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
HFPs	Hartree-Fock parameters
LRT	Linear Response Theory
MFT	Mean-Field Theory
SC	Superconductor
SSB	Spontaneous Symmetry Breaking
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.

1.2.2 Non-local bands renormalization in the same-spin sector

In the context of antiferromagnetism (Sec. **??**) we discussed the role of the non-local interaction $\hat{H}_V$ as a source of bands effective renormalization. One of the most interesting results was the on of Eq. (**??**), with the hopping parameter being rigidly shifted. In the present context, we aim to treat the non-local part similarly by using immediately the aforementioned results. Start from Eq. (**??**),

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

For the BCS ground state, it is immediate to see the only relevant contribution comes from

$$\mathbf{k} = -\mathbf{k}'$$

which gives the diagonal part of Eq. (**??**). We are then left with (half) the result of Eq. (**??**)

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}+\text{h.c.}\right]=\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma} \tag{1.9}$$

Recall Eq. (**??**): the structure term decomposes in harmonic waves, and this feature is particularly handy in order to decouple the $\mathbf{q}$ and $\mathbf{q}'$ parts, as we later do.

1.3 Superconducting solution in the Nambu formalism

As a first approach to anisotropic SC in the Hubbard model, let us discuss the superconducting solutions in the simple scenario where crystal translational invariance is preserved and thus the system can be treated by the means of common BCS. As will be discussed, the non-local attraction acts as a source of SC in all symmetry sectors.

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,

$$\phi_{\mathbf{k}}=\hat{\Psi}^{\dagger}_{\mathbf{k}}\begin{bmatrix}0&1\\0&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}}\qquad\phi^{\dagger}_{\mathbf{k}}=\hat{\Psi}^{\dagger}_{\mathbf{k}}\begin{bmatrix}0&0\\1&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}} \tag{1.10}$$

The full hamiltonian is then given by:

$$\hat{H}=\sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}h_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}\qquad h_{\mathbf{k}}\equiv\begin{bmatrix}\epsilon_{\mathbf{k}}&-\Delta^{*}_{\mathbf{k}}\\-\Delta_{\mathbf{k}}&-\epsilon_{\mathbf{k}}\end{bmatrix} \tag{1.11}$$

Next step is to perform the well-known Bogoliubov transform and reduce all the problem down to a simple ensemble of quantum pseudospins.

1.3.1 Bogoliubov transform and pseudospins picture

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

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

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

$$\begin{aligned}\hat{n}_{\mathbf{k}\uparrow}+\hat{n}_{-\mathbf{k}\downarrow}&=\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}+\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow} &(1.12)\\ &=\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}-\hat{c}_{-\mathbf{k}\downarrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}+\mathbb{I}\\ &=\hat{\Psi}^{\dagger}_{\mathbf{k}}\tau^{z}\hat{\Psi}_{\mathbf{k}}+\mathbb{I} &(1.13)\end{aligned}$$

and then it follows

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

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

$$\mathbf{b}_{\mathbf{k}}\equiv\begin{bmatrix}-\text{Re}\{\Delta_{\mathbf{k}}\}\\-\text{Im}\{\Delta_{\mathbf{k}}\}\\\epsilon_{\mathbf{k}}-\mu\end{bmatrix} \tag{1.14}$$

[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.

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

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\in \mathrm{BZ}} \mathbf{b}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}} = \begin{bmatrix} \hat{s}^x_{\mathbf{k}} \\ \hat{s}^y_{\mathbf{k}} \\ \hat{s}^z_{\mathbf{k}} \end{bmatrix} \tag{1.15}$$

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

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

the general diagonalizer will be an orthogonal rotation matrix

$$\begin{aligned} W_{\mathbf{k}} &= e^{i\left(\theta_{\mathbf{k}} - \frac{\pi}{2}\right)\tau^y} e^{i\zeta_{\mathbf{k}}\tau^z} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \\ \cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} e^{i\zeta_{\mathbf{k}}} & \\ & e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\cos\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \\ \cos\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\sin\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \end{aligned} \tag{1.16}$$

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.

