S}_a} \hat{h}_V^{(i)}}^{\hat{H}_V^{\uparrow\downarrow}} + \overbrace{\sum_{i\in\mathcal{S}_b} \hat{h}_V^{(i)}}^{\hat{H}_V^{\downarrow\uparrow}} \\ &= \sum_{i\in\mathcal{S}} \hat{h}_V^{(i)}\end{aligned} \qquad \hat{h}_V^{(i)} = -V \sum_{\ell=x,y} (\hat{n}_{i\uparrow}\hat{n}_{i+\delta_\ell\downarrow} + \hat{n}_{i\uparrow}\hat{n}_{i-\delta_\ell\downarrow})$$

Here the notation of Fig. **??** is used. The two-dimensional lattice is regular-square. For each site i in a given sublattice, the nearest neighbors sites are four – all in the other sublattice. The notation used is $i \pm \delta_x$, $i \pm \delta_y$ as in Fig. 1.1. Similarly, the Ferromagnetic hamiltonian decomposes as

$$\hat{H}_V^{(\mathrm{F})} = -V \sum_{i\in\mathcal{S}_a} \sum_{\ell=x,y} \sum_{\sigma} (\hat{n}_{i\sigma}\hat{n}_{i+\delta_\ell\sigma} + \hat{n}_{i\sigma}\hat{n}_{i-\delta_\ell\sigma})$$

Note here the summation only on one sublattice. As will be shown in Sec. 1.2.5, under MFT it makes sense to approximate

$$\hat{H}_V \simeq \hat{H}_V^{(\mathrm{AF})}$$

thus neglecting ferromagnetic contribution to Cooper instability. The non-local interaction contribution to energy, as a function of the $T = 0$ full hamiltonian ground-state[2] $|\Psi\rangle$, is given by

$$\begin{aligned}E_V[\Psi] &= \langle\Psi|\hat{H}_V|\Psi\rangle \\ &= -V \sum_{i\in\mathcal{S}} \sum_{\ell=x,y} \langle \hat{n}_{i\uparrow}\hat{n}_{i+\delta_\ell\downarrow} + \hat{n}_{i\uparrow}\hat{n}_{i-\delta_\ell\downarrow}\rangle\end{aligned}$$

Shorthand notation has been used: $\langle\Psi|\cdot|\Psi\rangle = \langle\cdot\rangle$. Consider one specific term, say, $\hat{n}_{i\uparrow}\hat{n}_{i+\delta_x\downarrow}$. Wick's Theorem states that, if the expectation value is performed onto a coherent state,

$$\begin{aligned}\langle \hat{n}_{i\uparrow}\hat{n}_{i+\delta_x\downarrow}\rangle &= \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i+\delta_x\downarrow}^\dagger \hat{c}_{i+\delta_x\downarrow}\hat{c}_{i\uparrow}\rangle \\ &= \underbrace{\langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i+\delta_x\downarrow}^\dagger\rangle\langle \hat{c}_{i+\delta_x\downarrow}\hat{c}_{i\uparrow}\rangle}_{\text{Cooper}} - \underbrace{\langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i+\delta_x\downarrow}\rangle\langle \hat{c}_{i+\delta_x\downarrow}^\dagger \hat{c}_{i\uparrow}\rangle}_{\text{Fock}} + \underbrace{\langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow}\rangle\langle \hat{c}_{i+\delta_x\downarrow}^\dagger \hat{c}_{i+\delta_x\downarrow}\rangle}_{\text{Hartree}}\end{aligned}$$

As a first approximation, the theorem is assumed to hold (which, in a BCS-like fashion, is equivalent to assuming for the ground-state to be a coherent state). The last two terms account for single-particle interactions with a background field; they are relevant in the Hartree-Fock scheme, being

[1] This is also due to superexchange stabilization: the triplet contribution to hamiltonian is suppressed, and this cancels out the ferromagnetic terms $\hat{H}_V^{\sigma\sigma}$ while privileging the singlet configuration of the anti-ferromagnetic terms $\hat{H}_V^{\sigma\overline{\sigma}}$.

[2] Extensions to finite temperatures is simple: minimization must be carried out on free energy, while expectation values must be taken in a thermodynamic fashion.

direct-exchange contributions to single particle energies. The first term accounts for non-local electrons pairing, mimicking the Cooper term of BCS theory. The core assumption, here, is that only one of the HF and Bogoliubov pairings survive. Appendix **??** shows a situation dominated by HF terms. Here, I assume the symmetry to be broken by a Cooper term. Energy then is cast to the form

$$E_V[\Psi] = -V \sum_{i\in\mathcal{S}} \sum_{\ell=x,y} \left[\langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i+\delta_\ell\downarrow} \rangle \langle \hat{c}_{i+\delta_\ell\downarrow} \hat{c}_{i\uparrow} \rangle + \langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i-\delta_\ell\downarrow} \rangle \langle \hat{c}_{i-\delta_\ell\downarrow} \hat{c}_{i\uparrow} \rangle \right]$$

The ground-state must realize the condition

$$\frac{\delta}{\delta \langle \Psi |} E[\Psi] = 0$$

being $E[\Psi]$ the total energy (made up of the three terms of couplings t, U and V). [Expand derivation?] The functional derivative must be carried out in a variational fashion including a Lagrange multiplier, the latter accounting for state-norm conservation, as is done normally in deriving the Hartree-Fock approximation for the eigenenergies of the electron liquid [4, 5]. This approach leads to the conclusion that the (coherent) ground-state of the system must be an eigenstate of the mean-field effective hamiltonian:

$$\begin{aligned} \hat{H}^{(\mathrm{e})} = & -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \\ & - V \sum_{i\in\mathcal{S}} \sum_{\ell=x,y} \sum_{\delta=\pm\delta_\ell} \left[\langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i+\delta\downarrow} \rangle \hat{c}_{i+\delta\downarrow} \hat{c}_{i\uparrow} + \mathrm{h.c.} \right] \end{aligned} \tag{1.2}$$

