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

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Thesis for the Master's degree in Physics

Abstract

[To be continued...]

Contents

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List of symbols and abbreviations

AF	Anti-Ferromagnetic
BCS	Bardeen-Cooper-Schrieffer (theory)
DoF	Degree of Freedom
HF	Hartree-Fock
MFT	Mean-Field Theory
SC	Superconductor
T_c	Critical temperature

Introduction

This thesis project is about my favorite ice cream flavor. [To be continued...]

Chapter 1

Mean-field theory analysis of the EHM

This chapter is devoted to develop a Mean Field Theory (MFT) approximation of the Extended Hubbard model (EHM) 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 to discuss both the effects of the non-local term $\hat{H}_V$ onto the AF phase, as well as the insurgence of anisotropic superconductivity – 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 $\hat{H}_V$ in real-space, describing how such interaction can contribute to the hamiltonian as a symmetry-breaking term in given channels. In the following sections, we move to specific channels and study theoretically and numerically the effect of non-local attraction.

1.1 Mean-Field theory real space description

The general aim is to study the phase diagram of the model by comparing ground-state energies of different phases. The phases we consider here for the EHM are the Anti-Ferromagnetic ordering (AF), given by a non-uniform distribution of charge in each spin sector, and the Superconducting phase, described by a uniformly distributed charge allowing for Cooper pairing instabilities. For the EHM, three symmetries are "brekable":

1. Discrete translational invariance. By breaking explicitly this symmetry, the obtained state must show a Charge-Density Wave (CDW) ordering;

2. $\mathrm{U}^c(1)$ charge conservation. By breaking this symmetry, we allow for the total charge to fluctuate in the ground state;

3. SU(2) spin rotation symmetry. If this symmetry is broken, we allow for the ground state to exhibit a preferred spin direction.

4. Note that the SU(2) group contains a U(1) subgroup. SU(2) symmetry can be broken, selecting a particular vectorial direction for the order parameter, and reduced to a smaller $\mathrm{U}^z(1)$ symmetry which is essentially expressed by the conservation of the *magnitude* of the order parameter.

The last point is important: for the AF phase, for example, there is no need for the magnetization vector to be directed along the *real* z-axis, which is the one perpendicular to the lattice plane. SU(2) symmetry breaks when (staggered) magnetization is established along a particular direction, but

Symmetry group	Operations
Point group	Discrete translations on lattice
$\mathrm{U}^c(1)$	Charge-conserving global phase shifts
SU(2)	Three-dimensional rotations in spin space
$\mathrm{U}^z(1)$	Reduced two-dimensional rotations around Néel z-axis in spin space

Table 1.1 | Model symmetries and relative group operations. Note that $U^c(1)$ represents the charge conserving group, while $\mathrm{U}^z(1)$ represents the subgroup obtained by breaking the SU(2) symmetry with a vector order parameter and preserving its amplitude.

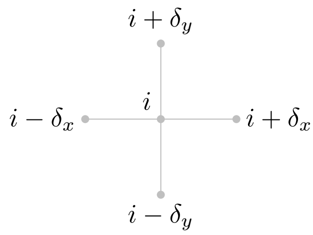


Figure 1.1 | Schematic representation of the four NNs of a given site i for a planar square lattice.

spin rotations around said direction still are ground state symmetries. The symmetries are reported synthetically in Tab. 1.1.

Different phases are described by different order parameters, each one exhibiting a specific symmetry subset from the initial set, while the rest are broken. Ferromagnetic state perform $\mathrm{SU}(2) \to \mathrm{U}^z(1)$ symmetry breaking, Anti-Ferromagnetic also break translational invariance (reducing it to a smaller symmetry, relative to double-sized unitary cells). Basic superconducting models do not break translational invariance and can preserve full SU(2) symmetry, while breaking $\mathrm{U}^c(1)$ charge conservation.

App. **??** describes in detail the MFT treatment of the pure Hubbard model, $\hat{H}_t + \hat{H}_U$ and its AF phase; the key passage is there given by the approximation

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \simeq \hat{n}_{i\uparrow}\langle\hat{n}_{i\downarrow}\rangle + \langle\hat{n}_{i\uparrow}\rangle\hat{n}_{i\downarrow} + (\text{constants}) \tag{1.1}$$

from which the AF structure is simply recovered. However, to perform the above approximation coherently, we are implementing Wick's Theorem on the generic term:

$$\langle\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{j\sigma'}\hat{c}_{i\sigma}\rangle \simeq \underbrace{\langle\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\rangle\langle\hat{c}_{j\sigma'}\hat{c}_{i\sigma}\rangle}_{\text{Cooper}} - \underbrace{\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma'}\rangle\langle\hat{c}^\dagger_{j\sigma'}\hat{c}_{i\sigma}\rangle}_{\text{Fock}} + \underbrace{\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma'}\hat{c}_{j\sigma'}\rangle}_{\text{Hartree}} \tag{1.2}$$

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 AF ground state breaks translational invariance and reduces rotational symmetry, $\mathrm{SU}(2) \to \mathrm{U}^z(1$. Thus, of the three terms above:

- Cooper fluctuations are suppressed, because they break charge conservation;
- Similarly the Fock term is null as well because if $i = j$ and $\sigma' = \overline{\sigma}$ (as is for the local interaction, which contains the operator $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$) the expectation values involved are describing a process breaking the survivor $\mathrm{U}^z(1)$ spin symmetry.

Thus, correctly, the Wick's decomposition of Eq. (1.1) only involves Hartree-terms of Eq. (1.2). In general, however, the three terms need to be considered altogether: this is what is done in the next section.

[Insert here a comment anticipating the discussion of different symmetry structures (s,s^*, p_x, p_y, $d_{x^2-y^2}$).]

1.1.1 The non-local term as a source of symmetry-breaking interactions

Consider now the NN non-local term,

$$\hat{H}_V \equiv -V \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \tag{1.3}$$

Evidently the hamiltonian can be decomposed in various spin terms,

$$\begin{aligned} \hat{H}_V &= \sum_{\sigma\sigma'} \hat{H}_V^{\sigma\sigma'} \\ &= \underbrace{\hat{H}_V^{\uparrow\uparrow} + \hat{H}_V^{\downarrow\downarrow}}_{\text{Same-spin}} + \underbrace{\hat{H}_V^{\uparrow\downarrow} + \hat{H}_V^{\downarrow\uparrow}}_{\text{Opposite-spin}} \end{aligned}$$

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 opposite-spin (o.s.) 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 $\mathcal{S}_b$. The o.s. 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. **??**)

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

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 same-spin (s.s.) hamiltonian decomposes as

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

Note here the summation only on one sublattice. The non-local interaction contribution to energy, as a function of the $T = 0$ full hamiltonian ground-state[1] $|\Psi\rangle$, is given by

$$\begin{aligned} E_V[\Psi] &= \langle \Psi | \hat{H}_V | \Psi \rangle \\ &= -V \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \rangle \\ &= \underbrace{-V \sum_{\langle ij \rangle} \sum_{\sigma} \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma} \rangle}_{\text{s.s.}} \underbrace{-V \sum_{\langle ij \rangle} \sum_{\sigma} \langle \hat{n}_{i\sigma} \hat{n}_{j\overline{\sigma}} \rangle}_{\text{o.s.}} \end{aligned}$$

Shorthand notation has been used: $\langle \Psi | \cdot | \Psi \rangle = \langle \cdot \rangle$. 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].