1.3.2 BCS ground state properties

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

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

Using Eq. (**??**),

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

where in the Fermi-Dirac function chemical potential was set to zero, because it already was included in the diagonalized hamiltonian. Recalling Eq. (**??**), it follows for $i = 1$, $j = 2$

$$\langle \hat{\phi}^\dagger_{\mathbf{k}} \rangle = [W_{\mathbf{k}}]_{11}[W^\dagger_{\mathbf{k}}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21}[W^\dagger_{\mathbf{k}}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.17}$$

$$= \frac{1}{2}\sin\left(2\theta_{\mathbf{k}}\right) e^{i2\zeta_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{1.18}$$

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

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

Similarly, for $i = 1$, $j = 1$

$$\langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \rangle = [W_{\mathbf{k}}]_{11} [W^\dagger_{\mathbf{k}}]_{11} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21} [W^\dagger_{\mathbf{k}}]_{12} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.19}$$

$$= \sin^2\theta_{\mathbf{k}} f\left(-E_{\mathbf{k}}; \beta, 0\right) + \cos^2\theta_{\mathbf{k}} f\left(E_{\mathbf{k}}; \beta, 0\right)$$

$$= \sin^2\theta_{\mathbf{k}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) + f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.20}$$

and for $i = 2$, $j = 2$

$$\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} \rangle = [W_{\mathbf{k}}]_{12} [W^\dagger_{\mathbf{k}}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{22} [W^\dagger_{\mathbf{k}}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.21}$$

$$= \cos^2\theta_{\mathbf{k}} f\left(-E_{\mathbf{k}}; \beta, 0\right) + \sin^2\theta_{\mathbf{k}} f\left(E_{\mathbf{k}}; \beta, 0\right)$$

$$= \cos^2\theta_{\mathbf{k}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) + f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.22}$$

Gap function. Eqns. (1.17), (1.18) 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

$$\Delta_{\mathbf{k}} \equiv \frac{1}{2} \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \frac{|\Delta_{\mathbf{k}'}|}{\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}} \exp\left\{i \arctan\left(\frac{\mathrm{Im}\{\Delta_{\mathbf{k}'}\}}{\mathrm{Re}\{\Delta_{\mathbf{k}'}\}}\right)\right\} \tanh\left(\frac{\beta}{2}\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}\right)$$

$$= \frac{1}{2} \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \frac{\Delta_{\mathbf{k}'}}{\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}} \tanh\left(\frac{\beta}{2}\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}\right) \tag{1.23}$$

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.

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

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

Proceed as previously, and from Eq. (1.13),

$$\langle \hat{n}_{\mathbf{k}\uparrow} \rangle + \langle \hat{n}_{-\mathbf{k}\downarrow} \rangle = 1 + \langle \hat{\Psi}^\dagger_{\mathbf{k}} \tau^z \hat{\Psi}_{\mathbf{k}} \rangle$$

$$= 1 + \left(|[W_{\mathbf{k}}]_{11}|^2 - |[W_{\mathbf{k}}]_{12}|^2\right) f\left(-E_{\mathbf{k}}; \beta, 0\right)$$

$$+ \left(|[W_{\mathbf{k}}]_{21}|^2 - |[W_{\mathbf{k}}]_{22}|^2\right) f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{1.24}$$

$$= 1 - \cos\left(2\theta_{\mathbf{k}}\right) \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{1.25}$$

coherently with Eqns. (1.20) and (1.22). 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. (1.24) directly on the diagonalization matrix of $h_{\mathbf{k}}$.

