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

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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

Part I

Mean-Field-Theory analysis

Chapter 1

Superconducting instability

This chapter is devoted to studying the superconducting phase of the system. The only symmetry we assume to break is the $\mathrm{U}^{\mathrm{c}}(1)$ charge symmetry, thus allowing for superconducting fluctuations. As is described thoroughly in Sec. **??**, 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.]

1.1 Cooper fluctuations in the EHM

Let us start once again from the general EHM of Eq. (**??**),

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

As is discussed in Sec. **??**, when applying Wick's theorem the resulting terms break the natural symmetries of the model. The superconducting symmetry we study breaks just the $\mathrm{U}^{\mathrm{c}}(1)$ charge conservation. Now, when dealing with superconducting Cooper pairing we need to account also for the spatial structure of the Cooper pair itself. Consider the generic Cooper fluctuation

$$\langle \hat{c}^\dagger_{i\sigma} \hat{c}^\dagger_{j\sigma'} \rangle \quad \text{with } i, j \text{ NN}$$

From basic Quantum Mechanics we know the summation rules of the spin algebra $\mathfrak{su}(2)$,

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

The two pairing channels are, at this level, the singlet channel associated to total spin 0 and the triplet channel associated to total spin 1. If we impose a specific spatial symmetry on the hamiltonian the ground state wavefunction will follow naturally, and the pairing channel will be the one providing a total anti-symmetry to the full wavefunction. This gives a selection rule over the relevant pairings: if we work with space symmetric structures – say, s^*-wave or d-wave – the pairing will happen in singlet channel, allowing us to eliminate the triplet pairing. This concept is summarized in Tab. 1.1.

[Add: Cooper pairing considerations in the pure Hubbard model.]

1.2 Cooper fluctuations in the opposite-spin sector

This section deals with Cooper fluctuations induced by the o.s. part of the non-local hamiltonian –referring to the notation of Eq. (**??**)– somewhat the simplest form of Cooper pairing. This sector

Spatial structure	Pairing channel	Relevant pairing
Symmetric wave function	Singlet pairing	Just $\langle \hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\bar{\sigma}}\rangle$
Anti-symmetric wave function	Triplet pairing	Both $\langle \hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\bar{\sigma}}\rangle$ and $\langle \hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma}\rangle$

Table 1.1 | Relation of the Cooper pairing channell with the wavefunction spatial symmetry (intended as the inversion $(x, y) \to (-x, -y)$).

contributes both to singlet pairing and triplet pairing. Considering Cooper fluctuations in the singlet channel, we need to break $\mathrm{U^c}(1)$ symmetry imposing space inversion symmetry, while for the triplet anti-symmetry is required. Let us now break down the MFT discussion for the local and non-local interactions.

Local interaction U. Consider first the local part,

$$\hat{H}_U = U\sum_{i\in\mathcal{S}} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \simeq U\sum_{i\in\mathcal{S}}\Big[\langle \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\rangle \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\langle \hat{c}_{i\downarrow}\hat{c}_{i\uparrow}\rangle\Big]$$

and use the result of Eq. (**??**),

$$\hat{H}_U \simeq \frac{U}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\Big[\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\rangle \hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow} + \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\langle \hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow}\rangle\Big]$$

We are not breaking translational invariance, thus only Cooper fluctuations with net zero total momentum are allowed. This means only $\mathbf{K} = \mathbf{0}$ contributes. Define the pairing operator

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

Then the non local repulsion reduces to the ordinary BCS-like interaction,

$$\hat{H}_U \simeq \sum_{\mathbf{k}}\Big[\mathcal{U}_{\mathbf{k}}\hat{\phi}_{\mathbf{k}} + \mathcal{U}^*_{\mathbf{k}}\hat{\phi}^\dagger_{\mathbf{k}}\Big] \tag{1.1}$$

where the MFT parameter $\mathcal{U}_{\mathbf{k}}$ must satisfy the self-consistency equation

$$\mathcal{U}_{\mathbf{k}} \equiv \frac{U}{L_xL_y}\sum_{\mathbf{k}}\langle \hat{\phi}^\dagger_{\mathbf{k}}\rangle \tag{1.2}$$

Note that $\mathcal{U}_{\mathbf{k}}$ is actually momentum independent. This is due to the fact that the repulsion is completely localized.