The pairing correlation function is defined across each bond as the pairing expectation

$$g_{ij} \equiv \langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{j\downarrow} \rangle$$

The effective hamiltonian reads:

$$\hat{H}^{(\mathrm{e})} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - V \sum_{\langle ij \rangle} \left[g_{ij} \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} + g^*_{ij} \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{j\downarrow} \right] \tag{1.3}$$

As in standard BCS theory, this hamiltonian – being quadratic in the electronic operators – can be diagonalized via a Bogoliubov rotation. Superconducting pairing can arise both from the local U term and from the non-local V term. In next sections it is assumed the V term generates dominant superconductivity via its weak non-local pairing.

1.1.2 Mean-field treatment of the local term

The mean-field description of the local (on-site) U interaction is given in detail in App. **??**, along with a simple numerical analysis of the insurgence of antiferromagnetic ordering in a Hartree-Fock approximation scheme. Here the Cooper pairing is likewise assumed to dominate. Performing an analysis analogous to the one carried out in last section, we get the decoupling

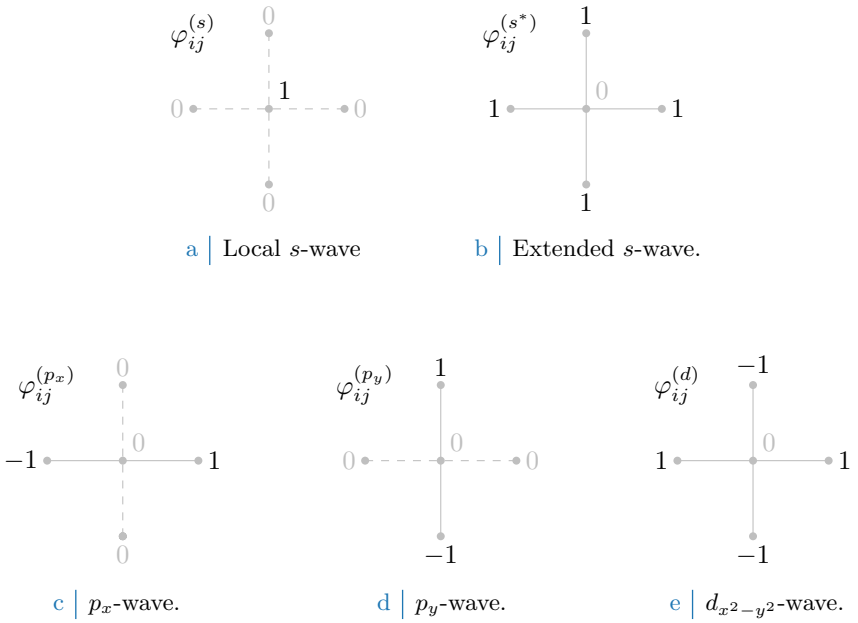
$$U \sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \simeq U \sum_{i\sigma} \left[f_i \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + f^*_i \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i\downarrow} \right]$$

being

$$f_i \equiv \langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i\downarrow} \rangle$$

Collect f and g in the unique function of two variables:

$$C(i,j) = \begin{cases} f_i & \text{if} \quad i = j \\ g_{ij} & \text{if} \quad |i-j| = 1 \\ (\cdots) & \text{otherwise} \end{cases}$$



a | Local s-wave b | Extended s-wave.

c | p_x-wave. d | p_y-wave. e | $d_{x^2-y^2}$-wave.

Figure 1.2 | Form factors at different topologies, as listed in Tab. 1.1. In figures five sites are represented: the hub site i and its four NN. Solid lines represent non-zero values for $\varphi_{\boldsymbol{\delta}}$, while dashed lines represent vanishing factors.

which expresses the generic correlator $\langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \rangle$. The correlator for $|i-j|>1$ is left unexpressed, and supposed to be subdominant. The decoupled hamiltonian, apart from pure energy shifts and suppressed terms, is given by

$$\hat{H}^{(\mathrm{e})} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \left[f_i \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + f_i^* \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \right] - V \sum_{\langle ij \rangle} \left[g_{ij} \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} + g_{ij}^* \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \right] \tag{1.4}$$

[To be continued...]

1.1.3 Topological correlations

Topology plays an important role in establishing SC, giving rise to anisotropic pairing as well as real space structures for the Cooper pairs. The correlator g_{ij} is a function of position, specifically of its variables difference $\boldsymbol{\delta} \equiv \mathbf{x}_j - \mathbf{x}_i$. Over the square lattice with NN interaction, the latter can assume four values: $\boldsymbol{\delta} = \pm\boldsymbol{\delta}_x, \pm\boldsymbol{\delta}_y$. For a function of space defined over the four rim sites $\mathbf{x}_i \pm \boldsymbol{\delta}_\ell$ of Fig. 1.1, various symmetry structures can be defined under the planar rotations group SO(2). In other words, the function $g_{\boldsymbol{\delta}}$ can be decomposed in planar harmonics (which are simply the sine-cosine basis). Equivalently, given two NN sites i, j

$$g_{ij} = \sum_\gamma g^{(\gamma)} \varphi_{ij}^{(\gamma)}$$

where $g^{(\gamma)}$ are the g_{ij} symmetries-decomposition coefficients while $\varphi_{ij}^{(\gamma)}$ are the form factors listed in Tab. 1.1, a simple orthonormal rearrangement of the harmonics basis.