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

Opposite-spin terms. Consider first the o.s. terms: take e.g. the term $\hat{n}_{i\uparrow}\hat{n}_{i+\delta_x\downarrow}$. As in Eq. (1.2), Wick's Theorem states that, if the expectation value is performed onto a coherent state,

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

Identical decompositions are given for all others NNs. Of the three terms above:

- The Coooper term breaks $\mathrm{U}^c(1)$ charge symmetry, allowing for supeconducting instabilities;
- The Fock term breaks the $\mathrm{U}^z(1)$ symmetry, because it accounts for a site hop *plus* spin flip process;
- The Hartree term breaks translational invariance, because the mean-field to interact with is given by the local density. SU(2) symmetry is also broken, because we do not have spin DoF perfect degeneracy anymore, but $\mathrm{U}^z(1$ symmetry still holds.

Then, to look for AF instability only the Hartree term is to be accounted; instead, in superconducting instability only the Cooper term contributes. Note that for superconducting instabilities, due to superexchange mechanism (as explained in App. **??**) the o.s. term account for singlet pairing as well as zero-spin triplet pairing. Which channel is preferred, is a matter of thermodynamic advantage.

Same-spin terms. Consider then the same-spin terms: take e.g. the term $\hat{n}_{i\uparrow}\hat{n}_{i+\delta_x\uparrow}$. As above,

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

Identical consideration as in the above paragraph hold for each term. The only difference with the o.s. terms is given by the Fock term: since the spin-flip process is absent, now the Fock fluctuations actually contribute as an effective NN hopping term. In other words, this term does not break $\mathrm{U}^z(1$ symmetry and thus is perfectly legitimate, say, in AF or superconducting phase. As a final remark, notice that the superconducting instabilities of the s.s. terms account only for triplet pairing. The only possible superconducting ordering established by the means of these terms is odd in real space. Then s-wave and d-wave superconductivity cannot establish in this channel; p_ℓ-wave superconductivity, instead, can.

1.1.2 Reciprocal-space transform of the non-local interaction

It is useful to derive analytically the reciprocal-space form of the 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:

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

Then, the interaction at site j, spin σ with its NNs at spin σ' – indicated as $(j\sigma\sigma')$ – is given by

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

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

$$
\frac{1}{L_xL_y} \sum_{j\in\mathcal{S}_a} e^{i[(\mathbf{k}_1+\mathbf{k}_2)-(\mathbf{k}_3+\mathbf{k}_4)]\cdot\mathbf{x}_j} = \frac{1}{2}\delta_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_3+\mathbf{k}_4}
$$

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

$$
\begin{aligned}
\hat{H}_V &= \sum_{j\in\mathcal{S}_a} \sum_{\sigma\sigma'} (j\sigma\sigma') \\
&= -\frac{V}{L_xL_y} \sum_{\sigma\sigma'} \sum_{\ell=x,y} \sum_{\mathbf{K},\mathbf{k},\mathbf{k}'} \cos\left(\delta\mathbf{k}\cdot\boldsymbol{\delta}_\ell\right) \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma'}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma'}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma} \\
&= -\frac{V}{L_xL_y} \sum_{\sigma\sigma'} \sum_{\mathbf{K},\mathbf{k},\mathbf{k}'} \left[\cos\left(\delta k_x\right)+\cos\left(\delta k_y\right)\right] \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma'}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma'}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma}
\end{aligned}
\tag{1.4}
$$

Different Wick contraction schemes lead to different results:

$$
c^\dagger_{\mathbf{K}+\mathbf{k}\sigma}c^\dagger_{\mathbf{K}-\mathbf{k}\sigma'}c_{\mathbf{K}-\mathbf{k}'\sigma'}c_{\mathbf{K}+\mathbf{k}'\sigma} \qquad \text{Cooper contraction} \tag{1.5}
$$

$$
c^\dagger_{\mathbf{K}+\mathbf{k}\sigma}c^\dagger_{\mathbf{K}-\mathbf{k}\sigma'}c_{\mathbf{K}-\mathbf{k}'\sigma'}c_{\mathbf{K}+\mathbf{k}'\sigma} \qquad \text{Fock contraction} \tag{1.6}
$$

$$
c^\dagger_{\mathbf{K}+\mathbf{k}\sigma}c^\dagger_{\mathbf{K}-\mathbf{k}\sigma'}c_{\mathbf{K}-\mathbf{k}'\sigma'}c_{\mathbf{K}+\mathbf{k}'\sigma} \qquad \text{Hartree contraction} \tag{1.7}
$$

which will be used explicitly later on.

1.2 Anti-Ferromagnetic instability

In this section, the effect of the non-local interaction on the antiferromagnetic phase is discussed. The MFT derivation for the "standard" Hubbard Model is discussed in App. ??. Recalling the main results, the Anti-Ferromagnetic phase specified by the Ansatz (??) (which is explicitly breaking translational invariance in each spin sector, while preserving $\mathrm{U}^z(1)$ and $\mathrm{U}^c(1)$ symmetries) reduces the hamiltonian to the form of Eq. (??)

$$
\hat{H}_t + \hat{H}_U \overset{\mathrm{MFT}}{\simeq} -t \sum_{\langle\mathbf{r}\mathbf{r}'\rangle} \sum_{\sigma} \hat{c}^\dagger_{\mathbf{r}\sigma}\hat{c}_{\mathbf{r}'\sigma} + nU \sum_{\mathbf{r}} \left[\hat{n}_{\mathbf{r}\uparrow}+\hat{n}_{\mathbf{r}\downarrow}\right] - mU \sum_{\mathbf{r}} (-1)^{x+y} \left[\hat{n}_{\mathbf{r}\uparrow}-\hat{n}_{\mathbf{r}\downarrow}\right]
$$

In reciprocal space, the hamiltonian decomposes as in Eq. (??),

$$
\hat{H}_t + \hat{H}_U \overset{\mathrm{MFT}}{\simeq} \sum_{\mathbf{k}\in\mathrm{MBZ}} \sum_{\sigma} \hat{\Psi}^\dagger_{\mathbf{k}\sigma} h_{\mathbf{k}\sigma} \hat{\Psi}_{\mathbf{k}\sigma} \quad \text{being} \quad h_{\mathbf{k}\sigma} \equiv \begin{bmatrix} \epsilon_{\mathbf{k}} & -\Delta_\sigma \\ -\Delta_\sigma & -\epsilon_{\mathbf{k}} \end{bmatrix}
$$

and $\Delta_\uparrow = mU$, $\Delta_\downarrow = -mU$. Nambu spinorial formulation is used,

$$\hat{\Psi}_{\mathbf{k}\sigma} \equiv \begin{bmatrix} \hat{c}_{\mathbf{k}\sigma} \\ \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma} \end{bmatrix}$$

and the free electrons energy is simply the tight binding energy

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

which is spin-invariant. The MFT description of the model reduces to a gas of free "γ-fermions", described by the Nambu spinor of Eq. (**??**),

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

where

$$W_{\mathbf{k}\sigma} = \begin{bmatrix} -\sin\theta_{\mathbf{k}\sigma} & -\cos\theta_{\mathbf{k}\sigma} \\ \cos\theta_{\mathbf{k}\sigma} & -\sin\theta_{\mathbf{k}\sigma} \end{bmatrix} \quad \text{and} \quad \sin 2\theta_{\mathbf{k}\sigma} \equiv \frac{\Delta_\sigma}{E_{\mathbf{k}}}$$

These fermions populate the two bands $\pm E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$. The entire system is mapped onto an ensemble of pseudo-spins, each subject to a pseudo-field, as in Fig. 1.2. To diagonalize the system essentially means to align each pseudo-spin with the z axis. Within on the notation of Fig. **??**, the following expectations values hold:

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^x\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\theta_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{1.8}$$

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^y\hat{\Psi}_{\mathbf{k}\sigma}\rangle = 0 \tag{1.9}$$