Ground state at zero temperature. Let $\beta \to +\infty$. The basic BCS grond state is well known and identical in the present discussion. It is easily obtained by considering the zero-temperature ground state of the pseudospin hamiltonian of Eq. (1.11),

$$|\mathrm{BCS}\rangle = \bigotimes_{\mathbf{k}} |2\theta_{\mathbf{k}}\rangle$$

where $|2\theta_{\mathbf{k}}\rangle$ is the up-state for the $\mathbf{k}$-th rotated pseudospin operator $\hat{\Gamma}^\dagger_{\mathbf{k}} \tau^z \hat{\Gamma}_{\mathbf{k}}$ (consider a diagram analogous to Fig. **??**). Said state can be expressed, making use of the non-rotated pseudospin operator $\hat{\Psi}^\dagger_{\mathbf{k}} \tau^z \hat{\Psi}_{\mathbf{k}}$ up and down states

$$\text{up: } |\Uparrow_{\mathbf{k}}\rangle \qquad \text{down: } |\Downarrow_{\mathbf{k}}\rangle$$

by the means of a simple Bloch's representation [Redo this computation...],

$$|2\theta_{\mathbf{k}}\rangle = \cos\theta_{\mathbf{k}}\,|\Downarrow_{\mathbf{k}}\rangle - \sin\theta_{\mathbf{k}}\,|\Uparrow_{\mathbf{k}}\rangle$$

[To be continued...]

Evidently it holds, in the rotated frame,

$$\left[\hat{\Psi}^{\dagger}_{\mathbf{k}}\tau^{z}\hat{\Psi}_{\mathbf{k}} + \mathbb{I}\right]|\Uparrow_{\mathbf{k}}\rangle = 2\,|\Uparrow_{\mathbf{k}}\rangle$$

1.3.3 Renormalization of the bare bands

We now deal with the renormalization of bare bands anticipated in Sec. 1.2.2. Taking together Eqns. (1.9), (1.17) and (1.18) we get:

$$\begin{aligned} V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} + \text{h.c.}\right] &= \frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\left[\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right)\right] \\ &\times\left[\left(\sin^2\theta_{\mathbf{q}}\tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) + f\left(E_{\mathbf{q}};\beta,0\right)\right)\hat{c}^{\dagger}_{\mathbf{q}'\uparrow}\hat{c}_{\mathbf{q}'\uparrow}\right. \\ &\left. + \left(1-\cos^2\theta_{-\mathbf{q}}\tanh\left(\frac{\beta E_{-\mathbf{q}}}{2}\right) - f\left(E_{-\mathbf{q}};\beta,0\right)\right)\hat{c}^{\dagger}_{\mathbf{q}'\downarrow}\hat{c}_{\mathbf{q}'\downarrow}\right] \end{aligned} \tag{1.26}$$

Spatial inversion symmetry guarantees

$$\cos^2\theta_{-\mathbf{q}} = \cos^2\theta_{\mathbf{q}} \quad \text{as well as} \quad E_{-\mathbf{q}} = E_{\mathbf{q}}$$

By simple algebraic manipulation is easy to see:

$$\begin{aligned} 1-\cos^2\theta_{\mathbf{q}}\tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) - f\left(E_{\mathbf{q}};\beta,0\right) &= \sin^2\theta_{\mathbf{q}}\tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) + 1 - \tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) - f\left(E_{\mathbf{q}};\beta,0\right) \\ &= \sin^2\theta_{\mathbf{q}}\tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) + f\left(E_{\mathbf{q}};\beta,0\right) \end{aligned}$$

Since

$$\begin{aligned} \sin^2\theta_{\mathbf{q}} &= \frac{1-\cos(2\theta_{\mathbf{q}})}{2} \\ &= \frac{1}{2} - \frac{\xi_{\mathbf{q}}}{2\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2}} \end{aligned}$$

Let now:

$$g_{\mathbf{q}} \equiv \left[\frac{1}{2} - \frac{\xi_{\mathbf{q}}}{2\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2}}\right]\tanh\left(\frac{\beta}{2}\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2}\right) + f\left(\sqrt{\xi^2_{\mathbf{q}} + |\Delta_{\mathbf{q}}|^2};\beta,0\right) \tag{1.27}$$

Thus,

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} + \text{h.c.}\right] = \frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right)\right]g_{\mathbf{q}}\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}$$