SC is established with a given symmetry – which means, symmetry breaking in the phase transition proceeds in a specific channel. Conventional BCS superconductivity arises from the only possible spatial structure of the local pairing, s-wave – here appearing as a local term (Fig. 1.2a) and extended on a non-local term (Fig. 1.2b). Cuprates exhibit a tendency towards $d_{x^2-y^2}$ SC, while other materials towards p-wave types – eventually with some chirality, as is the case for $p_x \pm ip_y$ SCs. To establish SC under a certain symmetry γ means that Cooper pairs acquire said symmetry – which implies, for correlations, $g^{(\gamma')} = g^{(\gamma)} \delta_{\gamma\gamma'}$. and $g_{ij} \propto \varphi_{ij}^{(\gamma)}$.

Structure	Form factor	Graph
s-wave	$\varphi_{ij}^{(s)} = \delta_{ij}$	Fig. 1.2a
Extended s-wave	$\varphi_{ij}^{(s^*)} = \delta_{j=i+\delta_x} + \delta_{j=i-\delta_x} + \delta_{j=i+\delta_y} + \delta_{j=i-\delta_y}$	Fig. 1.2b
p_x-wave	$\varphi_{ij}^{(p_x)} = \delta_{j=i+\delta_x} - \delta_{j=i-\delta_x}$	Fig. 1.2c
p_y-wave	$\varphi_{ij}^{(p_y)} = \delta_{j=i+\delta_y} - \delta_{j=i-\delta_y}$	Fig. 1.2d
$d_{x^2-y^2}$-wave	$\varphi_{ij}^{(d)} = \delta_{j=i+\delta_x} + \delta_{j=i-\delta_x} - \delta_{j=i+\delta_y} - \delta_{j=i-\delta_y}$	Fig. 1.2e

Table 1.1 First four spatial structures for the correlation function $C(i,j)$. In the middle column, all spatial dependence is included in the δs, while $f^s, g^{(\gamma)} \in \mathbb{C}$. The last column indicates the graph representation of each contribution given in Fig. **??**. Subscript x^2-y^2 is omitted for notational clarity.

1.2 Mean-Field theory reciprocal space description

In this BCS-like approach, a self-consistent equation for the gap function must be retrieved in order to further investigate the model and extract the conditions for the formation of a superconducting phase with a given pairing topology. In order to do so, let me take a step back and perform explicitly the Fourier-transform of the various terms of Eq. **??**.

1.2.1 Kinetic term

The kinetic part is trivial to transform. The followed convention is

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{L_x L_y}} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{x}_j} \hat{c}_{\mathbf{k}\sigma}$$

Calculation is carried out in App. **??**. Let

$$\epsilon_{\mathbf{k}} \equiv -2t\left[\cos(k_x\delta_x) + \cos(k_y\delta_y)\right]$$

then we have

$$\begin{aligned} -t\sum_{\langle ij\rangle}\sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} \\ &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \left[\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} + \hat{c}_{\mathbf{k}\downarrow}^\dagger \hat{c}_{\mathbf{k}\downarrow}\right] \\ &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \left[\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}\downarrow}^\dagger\right] \end{aligned}$$

In last passage I used fermionic anti-commutation rules and reversed the sign of the mute variable. This will become useful later.

1.2.2 Non-local attraction

Consider a generic bond, say, the one connecting sites j and $j \pm \delta_\ell$ (variable i is here referred to as the imaginary unit to avoid confusion). $\mathbf{x}_j$ is the 2D notation for the position of site j, while $\boldsymbol{\delta}_\ell$ is the 2D notation for the lattice spacing previously indicated as δ_ℓ. Fourier transform it according to the convention

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{L_x L_y}} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{x}_j} \hat{c}_{\mathbf{k}\sigma}$$

Then:

$$\begin{aligned} \hat{n}_{j\uparrow}\hat{n}_{j\pm\delta_\ell\downarrow} &= \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\pm\delta_\ell\downarrow}^\dagger \hat{c}_{j\pm\delta_\ell\downarrow} \hat{c}_{j\uparrow} \\ &= \frac{1}{(L_x L_y)^2} \sum_{\nu=1}^{4} \sum_{\mathbf{k}_\nu\in \mathrm{BZ}} e^{i[(\mathbf{k}_1+\mathbf{k}_2)-(\mathbf{k}_3+\mathbf{k}_4)]\cdot\mathbf{x}_j} e^{\pm i(\mathbf{k}_2-\mathbf{k}_3)\cdot\boldsymbol{\delta}_\ell} \hat{c}_{\mathbf{k}_1\uparrow}^\dagger \hat{c}_{\mathbf{k}_2\downarrow}^\dagger \hat{c}_{\mathbf{k}_3\downarrow} \hat{c}_{\mathbf{k}_4\uparrow} \end{aligned}$$