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Psi}_{\mathbf{k}\sigma}\rangle = -\cos(2\theta_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{1.10}$$

and since the γ-fermions are free and in the rotated frame the pseudo-field points "up",

$$\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle = \frac{1}{2}\left[f\left(-E_{\mathbf{k}};\beta,\tilde{\mu}\right) - f\left(E_{\mathbf{k}};\beta,\tilde{\mu}\right)\right]$$

Consider now the non-local interaction $\hat{H}_V$: since only translational invariance is broken in the AF phase, the only relevant contributions coming from Wick's decomposition are Hartree terms and the same-spin Fock term. The net effect obtained by including this interaction, as I will explain, is a renormalization of the various quantities,

$$\epsilon_{\mathbf{k}} \to \tilde{\epsilon}_{\mathbf{k}\sigma} \qquad E_{\mathbf{k}} \to \tilde{E}_{\mathbf{k}\sigma} \qquad \Delta_\sigma \to \tilde{\Delta}_{\mathbf{k}\sigma} \qquad \theta_{\mathbf{k}\sigma} \to \tilde{\theta}_{\mathbf{k}\sigma} \qquad W_{\mathbf{k}\sigma} \to \tilde{W}_{\mathbf{k}\sigma}$$

The band energies renormalization is simply

$$\tilde{E}_{\mathbf{k}\sigma} \equiv \sqrt{\tilde{\epsilon}^2_{\mathbf{k}\sigma} + |\tilde{\Delta}_{\mathbf{k}\sigma}|^2}$$

and the following relations hold:

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^x\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\tilde{\theta}_{\mathbf{k}})\sin(2\tilde{\zeta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{1.11}$$

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^y\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\tilde{\theta}_{\mathbf{k}})\cos(2\tilde{\zeta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{1.12}$$

$$\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Psi}_{\mathbf{k}\sigma}\rangle = -\cos(2\tilde{\theta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{1.13}$$

with:

$$\sin(2\tilde{\xi}_{\mathbf{k}}) = \frac{\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\}}{|\tilde{\Delta}_{\mathbf{k}}|} \qquad \cos(2\tilde{\xi}_{\mathbf{k}}) = \frac{\mathrm{Im}\{\tilde{\Delta}_{\mathbf{k}}\}}{|\tilde{\Delta}_{\mathbf{k}}|} \qquad \sin(2\tilde{\theta}_{\mathbf{k}}) = \frac{|\tilde{\Delta}_{\mathbf{k}}|}{\tilde{E}_{\mathbf{k}}} \qquad \cos(2\tilde{\theta}_{\mathbf{k}}) = \frac{\tilde{\epsilon}_{\mathbf{k}}}{\tilde{E}_{\mathbf{k}}} \tag{1.14}$$

The physical behavior is the same as for the pure Hubbard model. In next sections the different contributions to renormalization are treated.

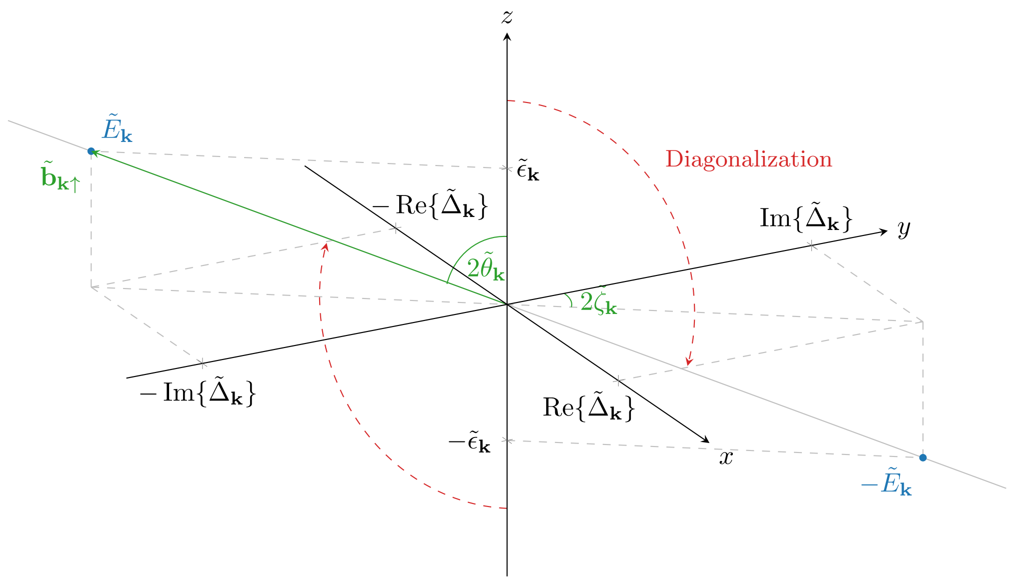


Figure 1.2 | Sketch of the diagonalization of the pseudo-spin problem. The dashed line represents the diagonalization given by the z-axis alignment with the field direction. In the top-right side of the picture are listed the expectation values of the original Nambu spinor.

1.2.1 Hartree renormalization of chemical potential and gap

The same-spin and opposite-spin non-local Hartree terms are

$$\underbrace{-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\sigma}+\hat{n}_{i\sigma}\langle\hat{n}_{j\sigma}\rangle\right]}_{\text{s.s.}}\underbrace{-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\overline{\sigma}}+\hat{n}_{i\sigma}\langle\hat{n}_{j\overline{\sigma}}\rangle\right]}_{\text{o.s.}}$$

Let $i\to\mathbf{r}=(x,y)$ and $j\to\mathbf{r}'=(x',y')$. Then, using the Ansatz of Eq. (**??**), summarized as

$$\langle\hat{n}_{\mathbf{r}\sigma}\rangle=n-(-1)^{x+y+\delta_{\sigma=\uparrow}}m$$

we get

$$\overbrace{-nV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}\left[\hat{n}_{\mathbf{r}'\sigma}+\hat{n}_{\mathbf{r}\sigma}\right]+mV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{\delta_{\sigma=\uparrow}}\left[(-1)^{x'+y'}\hat{n}_{\mathbf{r}'\sigma}+(-1)^{x+y}\hat{n}_{\mathbf{r}\sigma}\right]}^{\text{s.s.}}$$
$$\underbrace{-nV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}\left[\hat{n}_{\mathbf{r}'\overline{\sigma}}+\hat{n}_{\mathbf{r}\sigma}\right]+mV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}\left[(-1)^{x'+y'+\delta_{\overline{\sigma}=\uparrow}}\hat{n}_{\mathbf{r}'\overline{\sigma}}+(-1)^{x+y+\delta_{\sigma=\uparrow}}\hat{n}_{\mathbf{r}\sigma}\right]}_{\text{o.s.}}$$

For a square lattice, if $\mathbf{r}=(x,y)$ and $\mathbf{r}'=(x',y')$ are NNs evidently

$$(-1)^{x'+y'}=(-1)^{x+y+1}$$

Moreover,

$$(-1)^{\delta_{\overline{\sigma}=\uparrow}}=(-1)^{\delta_{\sigma=\uparrow}+1}$$

We obtain

$$\overbrace{-nV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}\left[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\sigma}\right]}^{\text{s.s. (density)}}+\overbrace{mV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}\left[\hat{n}_{\mathbf{r}\sigma}-\hat{n}_{\mathbf{r}'\sigma}\right]}^{\text{s.s. (magnetization)}}$$
$$\underbrace{-nV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}\left[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}\right]}_{\text{o.s. (density)}}+\underbrace{mV\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}\left[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}\right]}_{\text{o.s. (magnetization)}} \quad (1.15)$$

In the above expressions the various contribution have been separated in "density" contributions and "magnetization" contributions. Let me deal with these separately.

