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(s) of freedom
HF	Hartree-Fock
HFP(s)	Hartree-Fock parameter(s)
LRT	Linear Response Theory
MFT	Mean-Field Theory
NN(s)	Nearest neighbor(s)
RWC(s)	Relevant Wick's contraction(s)
RMP(s)	Renormalized model parameter(s)
SC	Superconductor
SSB	Spontaneous symmetry breaking
T_c	Critical temperature

Chapter 1

The normal phase

This chapter is devoted to the MFT analysis of the "normal phase", which is, the one where interacting electrons do not develop an antiferromagnetic or superconducting gap, although undergoing an effective non-trivial transformation. What will be derived here, in particular the hopping renormalization effect, constitutes a peculiarity of effective MFT treatment of the EHM and will be the groundwork of following analyses. Note that this chapter is structured in such a way that what is derived here mathematically is recovered and expanded to more complex phases in next chapters.

1.1 Theoretical description of the "normal" phase

The normal phase is simply the one where no symmetry is broken, and the many-body ground state preserves the entire U(2) structure of Eq. (**??**) as well as translational symmetry. Thus, the normal phase is essentially given by the null gap limit of both the antiferromagnetic and superconducting phases. By discussing it separately now, we highlight a MFT feature of the EHM of particular interest. From Tabs. **??** and **??**, we know that the relevant Wick's contractions (RWCs) for this phase are

$\hat{H}_U$	Hartree contraction
$\hat{H}_V$ (o.s. sector)	Hartree contraction
$\hat{H}_V$ (s.s. sector)	Hartree and Fock contractions

and since the phase we are establishing obeys translational symmetry, we also know Hartree terms are essentially chemical potential shifts. Next section derives this effect in detail.

1.1.1 Hartree shift of μ

In the context of numerical simulations at fixed density, the chemical potential is determined self-consistently; thus any net effect that shifts μ is effectively ignored within the iterative algorithm. For the sake of completeness, we hereby derive the effect analytically.

Local repulsion. In the normal phase, the local repulsion $\hat{H}_U$ only contributes through Hartree-like RWCs,

$$\hat{H}_U \simeq U \sum_i [\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle - \langle \hat{n}_{i\downarrow} \rangle \langle \hat{n}_{i\uparrow} \rangle]$$

For a translationally invariant phase such as the normal phase, it holds

$$\langle \hat{n}_{i\sigma} \rangle = n \tag{1.1}$$

which gives immediately

$$\begin{aligned} \hat{H}_U &\simeq nU \sum_i [\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}] - U \sum_i n^2 \\ &= nU \times \hat{N} - E^{(\mathrm{N})}_{\mathrm{H}/U} \end{aligned}$$

being $\hat{N}$ the total number operator and $E^{(\mathrm{N})}_{\mathrm{H}/U}$ the "contraction energy" (also known as double counting term) due to the Hartree (H) contraction of the U repulsion,

$$E^{(\mathrm{N})}_{\mathrm{H}/U} = nU \times L_x L_y \tag{1.2}$$

which correctly is a linearly extensive quantity. The chemical potential is corrected by

$$\mu \to \mu - nU \tag{1.3}$$

The non-local attraction further corrects μ.

Non-local attraction. Let us break down $\hat{H}_V$ isolating its Hartree RWCs in both o.s. and s.s. sectors:

$$\hat{H}_V \simeq \overbrace{-V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{n}_{i\sigma} \rangle \hat{n}_{j\sigma} + \hat{n}_{i\sigma} \langle \hat{n}_{j\sigma} \rangle - \langle \hat{n}_{i\sigma} \rangle \langle \hat{n}_{j\sigma} \rangle \right]}^{\text{s.s.}} \underbrace{-V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{n}_{i\sigma} \rangle \hat{n}_{j\bar{\sigma}} + \hat{n}_{i\sigma} \langle \hat{n}_{j\bar{\sigma}} \rangle - \langle \hat{n}_{i\sigma} \rangle \langle \hat{n}_{j\bar{\sigma}} \rangle \right]}_{\text{o.s.}} + (\text{all the rest})$$

where "all the rest" collects all non-Hartree RWCs. Recalling the Ansatz of Eq. (1.1), we get

$$\hat{H}_V \simeq \underbrace{-nV \sum_{\langle ij \rangle} \sum_{\sigma} \left[\hat{n}_{j\sigma} + \hat{n}_{i\sigma} \right]}_{\text{s.s.}} \underbrace{-nV \sum_{\langle ij \rangle} \sum_{\sigma} \left[\hat{n}_{j\bar{\sigma}} + \hat{n}_{i\sigma} \right]}_{\text{o.s.}} - E^{(\mathrm{N})}_{\mathrm{H}/V} + (\text{all the rest})$$

with $E^{(\mathrm{N})}_{\mathrm{H}/V}$ the normal state shift to energy brought by $\hat{H}_V$,

$$E^{(\mathrm{N})}_{\mathrm{H}/V} = 2V \sum_{\langle ij \rangle} \sum_{\sigma} n^2 = 4n^2 V \times \frac{z}{2} L_x L_y \tag{1.4}$$