It follows,

$$\begin{aligned}\hat{h}_V^{(j)} &= -\frac{V}{(L_xL_y)^2}\sum_{\ell=x,y}\sum_{\nu=1}^{4}\sum_{\mathbf{k}_\nu\in\mathrm{BZ}} e^{i[(\mathbf{k}_1+\mathbf{k}_2)-(\mathbf{k}_3+\mathbf{k}_4)]\cdot\mathbf{x}_j} \\ &\qquad\qquad \times\left(e^{i(\mathbf{k}_2-\mathbf{k}_3)\cdot\boldsymbol{\delta}_\ell}+e^{-i(\mathbf{k}_2-\mathbf{k}_3)\cdot\boldsymbol{\delta}_\ell}\right)\hat{c}^\dagger_{\mathbf{k}_1\uparrow}\hat{c}^\dagger_{\mathbf{k}_2\downarrow}\hat{c}_{\mathbf{k}_3\downarrow}\hat{c}_{\mathbf{k}_4\uparrow} \\ &= -\frac{2V}{(L_xL_y)^2}\sum_{\ell=x,y}\sum_{\nu=1}^{4}\sum_{\mathbf{k}_\nu\in\mathrm{BZ}} e^{i[(\mathbf{k}_1+\mathbf{k}_2)-(\mathbf{k}_3+\mathbf{k}_4)]\cdot\mathbf{x}_j}\cos\left[(\mathbf{k}_2-\mathbf{k}_3)\cdot\boldsymbol{\delta}_\ell\right]\hat{c}^\dagger_{\mathbf{k}_1\uparrow}\hat{c}^\dagger_{\mathbf{k}_2\downarrow}\hat{c}_{\mathbf{k}_3\downarrow}\hat{c}_{\mathbf{k}_4\uparrow}\end{aligned}$$

The full non-local interaction is given by summing over all sites of $\mathcal{S}$. This gives back momentum conservation,

$$\frac{1}{L_xL_y}\sum_{j\in\mathcal{S}} e^{i[(\mathbf{k}_1+\mathbf{k}_2)-(\mathbf{k}_3+\mathbf{k}_4)]\cdot\mathbf{x}_j} = \delta_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}$$

Let $\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4=\mathbf{K}$, and define $\mathbf{k}$, $\mathbf{k}'$ such that

$$\mathbf{k}_1\equiv\mathbf{K}+\mathbf{k} \qquad \mathbf{k}_2\equiv\mathbf{K}-\mathbf{k} \qquad \mathbf{k}_3\equiv\mathbf{K}-\mathbf{k}' \qquad \mathbf{k}_4\equiv\mathbf{K}+\mathbf{k}' \qquad \delta\mathbf{k}\equiv\mathbf{k}-\mathbf{k}'$$

Sums over these variables must be intended as over the Brillouin Zone (BZ). Then, finally

$$\begin{aligned}\hat{H}_V &\simeq \sum_{j\in\mathcal{S}}\hat{h}_V^{(j)} \\ &= -\frac{2V}{L_xL_y}\sum_{\ell=x,y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\cos\left(\delta\mathbf{k}\cdot\boldsymbol{\delta}_\ell\right)\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow} \\ &= -\frac{2V}{L_xL_y}\sum_{\ell=x,y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\left[\cos\left(\delta k_x\delta_x\right)+\cos\left(\delta k_y\delta_y\right)\right]\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow}\end{aligned}$$

Eventually, in the second passage the prefactor 2 can be absorbed by reintroducing the spin DoF[3]. Taking in the mean-field approximation (with Cooper pair symmetry breaking), we get

$$\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow} \simeq \langle\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\rangle\hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow} + \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\langle\hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow}\rangle + \cdots$$

Take e.g. $\langle\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\rangle$: the only non-zero contribution can come from the $\mathbf{K}=\mathbf{0}$ term, as will be discussed self-consistently in Sec. 1.2.5. Then finally:

$$\hat{H}_V \simeq -\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\left[\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle\hat{\phi}_{\mathbf{k}'}+\langle\hat{\phi}_{\mathbf{k}}\rangle\hat{\phi}^\dagger_{\mathbf{k}'}\right]$$

having I defined the pairing operator

$$\hat{\phi}_{\mathbf{k}}\equiv\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow} \qquad \hat{\phi}^\dagger_{\mathbf{k}}\equiv\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}$$

and the two-body potential

$$V_{\mathbf{k}\mathbf{k}'} = \frac{2V}{L_xL_y}\left[\cos\left(\delta k_x\delta_x\right)+\cos\left(\delta k_y\delta_y\right)\right]$$

Now, consider the term

$$\begin{aligned}\cos\left(\delta k_x\delta_x\right)+\cos\left(\delta k_y\delta_y\right) &= \cos\left(k_x\delta_x\right)\cos\left(k'_x\delta_x\right)+\sin\left(k_x\delta_x\right)\sin\left(k'_x\delta_x\right) \\ &\quad +\cos\left(k_y\delta_y\right)\cos\left(k'_y\delta_y\right)+\sin\left(k_y\delta_y\right)\sin\left(k'_y\delta_y\right)\end{aligned}$$

For the sake of readability, the notations

$$c_\ell\equiv\cos\left(k_\ell\delta_\ell\right) \qquad s_\ell\equiv\sin\left(k_\ell\delta_\ell\right) \qquad c'_\ell\equiv\cos\left(k'_\ell\delta_\ell\right) \qquad s'_\ell\equiv\sin\left(k'_\ell\delta_\ell\right)$$

[3] Justification can be given in two ways: either commutating appropriately the $\hat{c}$ operators, or by carrying out the previous space sums independently over the two sublattices.