Density terms. Consider the *s.s.* and *o.s.* (density) terms of Expr. (1.15). Since

$$\sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} [\hat{n}_{\mathbf{r}\sigma} + \hat{n}_{\mathbf{r}'\sigma}] = \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} [\hat{n}_{\mathbf{r}\sigma} + \hat{n}_{\mathbf{r}'\overline{\sigma}}] = z\hat{N}$$

with $z = 4$ the lattice coordination factor, indicating the number of NNs per site, then the first and third terms of Expr. (1.15) contribute to a pure chemical potential shift. The renormalized chemical potential is:

$$\tilde{\mu} \equiv \mu + 2znV \tag{1.16}$$

Magnetization terms. The s.s. and o.s. (magnetization) terms of Expr. (1.15) are to be reduced to a renormalization of the gap function. Explicitly,

$$\begin{aligned} mV \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} (-1)^{x+y+\delta_{\sigma=\uparrow}} [\hat{n}_{\mathbf{r}\sigma} - \hat{n}_{\mathbf{r}'\sigma}] + mV \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} (-1)^{x+y+\delta_{\sigma=\uparrow}} [\hat{n}_{\mathbf{r}\sigma} + \hat{n}_{\mathbf{r}'\overline{\sigma}}] \\ = -2zmV \sum_{\mathbf{r}} (-1)^{x+y} [\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}] \end{aligned} \tag{1.17}$$

Consider now the last term of the pure Hubbard model under MFT approximations of Eq. (**??**),

$$-mU \sum_{\mathbf{r}} (-1)^{x+y} [\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}] \quad \text{(Local gap)}$$

Expr. (1.17) is formally identical, thus we obtain a contribution to the renormalization of the AF gap,

$$\Delta \to \Delta + 2zmV + \text{(s.s. contribution)} \tag{1.18}$$

This, together with Eq. (1.16), concludes the non-local Hartree reparametrization of the hamiltonian. Next section is devoted to analyzing the effect of the Fock term.

1.2.2 Fock renormalization of the hopping amplitude

From Wick's decomposition of $\hat{H}_V$, the only allowed Fock term comes from the same-spin part due to SU(2) symmetry selection rules. Said hamiltonian term is

$$V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} + \text{h.c.} \right] \tag{1.19}$$

(note the + sign in front of it). A bond-wise hopping amplitude can be defined,

$$\tilde{t}_{ij\sigma} \equiv t - V \langle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \rangle$$

In the AF phase, given some site i and a spin σ, evidently $\tilde{t}_{ij\sigma}$ must be identical for any NN site j. Over the planar square lattice, this implies that the quantity $\langle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \rangle$ exhibits s^*-wave symmetry (also referred to as "Extended s-wave symmetry"). Later in the text, different symmetry structures will be discussed thoroughly. For now, the s^*-wave symmetry is the one given in Tab. 1.2 and depicted in Fig. 1.4b. These considerations will become useful later. The effective diffusive hamiltonian is given by

$$\begin{aligned} \hat{H}_{\tilde{t}} &= \hat{H}_t + V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} + \text{h.c.} \right] \\ &= - \sum_{\langle ij \rangle} \sum_{\sigma} \left[\tilde{t}_{ij\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} \right] \end{aligned}$$

As will become clear in next section, not only the diffusive part of the hamiltonian actually is affected by the Fock renormalization; also the gap terms are effectively renormalized.

In reciprocal space, the effective hopping must be transformed as well. Consider the Fourier Transform given in Eq. (1.4), applied to Eq. (1.19),

$$\begin{aligned} V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} + \text{h.c.} \right] \\ = \frac{2V}{L_x L_y} \sum_{\mathbf{K},\mathbf{k},\mathbf{k}'} \sum_{\sigma} \left[\cos\left(\delta k_x\right) + \cos\left(\delta k_y\right) \right] \langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}'\sigma} \rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}'\sigma} \end{aligned} \tag{1.20}$$

where the 2 prefactor comes from recognizing that the h.c. generates an identical contribution to the full sum. In order to proceed, it is now necessary to understand how the AF phase is realized in reciprocal space. As is exposed in App. **??**, to impose an AF Ansatz of the form

$$\langle \hat{n}_{\mathbf{r}\sigma} \rangle = n - (-1)^{x+y+\delta_{\sigma=\uparrow}} m$$

leads to an AF ground-state of free fermions at temperature β described by the Nambu spinor of Eq. (**??**). All parameters are renormalized, thus we must account for renormalized band energies $\pm\tilde{E}_{\mathbf{k}\sigma}$ as well. The ground-state is realized by simply populating the two bands $\pm\tilde{E}_{\mathbf{k}\sigma}$ as

$$\bigotimes_{\mathbf{k}\in\text{MBZ}} \bigotimes_{\sigma} \left[\left(\hat{\gamma}^{(-)}_{\mathbf{k}\sigma}\right)^\dagger f(-\tilde{E}_{\mathbf{k}};\beta,\mu) + \left(\hat{\gamma}^{(+)}_{\mathbf{k}\sigma}\right)^\dagger f(\tilde{E}_{\mathbf{k}};\beta,\mu) \right] |\Omega\rangle$$

The $\hat{\gamma}$ operators are normalized superpositions of two $\hat{c}$ operators at points in reciprocal space separated by a $\boldsymbol{\pi}$ shift. It follows that the above state is ultimately a superposition of many-body pure states, each of which has either the $\mathbf{k}\sigma$ state occupied *or* the $\mathbf{k}+\boldsymbol{\pi}\sigma$ state for each $\mathbf{k} \in \text{MBZ}$, $\sigma \in \{\uparrow, \downarrow\}$. It follows that, when computing generically $\langle \hat{c}^\dagger_{\mathbf{k}_1\sigma} \hat{c}_{\mathbf{k}_2\sigma} \rangle$, such expectation value can be non-zero if and only if $\mathbf{k}_1 = \mathbf{k}_2 + n\boldsymbol{\pi}$, being $n \in \mathbb{Z}$. Going back to Eq. (1.20), this implies only two contributions are non-zero:

$$\mathbf{k} = -\mathbf{k}' \quad \text{or} \quad \mathbf{k} + \boldsymbol{\pi} = -\mathbf{k}'$$

Then Eq. (1.20) is reduced to:

$$\begin{aligned} \frac{2V}{L_x L_y} \sum_{\mathbf{K},\mathbf{k}} \sum_{\sigma} \left[\cos\left(2k_x\right) + \cos\left(2k_y\right) \right] \\ \Big[\underbrace{\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}\sigma} \rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}\sigma}}_{\text{Diagonal terms}} - \underbrace{\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}+\boldsymbol{\pi}\sigma} \rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}-\boldsymbol{\pi}\sigma}}_{\text{Off-diagonal terms}} \Big] \end{aligned} \tag{1.21}$$

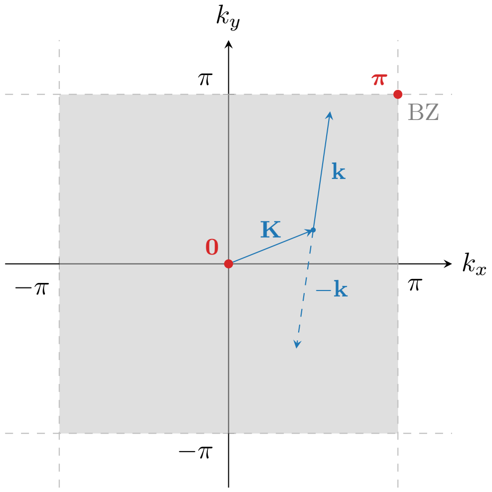
Now, the above equation presents *diagonal* and *off-diagonal* terms. Let me discuss them separately.