Non-local interaction V. The non-local attraction in the opposite-spin sector of $\hat{H}_V$ is given by

$$\hat{H}^{(\mathrm{o.s.})}_V = -V\sum_{\langle ij\rangle}\sum_{\sigma}\hat{n}_{i\sigma}\hat{n}_{j\bar{\sigma}}$$

which, using Eq. (**??**) and performing Wick's contractions, reduces to:

$$\begin{aligned}\hat{H}^{(\mathrm{o.s.})}_V &= -V\sum_{i\in\mathcal{S}}\sum_{\ell=x,y}\sum_{\delta=\pm\delta_\ell}\hat{n}_{i\uparrow}\hat{n}_{i+\delta\downarrow}\\ &\simeq -V\sum_{i\in\mathcal{S}}\sum_{\ell=x,y}\sum_{\delta=\pm\delta_\ell}\Big[\langle \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i+\delta\downarrow}\rangle \hat{c}_{i+\delta\downarrow}\hat{c}_{i\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i+\delta\downarrow}\langle \hat{c}_{i+\delta\downarrow}\hat{c}_{i\uparrow}\rangle\Big]\end{aligned}$$

Using Eq. (**??**) we can move to reciprocal space,

$$\begin{aligned}\hat{H}^{(\mathrm{o.s.})}_V \simeq -\frac{V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}&\left[\cos\left(\delta k_x\right) + \cos\left(\delta k_y\right)\right]\\ &\times\Big[\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\rangle \hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow} + \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\downarrow}\langle \hat{c}_{\mathbf{K}-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{K}+\mathbf{k}'\uparrow}\rangle\Big]\end{aligned}$$

Identical considerations as above hold, and just the $\mathbf{K} = \mathbf{0}$ term contributes. We have finally

$$\hat{H}_V^{(\mathrm{o.s.})} \simeq -\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \left[\langle \hat{\phi}_{\mathbf{k}}^\dagger \rangle \hat{\phi}_{\mathbf{k}'} + \langle \hat{\phi}_{\mathbf{k}} \rangle \hat{\phi}_{\mathbf{k}'}^\dagger \right]$$

where the two-body potential was defined

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

Making use of the decomposition of Eq. (**??**), the two-body potential becomes

$$\begin{aligned} V_{\mathbf{k}\mathbf{k}'} &= \frac{V}{2L_x L_y} \sum_\gamma \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*} \\ &= \sum_\gamma V^{(\gamma)} \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*} \end{aligned}$$

being $\gamma \in \{s^*, p_x, p_y, d_{x^2-y^2}\}$ and $\varphi_{\mathbf{k}}^{(\gamma)}$ the reciprocal-space expressions for the form factors of Tab. **??**, listed explicitly in Tab. **??**, 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

$$\mathcal{V}_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle \hat{\phi}_{\mathbf{k}'}^\dagger \rangle \tag{1.3}$$

one gets immediately

$$\hat{H}_V \simeq -\sum_{\mathbf{k}} \left[\mathcal{V}_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k}}^* \hat{\phi}_{\mathbf{k}}^\dagger \right] \tag{1.4}$$

To assume symmetry is broken in a specific symmetry channel γ means precisely to assume $\langle \hat{\phi}_{\mathbf{k}} \rangle \propto \varphi_{\mathbf{k}}^{(\gamma)}$. Of course, in Eq. (1.3) only the γ component of the potential survives, implying the gap function acquires the same symmetry,

$$\mathcal{V}_{\mathbf{k}} \propto \sum_{\mathbf{k}'} \varphi_{\mathbf{k}}^{(\gamma)} \varphi_{\mathbf{k}'}^{(\gamma)*} \varphi_{\mathbf{k}'}^{(\gamma)} \propto \varphi_{\mathbf{k}}^{(\gamma)}$$

where orthonormality of the $\varphi_{\mathbf{k}}^{(\gamma)}$ functions of Tab. **??** was used. Thus, assuming to have superconductivity in a given sector γ, the self consistency equation reads

$$\forall \gamma \in \{s^*, p_x, p_y, d_{x^2-y^2}\} \qquad \mathcal{V}_{\mathbf{k}}\big|_\gamma \equiv \frac{V}{2L_x L_y} \sum_{\mathbf{k}} \varphi_{\mathbf{k}}^{(\gamma)} \langle \hat{\phi}_{\mathbf{k}}^\dagger \rangle \tag{1.5}$$

Now we merge the two interaction in a single gap function.

1.2.1 Full gap function and self-consistency equations

Define the full gap function as the sum of both contributions,

$$\Delta_{\mathbf{k}} \equiv \mathcal{V}_{\mathbf{k}} - \mathcal{U}_{\mathbf{k}} \tag{1.6}$$

The full self-consistency equation is given by the simple combination of Eqns. (1.2) and (1.5),

$$\Delta_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'} \right] \langle \hat{\phi}_{\mathbf{k}'}^\dagger \rangle \quad \text{with} \quad V^{(s)} = -\frac{U}{2L_x L_y} \tag{1.7}$$

The gap function decomposes in symmetry channels as well,

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

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

Table 1.2 | Symmetry resolved self-consistency equations for the MFT parameters $\Delta^{(\gamma)}$, based on Eq. (1.7) and (1.8). By computing $\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle$, it is possible to reconstruct the various components of the gap function.