Structure	Structure factor	Graph
s-wave	$\varphi_{\mathbf{k}}^{(s)} = 1$	Fig. 1.2a
Extended s-wave	$\varphi_{\mathbf{k}}^{(s^*)} = \cos k_x + \cos k_y$	Fig. 1.2b
p_x-wave	$\varphi_{\mathbf{k}}^{(p_x)} = i\sqrt{2}\sin k_x$	Fig. 1.2c
p_y-wave	$\varphi_{\mathbf{k}}^{(p_y)} = i\sqrt{2}\sin k_y$	Fig. 1.2d
$d_{x^2-y^2}$-wave	$\varphi_{\mathbf{k}}^{(d)} = \cos k_x - \cos k_y$	Fig. 1.2e

Table 1.2 | Structure factors derived from the correlation structures of Tab. **??**. The functions hereby defined are orthonormal, and define the various components of the non-local topological effective potential.

are used. Group the four terms above,

$$\underbrace{\left(c_x c'_x + c_y c'_y\right)}_{\text{Symmetric}} + \underbrace{\left(s_x s'_x + s_y s'_y\right)}_{\text{Anti-symmetric}} \tag{1.5}$$

The first two exhibit inversion symmetry for both arguments $\mathbf{k}$, $\mathbf{k}'$; the second two exhibit anti-symmetry. Decoupling the symmetric part,

$$c_x c'_x + c_y c'_y = \frac{1}{2}(c_x + c_y)(c'_x + c'_y) + \frac{1}{2}(c_x - c_y)(c'_x - c'_y)$$

which finally gives:

$$\begin{aligned}
\cos(\delta k_x \delta_x) + \cos(\delta k_y \delta_y) = {} & \frac{1}{2}(c_x + c_y)(c'_x + c'_y) && (s^*\text{-wave}) \\
& + s_x s'_x && (p_x\text{-wave}) \\
& + s_y s'_y && (p_y\text{-wave}) \\
& + \frac{1}{2}(c_x - c_y)(c'_x - c'_y) && (d_{x^2-y^2}\text{-wave})
\end{aligned}$$

In other words, the two-body potential decomposes as

$$\begin{aligned}
V_{\mathbf{k}\mathbf{k}'} &= \sum_\gamma V^{(\gamma)} \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*} \qquad \text{where} \quad \gamma = s^*, p_x, p_y, d_{x^2-y^2} \\
&= \frac{V}{L_x L_y} \sum_\gamma \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*}
\end{aligned}$$

being $\varphi_{\mathbf{k}}^{(\gamma)}$ the reciprocal-space expressions for the form factors of Tab. 1.1, listed explicitly in Tab. 1.2, and $V_{\mathbf{k}\mathbf{k}'}^{(\gamma)}$ the symmetry-resolved components of the non-local attraction. Then the two-body potential has been decomposed in its planar symmetry components, each of which will naturally couple only to identically structured parameters in the full hamiltonian.

Define now the non-local gap function

$$\mathcal{V}_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle \hat{\phi}^\dagger_{\mathbf{k}'} \rangle \tag{1.6}$$

one gets immediately

$$\hat{H}_V \simeq -\sum_{\mathbf{k}} \left[\mathcal{V}_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} + \mathcal{V}^*_{\mathbf{k}} \hat{\phi}^\dagger_{\mathbf{k}} \right] \tag{1.7}$$

To assume symmetry is broken in a specific symmetry channel γ means precisely to assume $g_{ij} \propto \varphi_{ij}^{(\gamma)}$, which in turn implies $\langle \hat{\phi}_{\mathbf{k}} \rangle \propto \varphi_{\mathbf{k}}^{(\gamma)}$. Of course, in Eq. (1.6) only the γ component of the potential survives, implying the gap function acquires the same symmetry,

$$\begin{aligned}
\mathcal{V}_{\mathbf{k}} &\propto \sum_{\mathbf{k}'} \frac{V}{L_x L_y} \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*} \varphi_{\mathbf{k}'}^{(\gamma)} \\
&\propto \varphi_{\mathbf{k}}^{(\gamma)}
\end{aligned}$$

where I used orthonormality of the $\varphi_{\mathbf{k}}^{(\gamma)}$ functions.

1.2.3 Local interaction and gap function

A very similar argument can be carried out for the local U term. Without delving in too many details, the local gap $\mathcal{U}_{\mathbf{k}}$ is given by

$$\mathcal{U}_{\mathbf{k}} \equiv \frac{U}{2L_xL_y}\sum_{\mathbf{k}}\langle\hat{\phi}_{\mathbf{k}}\rangle \tag{1.8}$$

evidently independent of $\mathbf{k}$, correctly. Identical considerations as in the above section hold for the local gap. The local part of the hamiltonian then gets

$$\hat{H}_U \simeq \sum_{\mathbf{k}}\left[\mathcal{U}_{\mathbf{k}}\hat{\phi}_{\mathbf{k}} + \mathcal{U}_{\mathbf{k}}^*\hat{\phi}_{\mathbf{k}}^\dagger\right] \tag{1.9}$$

and the full gap function is simply

$$\Delta_{\mathbf{k}} \equiv \mathcal{V}_{\mathbf{k}} - \mathcal{U}_{\mathbf{k}} \tag{1.10}$$

Notice here that the only possible topology here is s-wave; define trivially the s-wave component of the total two-body interaction,

$$V^{(s)} = -\frac{U}{2L_xL_y}$$

Then the full effective interaction is collected in

$$\begin{aligned}\hat{H}_U + \hat{H}_V &\simeq -\sum_{\gamma}\sum_{\mathbf{k},\mathbf{k}'}V^{(\gamma)}\varphi_{\mathbf{k}}^{(\gamma)}\varphi_{\mathbf{k}'}^{(\gamma)*}\left[\langle\hat{\phi}_{\mathbf{k}}^\dagger\rangle\hat{\phi}_{\mathbf{k}'} + \langle\hat{\phi}_{\mathbf{k}}\rangle\hat{\phi}_{\mathbf{k}'}^\dagger\right]\\ &= -\sum_{\mathbf{k}}\left[\Delta_{\mathbf{k}}\hat{\phi}_{\mathbf{k}} + \Delta_{\mathbf{k}}^*\hat{\phi}_{\mathbf{k}}^\dagger\right]\end{aligned}$$