Diagonal terms. The diagonal terms of Eq. (1.21) are simple density interactions with the mean density field. Consider Fig. 1.3a: density at vector $\mathbf{q} \equiv \mathbf{K} + \mathbf{k}$ interacts with the mean density at vector $\mathbf{q}' \equiv \mathbf{K} - \mathbf{k}$. These variables are depicted in Fig. 1.3b. Apply the variable change in the diagonal part of Eq. (1.21),

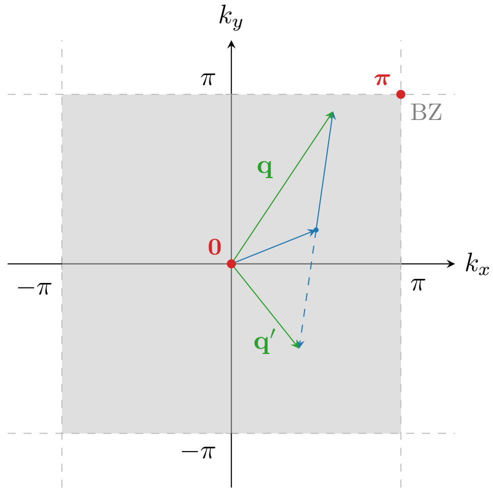
$$\begin{aligned} \frac{2V}{L_x L_y} \sum_{\mathbf{q},\mathbf{q}'} \sum_{\sigma} \left[\cos\left(2k_x\right) + \cos\left(2k_y\right) \right] \langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}\sigma} \rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}\sigma} \\ = \frac{2V}{L_x L_y} \sum_{\mathbf{q},\mathbf{q}'} \sum_{\sigma} \left[\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right) \right] \langle \hat{c}^\dagger_{\mathbf{q}\sigma} \hat{c}_{\mathbf{q}\sigma} \rangle \hat{c}^\dagger_{\mathbf{q}'\sigma} \hat{c}_{\mathbf{q}'\sigma} \end{aligned} \tag{1.22}$$

being for $\ell = x, y$

$$\begin{aligned} \delta q_\ell &\equiv q_\ell - q'_\ell \\ &= (K_\ell + k_\ell) - (K_\ell - k_\ell) \\ &= 2k_\ell \end{aligned}$$



a | Generic vectors.



b | Change of variables.

Figure 1.3 | Representation of the vectors involved in the diagonal terms of Eq. (1.21). In Fig. 1.3a generic vectors are considered, cycling over all values of $\mathbf{K}, \mathbf{k} \in$ BZ. In Fig. 1.3b is depicted the variables change to the new vectors $\mathbf{q}, \mathbf{q}'$.

Decompose the form factor,

$$\begin{aligned}
\cos(\delta q_x) + \cos(\delta q_y) = {} & \frac{1}{2}(\cos q_x + \cos q_y)(\cos q_x' + \cos q_y') && (s^*\text{-wave}) \\
& + \sin q_x \sin q_x' && (p_x\text{-wave}) \\
& + \sin q_y \sin q_y' && (p_y\text{-wave}) \\
& + \frac{1}{2}(\cos q_x - \cos q_y)(\cos q_x' - \cos q_y') && (d_{x^2-y^2}\text{-wave})
\end{aligned}$$

where all contributions are classified by their symmetry structure. These structure are listed and then later on dealt with in Tab. 1.3, in the context of anisotropic pairing and topological superconductivity. For now, all that matters is that, in the AF phase, $\langle \hat{c}^\dagger_{\mathbf{q}\sigma} \hat{c}_{\mathbf{q}\sigma} \rangle$ must be s^*-wave symmetric, as anticipated in the starting discussion of Sec. 1.2.2. This is due to the fact that of the four symmetries listed above, only the first one exhibits both x, y reflections symmetry and $\pi/2$ rotational invariance. It follows, only the s^*-wave component when coupled to $\langle \hat{c}^\dagger_{\mathbf{q}\sigma} \hat{c}_{\mathbf{q}\sigma} \rangle$ in Eq. (1.22) gives a non-null contribution, reducing the latter to

$$\begin{aligned}
& \frac{2V}{L_x L_y} \sum_{\mathbf{q},\mathbf{q}'} \sum_{\sigma} \left[\cos(\delta q_x) + \cos(\delta q_y)\right] \langle \hat{c}^\dagger_{\mathbf{q}\sigma} \hat{c}_{\mathbf{q}\sigma} \rangle \hat{c}^\dagger_{\mathbf{q}'\sigma} \hat{c}_{\mathbf{q}'\sigma} \\
& \qquad = \frac{V}{L_x L_y} \sum_{\mathbf{q}'\sigma} \left(\cos q_x' + \cos q_y'\right) \hat{c}^\dagger_{\mathbf{q}'\sigma} \hat{c}_{\mathbf{q}'\sigma} \sum_{\mathbf{q}} \left(\cos q_x + \cos q_y\right) \langle \hat{c}^\dagger_{\mathbf{q}\sigma} \hat{c}_{\mathbf{q}\sigma} \rangle
\end{aligned} \tag{1.23}$$

Note that, for two vectors separated by a $\boldsymbol{\pi}$ shift,

$$\cos q_x + \cos q_y = -\cos(q_x + \pi) - \cos(q_y + \pi)$$

Because of this feature, changing the variables names $\mathbf{q}' \to \mathbf{k}$, $\mathbf{q} \to \mathbf{k}'$ for the sake of general aesthetic coherence, it becomes evident that the above equation gives the bands renormalization:

$$\begin{aligned}
\epsilon_{\mathbf{k}} &\equiv -2t\left(\cos k_x + \cos k_y\right) \\
\tilde{\epsilon}_{\mathbf{k}} &\equiv \epsilon_{\mathbf{k}} + \left[\frac{1}{2L_x L_y} \sum_{\mathbf{k}'} \left(\cos k_x' + \cos k_y'\right) \langle \hat{c}^\dagger_{\mathbf{k}'\sigma} \hat{c}_{\mathbf{k}'\sigma} \rangle \right] \times 2V\left(\cos k_x + \cos k_y\right)
\end{aligned}$$

Note that on the left-hand side $\tilde{\epsilon}_{\mathbf{k}}$ is independent of σ. To explain this, let:

$$w^{(\mathbf{0})}_\sigma \equiv \frac{1}{2L_x L_y} \sum_{\mathbf{k}\in\text{BZ}} \left(\cos k_x + \cos k_y\right) \langle \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \rangle$$

By simple symmetry considerations, it must be $\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle = \langle \hat{c}^\dagger_{\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\downarrow}\rangle$ (as is later seen explicitly). Then,

$$w^{(\mathbf{0})}_\uparrow = w^{(\mathbf{0})}_\downarrow \equiv w^{(\mathbf{0})}$$

The computation can be simplified:

$$\begin{aligned}
w^{(\mathbf{0})} &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}} (\cos k_x + \cos k_y)\,\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle \\
&= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}} (\cos k_x + \cos k_y)\,\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} - \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\rangle \\
&= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}} (\cos k_x + \cos k_y)\,\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow}\tau^z\hat{\Psi}_{\mathbf{k}\uparrow}\rangle \\
&= -\frac{1}{4L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}} (\cos k_x + \cos k_y)\,\frac{\tilde{\epsilon}_\mathbf{k}}{\tilde{E}_\mathbf{k}}\left[f\left(-\tilde{E}_\mathbf{k};\beta,\tilde{\mu}\right) - f\left(\tilde{E}_\mathbf{k};\beta,\tilde{\mu}\right)\right]
\end{aligned} \tag{1.24}$$

where in the second passage the sign change is due to the presence of the structure factor, and in the fourth passage Eq. (1.13) and the relations (1.14) have been used. It follows, finally, that the hopping parameter gets effectively renormalized:

$$\tilde{t} \equiv t - w^{(\mathbf{0})}V \tag{1.25}$$

The full effective MFT hamiltonian is spin-independent, then similarly the renormalized parameters cannot exhibit spin dependency. This justifies the fact that $\tilde{t}$ is spin-independent, and so is $\tilde{\epsilon}_\mathbf{k}$.