If SC arises in a specific symmetry channel, $\Delta_{\mathbf{k}}$ will show the same symmetry. It follows, due to orthonormality and using Eq. (1.7),

$$\begin{aligned}\Delta^{(\gamma)} &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\Delta_{\mathbf{k}}\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\sum_{\mathbf{k}'}\left[V^{(s)}+V_{\mathbf{k}\mathbf{k}'}\right]\langle\hat{\phi}^\dagger_{\mathbf{k}'}\rangle\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\sum_{\mathbf{k}'\gamma'}V^{(\gamma')}\varphi^{(\gamma')}_{\mathbf{k}}\varphi^{(\gamma')*}_{\mathbf{k}'}\langle\hat{\phi}^\dagger_{\mathbf{k}'}\rangle\\ &= V^{(\gamma)}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle\end{aligned} \tag{1.8}$$

This result provides a set of self-consistency equations for each symmetry channel, listed in Tab. 1.2. 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.

1.2.2 Nambu formalism and Bogoliubov transform

Define the Nambu spinor[1] as in BCS

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

Evidently,

$$\phi_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}}\begin{bmatrix}0&1\\0&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}} \qquad \phi^\dagger_{\mathbf{k}} = \hat{\Psi}^\dagger_{\mathbf{k}}\begin{bmatrix}0&0\\1&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}} \tag{1.9}$$

The full hamiltonian is then given by:

$$\hat{H} = \sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}h_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}} \qquad h_{\mathbf{k}} \equiv \begin{bmatrix}\epsilon_{\mathbf{k}} & -\Delta^*_{\mathbf{k}}\\ -\Delta_{\mathbf{k}} & -\epsilon_{\mathbf{k}}\end{bmatrix} \tag{1.10}$$

[1] 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.

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 $L_x L_y$ 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

$$\begin{aligned} \hat{n}_{\mathbf{k}\uparrow} + \hat{n}_{-\mathbf{k}\downarrow} &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} + \hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow} \\ &= \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow} - \hat{c}_{-\mathbf{k}\downarrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \mathbb{I} \\ &= \hat{\Psi}^\dagger_{\mathbf{k}} \tau^z \hat{\Psi}_{\mathbf{k}} + \mathbb{I} \end{aligned} \tag{1.11}$$

and then it follows

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

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

$$\mathbf{b}_{\mathbf{k}} \equiv \begin{bmatrix} -\operatorname{Re}\{\Delta_{\mathbf{k}}\} \\ -\operatorname{Im}\{\Delta_{\mathbf{k}}\} \\ \epsilon_{\mathbf{k}} - \mu \end{bmatrix} \tag{1.12}$$

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

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\in \mathrm{BZ}} \mathbf{b}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}\sigma} = \begin{bmatrix} \hat{s}^x_{\mathbf{k}} \\ \hat{s}^y_{\mathbf{k}} \\ \hat{s}^z_{\mathbf{k}} \end{bmatrix} \tag{1.13}$$

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

$$\begin{aligned} W_{\mathbf{k}} &= e^{i\left(\theta_{\mathbf{k}} - \frac{\pi}{2}\right)\tau^y} e^{i\zeta_{\mathbf{k}}\tau^z} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \\ \cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} e^{i\zeta_{\mathbf{k}}} & \\ & e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\cos\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \\ \cos\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\sin\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \end{aligned} \tag{1.14}$$

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

$$\begin{aligned} \langle \phi_{\mathbf{k}}^{\dagger} \rangle &= [W_{\mathbf{k}}]_{11} [W_{\mathbf{k}}^{\dagger}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21} [W_{\mathbf{k}}^{\dagger}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) && (1.15) \\ &= \frac{1}{2} \sin\left(2\theta_{\mathbf{k}}\right) e^{i2\zeta_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) && (1.16) \end{aligned}$$

The last passage has been obtained by computing the matrix element from the explicit form of $W_{\mathbf{k}}$ of Eq. (1.14) 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. (1.15), (1.16) 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

$$\Delta_{\mathbf{k}} \equiv \frac{1}{2} \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'} \right] \frac{|\Delta_{\mathbf{k}}|}{\sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}} e^{i \operatorname{Im}\{\Delta_{\mathbf{k}}\} / \operatorname{Re}\{\Delta_{\mathbf{k}}\}} \tanh\left(\frac{\beta}{2} \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}\right) \tag{1.17}$$

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. 1.2.

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. (1.11),

$$\begin{aligned} \langle \hat{n}_{\mathbf{k}\uparrow} \rangle + \langle \hat{n}_{-\mathbf{k}\downarrow} \rangle &= 1 + \langle \hat{\Psi}_{\mathbf{k}}^{\dagger} \tau^z \hat{\Psi}_{\mathbf{k}} \rangle \\ &= 1 + \left(|[W_{\mathbf{k}}]_{11}|^2 - |[W_{\mathbf{k}}]_{12}|^2 \right) f\left(-E_{\mathbf{k}}; \beta, 0\right) \\ &\quad + \left(|[W_{\mathbf{k}}]_{21}|^2 - |[W_{\mathbf{k}}]_{22}|^2 \right) f\left(E_{\mathbf{k}}; \beta, 0\right) && (1.18) \\ &= 1 - \cos\left(2\theta_{\mathbf{k}}\right) \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) && (1.19) \end{aligned}$$

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

1.2.3 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:

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

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. 1.2.2 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...]