The full self-consistency equation is given by

$$\Delta_{\mathbf{k}} \equiv \sum_{\mathbf{k}'}\left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right]\langle\hat{\phi}_{\mathbf{k}'}^\dagger\rangle \tag{1.11}$$

The gap function decomposes in symmetry channels as well,

$$\Delta_{\mathbf{k}} = \sum_{\gamma}\Delta^{(\gamma)}\varphi_{\mathbf{k}}^{(\gamma)}$$

If SC arises in a specific symmetry channel, $\Delta_{\mathbf{k}}$ will show the same symmetry. It follows, due to orthonormality and using Eq. (1.11),

$$\begin{aligned}\Delta^{(\gamma)} &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi_{\mathbf{k}}^{(\gamma)*}\Delta_{\mathbf{k}}\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi_{\mathbf{k}}^{(\gamma)*}\sum_{\mathbf{k}'}\left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right]\langle\hat{\phi}_{\mathbf{k}'}^\dagger\rangle\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi_{\mathbf{k}}^{(\gamma)*}\sum_{\mathbf{k}'\gamma'}V^{(\gamma')}\varphi_{\mathbf{k}}^{(\gamma')}\varphi_{\mathbf{k}'}^{(\gamma')*}\langle\hat{\phi}_{\mathbf{k}'}^\dagger\rangle\\ &= V^{(\gamma)}\sum_{\mathbf{k}}\varphi_{\mathbf{k}}^{(\gamma)*}\langle\hat{\phi}_{\mathbf{k}}^\dagger\rangle\end{aligned} \tag{1.12}$$

This result provides a set of self-consistency equations for each symmetry channel, listed in Tab. 1.3. Notice that to reconstruct self-consistently the full s-wave phase transition, the actual gap function is given by

$$\Delta^{(s)} + \Delta^{(s^*)}(c_x + c_y)$$

The s-wave transition is the only one equipped of both the local and the non-local parts. Within this structure, we are finally able to move to Nambu formalism.

Structure	Self-consistency equation	Graph
s-wave	$\Delta^{(s)} = -\frac{U}{2L_xL_y}\sum_{\mathbf{k}}\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.2a
Extended s-wave	$\Delta^{(s^*)} = \frac{V}{L_xL_y}\sum_{\mathbf{k}}(c_x+c_y)\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.2b
p_x-wave	$\Delta^{(p_x)} = -i\sqrt{2}\frac{V}{L_xL_y}\sum_{\mathbf{k}} s_x\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.2c
p_y-wave	$\Delta^{(p_y)} = -i\sqrt{2}\frac{V}{L_xL_y}\sum_{\mathbf{k}} s_y\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.2d
$d_{x^2-y^2}$-wave	$\Delta^{(d)} = \frac{V}{L_xL_y}\sum_{\mathbf{k}}(c_x-c_y)\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.2e

Table 1.3 | Symmetry resolved self-consistency equations for the MFT parameters $\Delta^{(\gamma)}$, based on Eq. (1.11) and (1.12). By computing $\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$, it is possible to reconstruct the various components of the gap function.

1.2.4 Nambu formalism and Bogoliubov transform

Define the Nambu spinor[4] as in BCS

$$\hat{\Psi}_{\mathbf{k}} \equiv \begin{bmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^\dagger_{-\mathbf{k}\downarrow} \end{bmatrix}$$

Evidently,

$$\phi_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}}\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\hat{\Psi}_{\mathbf{k}} \qquad \phi^\dagger_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}}\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}\hat{\Psi}_{\mathbf{k}} \tag{1.13}$$

The full hamiltonian is then given by:

$$\hat{H} = \sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}h_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}} \qquad h_{\mathbf{k}} \equiv \begin{bmatrix} \epsilon_{\mathbf{k}} & -\Delta^*_{\mathbf{k}} \\ -\Delta_{\mathbf{k}} & -\epsilon_{\mathbf{k}} \end{bmatrix} \tag{1.14}$$

Let τ^α for $\alpha = x, y, z$ be the Pauli matrices. Define:

$$\hat{s}^\alpha_{\mathbf{k}} \equiv \hat{\Psi}^\dagger_{\mathbf{k}}\tau^\alpha\hat{\Psi}_{\mathbf{k}} \quad \text{for} \quad \alpha = x, y, z$$

As can be shown easily, these operators realize spin-1/2 algebra. $\hat{H}$ represents an ensemble of L_xL_y independent spins subject to pseudo-magnetic fields. Note that, differently form App. **??** where the chemical potential is inserted later (because in Nambu formalism it accounts for a diagonal term) here the chemical potential is part of the z component of the pseudo-magnetic field, since

$$\begin{aligned} \hat{n}_{\mathbf{k}\uparrow} + \hat{n}_{-\mathbf{k}\downarrow} &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow} \\ &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{-\mathbf{k}\downarrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \mathbb{I} \\ &= \hat{\Psi}^\dagger_{\mathbf{k}}\tau^z\hat{\Psi}_{\mathbf{k}} + \mathbb{I} \end{aligned} \tag{1.15}$$

and then it follows

$$\begin{aligned} -\mu\hat{N} &= -\mu\sum_{\mathbf{k}\in\mathrm{BZ}}[\hat{n}_{\mathbf{k}\uparrow} + \hat{n}_{-\mathbf{k}\downarrow}] \\ &= -\mu\sum_{\mathbf{k}\in\mathrm{BZ}}\hat{\Psi}^\dagger_{\mathbf{k}}\tau^z\hat{\Psi}_{\mathbf{k}} - \mu L_xL_y \end{aligned}$$

[4] Notice that the spinor is here differently defined with respect to App. **??**, where because of the HF prevalence in mean-field decoupling the spinor components were homogeneously fermions creations or destructions.