Off-diagonal terms. Consider the off-diagonal terms of Eq. (1.21). These contribute instead to the gap renormalization, being out of diagonal in the 2×2 hamiltonian matrix. Define $\mathbf{q}$, $\mathbf{q}'$ as in Fig. 1.3b, and rewrite

$$\begin{aligned}
&-\frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k}}\sum_{\sigma}\left[\cos(2k_x) + \cos(2k_y)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}+\boldsymbol{\pi}\sigma}\rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}-\boldsymbol{\pi}\sigma} \\
&\qquad = -\frac{2V}{L_xL_y}\sum_{\mathbf{q}}\langle \hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\rangle \sum_{\mathbf{q}'\sigma}\left[\cos(\delta q_x) + \cos(\delta q_y)\right]\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'+\boldsymbol{\pi}\sigma}
\end{aligned}$$

Identical considerations about the s^*-wave symmetry structure of the expectation value $\langle \hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\rangle$ as in the above paragraph hold. Once again renaming the variables $\mathbf{q}' \to \mathbf{k}$, $\mathbf{q} \to \mathbf{k}'$ for the sake of general aesthetic coherence, this gives

$$\begin{aligned}
&-\frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k}}\sum_{\sigma}\left[\cos(2k_x) + \cos(2k_y)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}+\boldsymbol{\pi}\sigma}\rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}-\boldsymbol{\pi}\sigma} \\
&\quad = -2V\left[\frac{1}{2L_xL_y}\sum_{\mathbf{k}'}\left(\cos k'_x + \cos k'_y\right)\langle \hat{c}^\dagger_{\mathbf{k}'\sigma}\hat{c}_{\mathbf{k}'+\boldsymbol{\pi}\sigma}\rangle\right]\sum_{\mathbf{k}\sigma}(\cos k_x + \cos k_y)\,\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma}
\end{aligned} \tag{1.26}$$

Because of this, the x component of the pseudo-magnetic field – the gap already renormalized by Eq. (1.18) when analyzing o.s. terms – takes up another renormalization contribution, finally giving

$$\tilde{\Delta}_{\mathbf{k}\sigma} \equiv m(U + 2zV)\times(-1)^{\delta_{\sigma=\uparrow}} + i2Vw^{(\boldsymbol{\pi})}_\sigma(\cos k_x + \cos k_y) \tag{1.27}$$

where

$$w^{(\boldsymbol{\pi})}_\sigma \equiv -\frac{i}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}}(\cos k_x + \cos k_y)\,\langle \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma}\rangle$$

As will be clear in few lines, $w^{(\boldsymbol{\pi})}_\sigma$ as is defined here is purely real (due to the presence of a $-i$ prefactor). This makes $\tilde{\Delta}_{\mathbf{k}\sigma}$ made of two contributions,

$$\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}\sigma}\} = m(U + 2zV)\times(-1)^{\delta_{\sigma=\uparrow}} \qquad \mathrm{Im}\{\tilde{\Delta}_{\mathbf{k}\sigma}\} = 2Vw^{(\boldsymbol{\pi})}_\sigma(\cos k_x + \cos k_y)$$

Now, since the gapped band value cannot depend on the spin index for symmetry reasons,

$$\tilde{E}_{\mathbf{k}} = \sqrt{\tilde{\epsilon}_{\mathbf{k}}^2 + |\tilde{\Delta}_{\mathbf{k}\sigma}|^2}$$

this implies necessarily $|\tilde{\Delta}_{\mathbf{k}\uparrow}| = |\tilde{\Delta}_{\mathbf{k}\downarrow}|$. This is possible either if $w_\uparrow^{(\boldsymbol{\pi})} = \pm w_\downarrow^{(\boldsymbol{\pi})}$. Actually, in the end the exact sign does not matter: all that matters is the gap amplitude $|\tilde{\Delta}_{\mathbf{k}\sigma}|$, thus we may restrict to $\sigma =\uparrow$ and omit from now on the spin index. [Not so sure about this.]. This then gives us the final result for the renormalized gap function,

$$\tilde{\Delta}_{\mathbf{k}} \equiv m(U + 2zV) + 2iw^{(\boldsymbol{\pi})}V\,(\cos k_x + \cos k_y) \tag{1.28}$$

This result, together with Eqns. (1.16) and (1.25), concludes the renormalization of all parameters due to the non-local interaction. To calculate $w^{(\boldsymbol{\pi})}$ self consistently, we may use:

$$\begin{aligned}
w^{(\boldsymbol{\pi})} &= -\frac{i}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}}(\cos k_x + \cos k_y)\,\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\rangle \\
&= -\frac{i}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}(\cos k_x + \cos k_y)\,\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle \\
&= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}(\cos k_x + \cos k_y)\,\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow}\tau^y\hat{\Psi}_{\mathbf{k}\uparrow}\rangle \\
&= \frac{1}{4L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}(\cos k_x + \cos k_y)\,\frac{\mathrm{Im}\{\tilde{\Delta}_{\mathbf{k}}\}}{\tilde{E}_{\mathbf{k}}}\left[f\left(-\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right) - f\left(\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)\right]
\end{aligned} \tag{1.29}$$

Notice that this expression is purely real, as promised, and contributes to the y component of the pseudo-field of Fig. 1.2.

1.2.3 Renormalized hamiltonian behavior

Summing up, the non-local interaction $\hat{H}_V$ when discussed within MFT affects the EHM hamiltonian by renormalizing the various parameters as:

$$\begin{aligned}
\tilde{\mu} &\equiv \mu + 2znV \\
\tilde{t} &\equiv t - w^{(\mathbf{0})}V \\
\tilde{\Delta}_{\mathbf{k}} &\equiv m(U + 2zV) + 2iw^{(\boldsymbol{\pi})}V\,[\cos(k_x) + \cos(k_y)]
\end{aligned}$$

Various details are to be noted. First, the non-local interaction both contributes by enlarging the real part of the gap [To be understood: why does a non-local attraction increase the gap?] as well as introducing a s^*-wave shaped imaginary gap. Interestingly, if

$$\left(w^{(\mathbf{0})}\right)^{-1} = V/t$$

the diffusive part of the hamiltonian drops to zero. For even larger values, diffusion becomes energetically expensive and V-induced localization appears.

The new set of Hartree-Fock parameters to be determined is given by the vector

$$\mathbf{v} \equiv \begin{bmatrix} m \\ w^{(\mathbf{0})} \\ w^{(\boldsymbol{\pi})} \end{bmatrix}$$

Its three components are self-consistently determined by Eqns. (1.24) and (1.29). The self-consistent equation for m comes from Eq. (**??**), and reads

$$\begin{aligned} m &= \frac{1}{2L_xL_y} \sum_{\mathbf{k}\in\mathrm{BZ}} \langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow} \rangle \\ &= \frac{1}{2L_xL_y} \sum_{\mathbf{k}\in\mathrm{MBZ}} \langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow} \tau^x \hat{\Psi}_{\mathbf{k}\uparrow} - \hat{\Psi}^\dagger_{\mathbf{k}\downarrow} \tau^x \hat{\Psi}_{\mathbf{k}\downarrow} \rangle \\ &= \frac{1}{L_xL_y} \sum_{\mathbf{k}\in\mathrm{MBZ}} \langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow} \tau^x \hat{\Psi}_{\mathbf{k}\uparrow} \rangle \\ &= \frac{1}{2L_xL_y} \sum_{\mathbf{k}\in\mathrm{MBZ}} \frac{\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\}}{\tilde{E}_{\mathbf{k}}} \left[f\left(-\tilde{E}_{\mathbf{k}}; \beta, \tilde{\mu}\right) - f\left(\tilde{E}_{\mathbf{k}}; \beta, \tilde{\mu}\right) \right] \end{aligned} \tag{1.30}$$

In the second passage $\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow} \tau^x \hat{\Psi}_{\mathbf{k}\uparrow} \rangle = -\langle \hat{\Psi}^\dagger_{\mathbf{k}\downarrow} \tau^x \hat{\Psi}_{\mathbf{k}\downarrow} \rangle$ has been used. In the third passage, relations (1.14) were inserted. The algorithm sketched in Sec. **??** remains essentially identical, with the *caveat* of defining three HF parameters, running for each a convergence analysis.