Recall now the result of Eq. (**??**),

$$\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right) = \frac{1}{2}\sum_{\gamma}\varphi^{(\gamma)}_{\mathbf{q}}\varphi^{(\gamma)*}_{\mathbf{q}'} \quad \text{for } \gamma \in \{s^*, p_x, p_y, d_{x^2-y^2}\}$$

which gives (sum over γ is intended within the aforementioned symmetries)

$$\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right)\right]g_{\mathbf{q}}\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma} = \frac{V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma,\gamma}\varphi^{(\gamma)}_{\mathbf{q}}\varphi^{(\gamma)*}_{\mathbf{q}'}g_{\mathbf{q}}\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma} \tag{1.28}$$

Evidently from Eq. (1.27), $g_{\mathbf{q}}$ is an even function of the momentum, a feature that ensures

$$\frac{1}{L_xL_y}\sum_{\mathbf{q}}\varphi^{(p_\ell)}_{\mathbf{q}}g_{\mathbf{q}} = 0 \quad \text{for } \ell \in \{x, y\}$$

General result. Let us now divide the discussion in two parts. First, let us deal with the theoretical general result of the above calculations. Define the s^* and $d_{x^2-y^2}$ components as

$$g^{(s^*)} \equiv \frac{1}{L_x L_y}\sum_{\mathbf{q}}(\cos q_x + \cos q_y) g_{\mathbf{q}} \qquad g^{(d)} \equiv \frac{1}{L_x L_y}\sum_{\mathbf{q}}(\cos q_x - \cos q_y) g_{\mathbf{q}}$$

and from Eq. (1.28) we get the final form

$$\frac{2V}{L_x L_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos(\delta q_x) + \cos(\delta q_y)\right] g_{\mathbf{q}} \hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma} = V\sum_{\mathbf{q}\sigma}\left[g^{(s^*)}(\cos q_x + \cos q_y) + g^{(d)}(\cos q_x - \cos q_y)\right]\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma} \tag{1.29}$$

This equation reduces fully the initial o.s. Fock component of $\hat{H}_V$ to a simpler, decoupled form. Here, similarly to what we observed for AF phase in Sec. **??**, the bare bands are renormalized,

$$\tilde{\epsilon}_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} + V\left[g^{(s^*)}(\cos q_x + \cos q_y) + g^{(d)}(\cos q_x - \cos q_y)\right] \tag{1.30}$$

As is done in next paragraph, the s^* is actually a rigid t renormalization, which however requires a little care.

Pure x-wave superconductivity. As long as we work in a precise sector ($s \oplus s^*$ as well as $d_{x^2-y^2}$) with a gap function completely contained in said symmetry sector, we can rule out the $d_{x^2-y^2}$-wave component of $g_{\mathbf{q}}$ from Eq. (1.30)

$$\frac{1}{L_x L_y}\sum_{\mathbf{q}}\varphi^{(d)}_{\mathbf{q}} g_{\mathbf{q}} = 0$$

The result above is valid only if $\Delta_{\mathbf{q}}$ is described only by a single symmetry harmonics. This is because under a rotation of angle $\pi/2$ the two functions behave differently:

$$(q_x, q_y) \to (-q_y, q_x) \quad : \quad \begin{cases} \varphi^{(d)}_{\mathbf{q}} \to -\varphi^{(d)}_{\mathbf{q}} \\ g_{\mathbf{q}} \to g_{\mathbf{q}} \end{cases}$$

The only remainder of Eq. (1.30) is its s^* part

$$\tilde{\epsilon}_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} + V g^{(s^*)}(\cos q_x + \cos q_y) \tag{1.31}$$

and since $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ we obtain an equation essentially identical to the one expressing the hopping renormalization in the AF phase, Eq. (**??**). Indeed, let $w \equiv g^{(s^*)}/2$ be the new HF parameter, we get

$$\tilde{t} \equiv t - wV \tag{1.32}$$

Once again the hopping parameter shift is rigid and controlled directly by V.

1.4 Results of the HF algorihtm

[To be continued...]

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