Then, adding a term $-\mu\hat{N}$ to $\hat{H}$, apart from an irrelevant total energy increase, changes the pseudo-field whose explicit form becomes

$$\mathbf{b}_{\mathbf{k}} \equiv \begin{bmatrix} -\operatorname{Re}\{\Delta_{\mathbf{k}}\} \\ -\operatorname{Im}\{\Delta_{\mathbf{k}}\} \\ \epsilon_{\mathbf{k}} - \mu \end{bmatrix} \tag{1.16}$$

This hamiltonian behaves as an ensemble of spins in local magnetic fields precisely as in Eq. (**??**),

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\in \mathrm{BZ}} \mathbf{b}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}\sigma} = \begin{bmatrix} \hat{s}^x_{\mathbf{k}} \\ \hat{s}^y_{\mathbf{k}} \\ \hat{s}^z_{\mathbf{k}} \end{bmatrix} \tag{1.17}$$

Proceed as in App. **??** and diagonalize via a rotation,

$$d_{\mathbf{k}} \equiv \begin{bmatrix} -E_{\mathbf{k}} & \\ & E_{\mathbf{k}} \end{bmatrix} \quad \text{being} \quad E_{\mathbf{k}} \equiv \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$$

and $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$. Given the pseudoangles

$$\tan(2\theta_{\mathbf{k}}) \equiv \frac{|\Delta_{\mathbf{k}}|}{\epsilon_{\mathbf{k}}} \qquad \tan(2\zeta_{\mathbf{k}}) \equiv \frac{\operatorname{Im}\{\Delta_{\mathbf{k}}\}}{\operatorname{Re}\{\Delta_{\mathbf{k}}\}}$$

the general diagonalizer will be an orthogonal rotation matrix

$$\begin{aligned} W_{\mathbf{k}} &= e^{i\left(\theta_{\mathbf{k}} - \frac{\pi}{2}\right)\tau^y} e^{i\zeta_{\mathbf{k}}\tau^z} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \\ \cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} e^{i\zeta_{\mathbf{k}}} & \\ & e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\cos\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \\ \cos\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\sin\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \end{aligned} \tag{1.18}$$

given by a rotation of angle $\zeta_{\mathbf{k}}$ around the z axis, to align the x axis with the field projection onto the xy plane, followed by a rotation around the y axis to anti-align with the pseudo-field. The MFT-BCS solution is given by a degenerate Fermi gas at ground state, whose quasi-particles occupy two bands $\pm E_{\mathbf{k}}$ and their fermionic operators are given by

$$\hat{\gamma}^{(-)}_{\mathbf{k}} \equiv \left[W_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}\right]_1 \qquad \hat{\gamma}^{(+)}_{\mathbf{k}} \equiv \left[W_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}\right]_2$$

The diagonalization operators are given by

$$\hat{\Gamma}_{\mathbf{k}} \equiv W_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}} \quad \text{where} \quad \hat{\Gamma}_{\mathbf{k}} = \begin{bmatrix} \hat{\gamma}^{(-)}_{\mathbf{k}} \\ \hat{\gamma}^{(+)}_{\mathbf{k}} \end{bmatrix}$$

then, using Eq. (**??**),

$$\left\langle [\hat{\Psi}^\dagger_{\mathbf{k}}]_i [\hat{\Psi}_{\mathbf{k}}]_j \right\rangle = [W_{\mathbf{k}}]_{1i}[W^\dagger_{\mathbf{k}}]_{j1} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{2i}[W^\dagger_{\mathbf{k}}]_{j2} f\left(E_{\mathbf{k}}; \beta, 0\right)$$

where in the Fermi-Dirac function chemical potential was set to zero, because it already was included in the diagonalized hamiltonian. Recalling Eq. (**??**), it follows

$$\langle \phi^\dagger_{\mathbf{k}} \rangle = [W_{\mathbf{k}}]_{11}[W^\dagger_{\mathbf{k}}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21}[W^\dagger_{\mathbf{k}}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.19}$$

$$= \frac{1}{2}\sin\left(2\theta_{\mathbf{k}}\right) e^{i2\zeta_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{1.20}$$

The last passage has been obtained by computing the matrix element from the explicit form of $W_{\mathbf{k}}$ of Eq. (1.18) and by the simple relation

$$\begin{aligned} \frac{1}{e^{-x}+1} - \frac{1}{e^{x}+1} &= \frac{e^x - 1}{e^x + 1} \\ &= \tanh\left(\frac{x}{2}\right) \end{aligned}$$

Eqns. (1.19), (1.20) give us both the algorithmic formula (first row) and its theoretical counterpart (second row) to compute the order parameters in the HF approach at each point in k-space (k_x, k_y). We can finally derive the BCS self-consistency equation

$$\Delta_{\mathbf{k}} \equiv \frac{1}{2}\sum_{\mathbf{k}'}\left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right]\frac{|\Delta_{\mathbf{k}}|}{\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}} e^{i\,\mathrm{Im}\{\Delta_{\mathbf{k}}\}/\,\mathrm{Re}\{\Delta_{\mathbf{k}}\}}\tanh\left(\frac{\beta}{2}\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}\right) \tag{1.21}$$

The whole point of the HF algorithm is to find an iterative solution for each symmetry channel, using the self-consistency equation projection of Tab. 1.3.