1.2.4 Results of the HF algorithm

An HF algorithm similar to the one sketched in Sec. **??** was run, now self-consistently on the entire HF vector $\mathbf{v}$. [Insert results of analysis.]

1.3 Superconducting instability

This section is devoted to studying the superconducting phase of the system. The only symmetry we assume to break is the U(1) charge symmetry, thus allowing for superconducting fluctuations. As is described thoroughly in Sec. 1.2.2, the hopping amplitude is renormalized because of the non-local attraction. The symmetry structure of the pairing mechanism determines the contributing Cooper fluctuations: for s-wave and d-wave superconductivity, only the o.s. Cooper term contributes; for p_ℓ-wave superconductivity, the s.s. term contributes as well. In the following sections, a derivation containing both Cooper terms is proposed.

[To be continued: separate singlet and triplet pairing channels, and describe them separately by the means of four-components Nambu spinors. Use selection rules to set $\Delta^{(p_\ell)} = 0$ in the singlet channel, in order to justify results obtained by a pure space-even simulation containing just the o.s. terms.]

1.3.1 Mean-field treatment of the non-local term

This approach leads to the conclusion that the (coherent) ground-state of the system must be an eigenstate of the mean-field effective hamiltonian:

$$\begin{aligned} \hat{H}^{(\mathrm{e})} = &- t \sum_{\langle ij \rangle} \sum_\sigma \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \\ &- V \sum_{i\in\mathcal{S}} \sum_{\ell=x,y} \sum_{\delta=\pm\delta_\ell} \left[\langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i+\delta\downarrow} \rangle \hat{c}_{i+\delta\downarrow} \hat{c}_{i\uparrow} + \mathrm{h.c.} \right] \end{aligned} \tag{1.31}$$

Note that I am here summing over $i \in \mathcal{S}$: this is the same as considering both the $\uparrow\downarrow$ *plus* the $\downarrow\uparrow$ terms of the o.s. hamiltonian involved in even-wave pairing. 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:

$$\hat{H}^{(\mathrm{e})} = -t \sum_{\langle ij \rangle} \sum_\sigma \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - V \sum_{\langle ij \rangle} \left[g_{ij} \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} + g^*_{ij} \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{j\downarrow} \right] \tag{1.32}$$

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.

1.3.2 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

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

being

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

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

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

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

$$\begin{aligned} \hat{H}^{(\mathrm{e})} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_{i} \left[f_i \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} + f_i^* \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \right] \\ - V \sum_{\langle ij \rangle} \left[g_{ij} \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} + g_{ij}^* \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \right] \end{aligned} \tag{1.33}$$

Next section is devoted to analyzing the consequences of choosing a specific topology (which is, symmetry structure) for the pairing correlations.

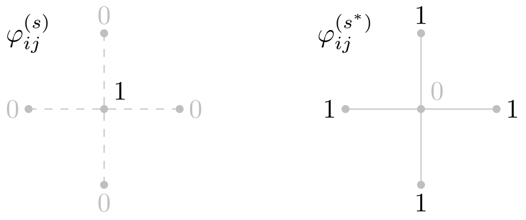
1.3.3 Topological correlations

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

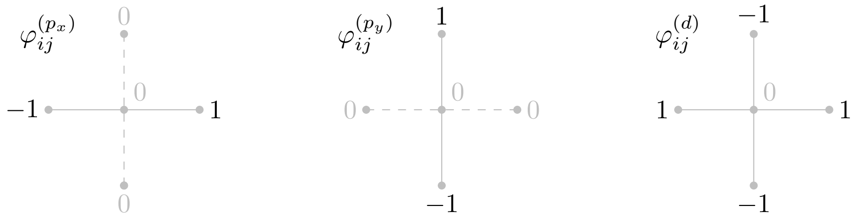
$$g_{ij} = \sum_{\gamma} g^{(\gamma)} \varphi_{ij}^{(\gamma)}$$

where $g^{(\gamma)}$ are the g_{ij} symmetries-decomposition coefficients while $\varphi_{ij}^{(\gamma)}$ are the form factors listed in Tab. 1.2, 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. 1.4a) and extended on a non-local term (Fig. 1.4b). 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 $g_{ij} \propto \varphi_{ij}^{(\gamma)}$.



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



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

Figure 1.4 | Form factors at different topologies, as listed in Tab. 1.2. 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.

Structure	**Form factor**	**Graph**
s-wave	$\varphi_{ij}^{(s)} = \delta_{ij}$	Fig. 1.4a
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. 1.4b
p_x-wave	$\varphi_{ij}^{(p_x)} = \delta_{j=i+\delta_x} - \delta_{j=i-\delta_x}$	Fig. 1.4c
p_y-wave	$\varphi_{ij}^{(p_y)} = \delta_{j=i+\delta_y} - \delta_{j=i-\delta_y}$	Fig. 1.4d
$d_{x^2-y^2}$-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. 1.4e

Table 1.2 | 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.

1.4 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. ??.

1.4.1 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

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

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

1.4.2 Non-local attraction

Consider now the result of Eq. (1.4). 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. 1.4.5. 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

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

Now, consider the term

$$
\cos\left(\delta k_x\right) + \cos\left(\delta k_y\right) = \cos k_x \cos k'_x + \sin k_x \sin k'_x + \cos k_y \cos k'_y + \sin k_y \sin k'_y
$$

For the sake of readability, the notations

$$
c_\ell \equiv \cos k_\ell \qquad s_\ell \equiv \sin k_\ell \qquad c'_\ell \equiv \cos k'_\ell \qquad s'_\ell \equiv \sin k'_\ell
$$

are used. Group the four terms above,

$$
\underbrace{\left(c_x c'_x + c_y c'_y\right)}_{\text{Symmetric}} + \underbrace{\left(s_x s'_x + s_y s'_y\right)}_{\text{Anti-symmetric}} \tag{1.34}
$$

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:

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

Structure	Structure factor	Graph
s-wave	$\varphi_{\mathbf{k}}^{(s)} = 1$	Fig. 1.4a
Extended s-wave	$\varphi_{\mathbf{k}}^{(s^*)} = \cos k_x + \cos k_y$	Fig. 1.4b
p_x-wave	$\varphi_{\mathbf{k}}^{(p_x)} = i\sqrt{2}\sin k_x$	Fig. 1.4c
p_y-wave	$\varphi_{\mathbf{k}}^{(p_y)} = i\sqrt{2}\sin k_y$	Fig. 1.4d
$d_{x^2-y^2}$-wave	$\varphi_{\mathbf{k}}^{(d)} = \cos k_x - \cos k_y$	Fig. 1.4e

Table 1.3 | 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.

In other words, the two-body potential decomposes as

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

being $\varphi_{\mathbf{k}}^{(\gamma)}$ the reciprocal-space expressions for the form factors of Tab. 1.2, listed explicitly in Tab. 1.3, 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

$$\mathcal{V}_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle \hat{\phi}_{\mathbf{k}'}^\dagger \rangle \tag{1.35}$$

one gets immediately

$$\hat{H}_V \simeq -\sum_{\mathbf{k}} \left[\mathcal{V}_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k}}^* \hat{\phi}_{\mathbf{k}}^\dagger \right] \tag{1.36}$$

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. (1.35) 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.

1.4.3 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

$$\mathcal{U}_{\mathbf{k}} \equiv \frac{U}{2 L_x L_y} \sum_{\mathbf{k}} \langle \hat{\phi}_{\mathbf{k}} \rangle \tag{1.37}$$

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

$$\hat{H}_U \simeq \sum_{\mathbf{k}} \left[\mathcal{U}_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} + \mathcal{U}_{\mathbf{k}}^* \hat{\phi}_{\mathbf{k}}^\dagger \right] \tag{1.38}$$

and the full gap function is simply

$$\Delta_{\mathbf{k}} \equiv \mathcal{V}_{\mathbf{k}} - \mathcal{U}_{\mathbf{k}} \tag{1.39}$$

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

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

Then the full effective interaction is collected in

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

The full self-consistency equation is given by

$$\Delta_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \langle \hat{\phi}^\dagger_{\mathbf{k}'}\rangle \tag{1.40}$$

The gap function decomposes in symmetry channels as well,

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

If SC arises in a specific symmetry channel, $\Delta_{\mathbf{k}}$ will show the same symmetry. It follows, due to orthonormality and using Eq. (1.40),

$$\begin{aligned}
\Delta^{(\gamma)} &= \frac{1}{L_x L_y} \sum_{\mathbf{k}} \varphi^{(\gamma)*}_{\mathbf{k}} \Delta_{\mathbf{k}} \\
&= \frac{1}{L_x L_y} \sum_{\mathbf{k}} \varphi^{(\gamma)*}_{\mathbf{k}} \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \langle \hat{\phi}^\dagger_{\mathbf{k}'}\rangle \\
&= \frac{1}{L_x L_y} \sum_{\mathbf{k}} \varphi^{(\gamma)*}_{\mathbf{k}} \sum_{\mathbf{k}'\gamma'} V^{(\gamma')} \varphi^{(\gamma')}_{\mathbf{k}} \varphi^{(\gamma')*}_{\mathbf{k}'} \langle \hat{\phi}^\dagger_{\mathbf{k}'}\rangle \\
&= V^{(\gamma)} \sum_{\mathbf{k}} \varphi^{(\gamma)*}_{\mathbf{k}} \langle \hat{\phi}^\dagger_{\mathbf{k}}\rangle
\end{aligned} \tag{1.41}$$

This result provides a set of self-consistency equations for each symmetry channel, listed in Tab. 1.4. 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.

1.4.4 Nambu formalism and Bogoliubov transform

Define the Nambu spinor[2] as in BCS

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

Evidently,

$$\phi_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \hat{\Psi}_{\mathbf{k}} \qquad \phi^\dagger_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \hat{\Psi}_{\mathbf{k}} \tag{1.42}$$

[2] 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.

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. 1.4a
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. 1.4b
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. 1.4c
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. 1.4d
$d_{x^2-y^2}$-wave	$\Delta^{(d)} = \frac{V}{L_xL_y}\sum_{\mathbf{k}}(c_x-c_y)\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$	Fig. 1.4e

Table 1.4 Symmetry resolved self-consistency equations for the MFT parameters $\Delta^{(\gamma)}$, based on Eq. (1.40) and (1.41). By computing $\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$, it is possible to reconstruct the various components of the gap function.

The full hamiltonian is then given by:

$$\hat{H} = \sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}h_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}} \qquad h_{\mathbf{k}} \equiv \begin{bmatrix}\epsilon_{\mathbf{k}} & -\Delta^*_{\mathbf{k}} \\ -\Delta_{\mathbf{k}} & -\epsilon_{\mathbf{k}}\end{bmatrix} \tag{1.43}$$

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

$$\begin{aligned}\hat{n}_{\mathbf{k}\uparrow} + \hat{n}_{-\mathbf{k}\downarrow} &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow} \\ &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{-\mathbf{k}\downarrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \mathbb{I} \\ &= \hat{\Psi}^\dagger_{\mathbf{k}}\tau^z\hat{\Psi}_{\mathbf{k}} + \mathbb{I}\end{aligned} \tag{1.44}$$

and then it follows

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

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

$$\mathbf{b}_{\mathbf{k}} \equiv \begin{bmatrix}-\mathrm{Re}\{\Delta_{\mathbf{k}}\} \\ -\mathrm{Im}\{\Delta_{\mathbf{k}}\} \\ \epsilon_{\mathbf{k}} - \mu\end{bmatrix} \tag{1.45}$$

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

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\in\mathrm{BZ}}\mathbf{b}_{\mathbf{k}}\cdot\hat{\mathbf{s}}_{\mathbf{k}} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}\sigma} = \begin{bmatrix}\hat{s}^x_{\mathbf{k}} \\ \hat{s}^y_{\mathbf{k}} \\ \hat{s}^z_{\mathbf{k}}\end{bmatrix} \tag{1.46}$$

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

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

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

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

the general diagonalizer will be an orthogonal rotation matrix

$$\begin{aligned} W_{\mathbf{k}} &= e^{i\left(\theta_{\mathbf{k}} - \frac{\pi}{2}\right)\tau^y} e^{i\zeta_{\mathbf{k}}\tau^z} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \\ \cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} e^{i\zeta_{\mathbf{k}}} & \\ & e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\cos\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \\ \cos\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\sin\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \end{aligned} \tag{1.47}$$

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. (**??**),

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

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

$$\langle \phi_{\mathbf{k}}^\dagger \rangle = [W_{\mathbf{k}}]_{11}[W_{\mathbf{k}}^\dagger]_{21} f\left(-E_{\mathbf{k}};\beta,0\right) + [W_{\mathbf{k}}]_{21}[W_{\mathbf{k}}^\dagger]_{22} f\left(E_{\mathbf{k}};\beta,0\right) \tag{1.48}$$

$$= \frac{1}{2}\sin\left(2\theta_{\mathbf{k}}\right) e^{i2\zeta_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{1.49}$$

The last passage has been obtained by computing the matrix element from the explicit form of $W_{\mathbf{k}}$ of Eq. (1.47) 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. (1.48), (1.49) 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

$$\Delta_{\mathbf{k}} \equiv \frac{1}{2}\sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \frac{|\Delta_{\mathbf{k}}|}{\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}} e^{i\,\mathrm{Im}\{\Delta_{\mathbf{k}}\}/\,\mathrm{Re}\{\Delta_{\mathbf{k}}\}} \tanh\left(\frac{\beta}{2}\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}\right) \tag{1.50}$$

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. 1.4.

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

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

I proceed in as done previously, and from Eq. (1.44),

$$\begin{aligned}
\langle \hat{n}_{\mathbf{k}\uparrow} \rangle + \langle \hat{n}_{-\mathbf{k}\downarrow} \rangle &= 1 + \langle \hat{\Psi}^{\dagger}_{\mathbf{k}} \tau^z \hat{\Psi}_{\mathbf{k}} \rangle \\
&= 1 + \left(|[W_{\mathbf{k}}]_{11}|^2 - |[W_{\mathbf{k}}]_{12}|^2 \right) f\left(-E_{\mathbf{k}}; \beta, 0\right) \\
&\quad + \left(|[W_{\mathbf{k}}]_{21}|^2 - |[W_{\mathbf{k}}]_{22}|^2 \right) f\left(E_{\mathbf{k}}; \beta, 0\right) && (1.51) \\
&= 1 - \cos\left(2\theta_{\mathbf{k}}\right) \tanh\left(\frac{\beta E_{\mathbf{k}}}{2} \right) && (1.52)
\end{aligned}$$

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. (1.51) directly on the diagonalization matrix of $h_{\mathbf{k}}$.

1.4.5 A short comment on self-consistency

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

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

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

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

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. 1.4.4 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.

1.5 Results of the HF algorihtm

[To be continued. . .]

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