Notice that the z component of the spin operators is related to density: using Eq. (**??**),

$$\langle\hat{\Psi}_{\mathbf{k}}^\dagger\tau^z\hat{\Psi}_{\mathbf{k}}\rangle = \left\langle[\hat{\Psi}_{\mathbf{k}}^\dagger]_1[\hat{\Psi}_{\mathbf{k}}]_1\right\rangle - \left\langle[\hat{\Psi}_{\mathbf{k}}^\dagger]_2[\hat{\Psi}_{\mathbf{k}}]_2\right\rangle$$

I proceed in as done previously, and from Eq. (1.15),

$$\begin{aligned}\langle\hat{n}_{\mathbf{k}\uparrow}\rangle + \langle\hat{n}_{-\mathbf{k}\downarrow}\rangle &= 1 + \langle\hat{\Psi}_{\mathbf{k}}^\dagger\tau^z\hat{\Psi}_{\mathbf{k}}\rangle \\ &= 1 + \left(|[W_{\mathbf{k}}]_{11}|^2 - |[W_{\mathbf{k}}]_{12}|^2\right) f\left(-E_{\mathbf{k}};\beta,0\right) \\ &\quad + \left(|[W_{\mathbf{k}}]_{21}|^2 - |[W_{\mathbf{k}}]_{22}|^2\right) f\left(E_{\mathbf{k}};\beta,0\right) \qquad (1.22) \\ &= 1 - \cos\left(2\theta_{\mathbf{k}}\right)\tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \qquad (1.23)\end{aligned}$$

The expectation value for the density is needed in order to extract the optimal chemical potential μ for the target density we aim to simulate at the given parametrization. This is numerically obtained by using Eq. (1.22) directly on the diagonalization matrix of $h_{\mathbf{k}}$.

1.2.5 A short comment on self-consistency

The Bogoliubov fermions in spinor representation satisfy obviously $\hat{\Psi}_{\mathbf{k}} = W_{\mathbf{k}}^\dagger\hat{\Gamma}_{\mathbf{k}}$. Consider e.g.

$$\langle\hat{c}_{\mathbf{k}\sigma}^\dagger\hat{c}_{-\mathbf{k}\sigma}^\dagger\rangle$$

which is a spin-symmetric anomalous Cooper pair. For simplicity, take $\sigma =\uparrow$. Expand:

$$\begin{aligned}\langle\hat{c}_{\mathbf{k}\uparrow}^\dagger\hat{c}_{-\mathbf{k}\uparrow}^\dagger\rangle &= \left\langle[\hat{\Psi}_{\mathbf{k}}^\dagger]_1[\hat{\Psi}_{-\mathbf{k}}^\dagger]_1\right\rangle \\ &= \left\langle[W_{\mathbf{k}}\hat{\Gamma}_{\mathbf{k}}^\dagger]_1[W_{-\mathbf{k}}\hat{\Gamma}_{-\mathbf{k}}^\dagger]_1\right\rangle\end{aligned}$$

This expectation value is taken over the ground-state, the latter being the vacuum of Γ fermions. Evidently the above expectation cannot assume non-zero values. Obviously the same holds for $\sigma =\downarrow$, and this argument explains why the Ferromagnetic terms of the hamiltonian decomposition do not contribute to Cooper instability. An identical argument, with the exchange

$$(\sigma,\sigma)\to(\uparrow,\downarrow) \quad\text{and}\quad (\mathbf{k},-\mathbf{k})\to(\mathbf{K}+\mathbf{k},\mathbf{K}-\mathbf{k}) \quad\text{with}\quad \mathbf{K}\neq\mathbf{0}$$

justifies why in Sec. 1.2.4 the only relevant contribution was given by $\mathbf{K} = \mathbf{0}$. In the next sections, the results of the self-consistent HF algorithm are exposed.

1.3 Results of the HF algorihtm

[To be continued...]

Bibliography

[1] Zhangkai Cao et al. *p-wave superconductivity induced by nearest-neighbor attraction in the square-lattice extended Hubbard model*. en. arXiv:2408.01113 [cond-mat]. Jan. 2025. DOI: 10.48550/arXiv.2408.01113. URL: http://arxiv.org/abs/2408.01113 (visited on 03/15/2025).

[2] Piers Coleman. *Introduction to Many-Body Physics*. Cambridge University Press, 2015.

[3] Michele Fabrizio. *A Course in Quantum Many-Body Theory*. Springer, 2022.

[4] Gabriele Giuliani and Giovanni Vignale. *Quantum Theory of the Electron Liquid*. Cambridge University Press, 2005.

[5] Giuseppe Grosso and Giuseppe Pastori Parravicini. *Solid State Physics*. Second Edition. Academic Press, 2014.

[6] J. E. Hirsch. "Two-dimensional Hubbard model: Numerical simulation study". In: *Phys. Rev. B* 31 (7 Apr. 1985), pp. 4403–4419. DOI: 10.1103/PhysRevB.31.4403. URL: https://link.aps.org/doi/10.1103/PhysRevB.31.4403.

[7] Robin Scholle et al. "Comprehensive mean-field analysis of magnetic and charge orders in the two-dimensional Hubbard model". In: *Phys. Rev. B* 108 (3 July 2023), p. 035139. DOI: 10.1103/PhysRevB.108.035139. URL: https://link.aps.org/doi/10.1103/PhysRevB.108.035139.