being $z = 4$ the coordination number for the 2D square lattice. Now, evidently both sums above are just a number operator,

$$\hat{H}_V \simeq -2nzV \times \hat{N} + (\text{all the rest})$$

This accounts for the final Hartree shift of μ,

$$\mu \to \mu + 2znV \tag{1.5}$$

Thus, when considering the net shift to μ due to both interactions combining Eqns. (1.3), (1.5), we get

$$\tilde{\mu} \equiv \mu + n(2zV - U) \tag{1.6}$$

This result remains valid in all phases discussed in this text: for the AF phase, the SDW character leaves this shift untouched, while the superconducting phase we are discussion is inherently translational invariant.

1.1.2 Fock hopping renormalization in the normal phase

The most relevant effect brought by the presence of $\hat{H}_V$ is hopping renormalization. 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. Let us focus only on this term when decomposing $\hat{H}$:

$$\hat{H}_V \simeq V \sum_{\langle ij \rangle} \sum_{\sigma} \left[\langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \rangle \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} + \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \langle \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \rangle - \langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} \rangle \langle \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \rangle \right] + (\text{all the rest}) \tag{1.7}$$

(note the + sign in front of the displayed term). 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 all phases considered in the present discussion, 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") given in Tab. **??** and depicted in Fig. **??**. This gives in turn that the hopping shift is rigid and the bands are rigidly renormalized by a self consistent parameter $w^{(\mathrm{N})}$,

$$t \to \tilde{t} \equiv t - w^{(\mathrm{N})}V \quad \Longrightarrow \quad \epsilon_{\mathbf{k}} \to \tilde{\epsilon}_{\mathbf{k}} = -2\tilde{t}\,(\cos k_x + \cos k_y)$$

The effective diffusive hamiltonian is given by

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

In reciprocal space, the effective hopping must be transformed as well. Consider the Fourier Transform $\mathcal{F}$ given in Eq. (**??**), applied to the displayed part of Eq. (1.7),

$$\begin{aligned}&V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle - \langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right] \\ &\qquad \overset{\mathcal{F}}{=} \frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\sum_{\sigma}\left[\cos(\delta k_x) + \cos(\delta k_y)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma}\rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma} - E^{(\mathrm{N})}_{\mathrm{F}/V} \quad (1.8)\end{aligned}$$

Here, the 2 prefactor comes from recognizing that the first two operators in square brackets in the first line generate identical contributions to the full sum; the double counting energy shift is given by

$$E^{(\mathrm{N})}_{\mathrm{F}/V} \equiv \frac{V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\sum_{\sigma}\left[\cos(\delta k_x) + \cos(\delta k_y)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma}\rangle\langle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma}\rangle \quad (1.9)$$

Up to this point, this derivation is general and will be re-used in next chapters. Here the specificity of the physical phase settles in: if we assume the normal state to be a free degenerate Fermi gas with renormalized bands, we get

$$\langle \hat{c}_{\mathbf{k}_1\sigma_1}\hat{c}_{\mathbf{k}_2\sigma_2}\rangle = \delta_{\mathbf{k}_1=\mathbf{k}_2}\delta_{\sigma_1=\sigma_2}f(\tilde{\epsilon}_{\mathbf{k}};\beta,\tilde{\mu})$$

being f the Fermi-Dirac distribution,

$$f(\epsilon;\beta,\mu) \equiv \frac{1}{e^{\beta(\epsilon-\mu)}+1}$$

It follows that Eq. (1.8) becomes

$$\begin{aligned}&V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle - \langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right] \\ &\qquad \overset{\mathcal{F}}{=} \frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k}}\sum_{\sigma}\left[\cos(2k_x) + \cos(2k_y)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}\sigma}\rangle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}\sigma} - E^{(\mathrm{N})}_{\mathrm{F}/V} \quad (1.10)\end{aligned}$$

since the only contribution comes from $\mathbf{k}' = -\mathbf{k}$. Let now $\mathbf{q} \equiv \mathbf{K} + \mathbf{k}$, $\mathbf{q}' \equiv \mathbf{K} - \mathbf{k}$. Being for $\ell = x, y$

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

Operator	Sector	RWCs	Net effect
$\hat{H}_U$		Hartree	μ shift
$\hat{H}_V$	o.s.	Hartree	μ shift
$\hat{H}_V$	s.s.	Hartree	μ shift
		Fock	t shift

Table 1.1

we reduce Eq. (1.8) to

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\Big[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\Big]$$
$$\overset{\mathcal{F}}{=}\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.11}$$

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

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

Thanks to this handy property, we reduce Eq. (1.11) to

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\Big[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\Big]$$
$$\overset{\mathcal{F}}{=}\sum_{\gamma}\left[\frac{1}{L_xL_y}\sum_{\mathbf{q}}\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\right]\times V\sum_{\mathbf{q}'}\varphi^{(\gamma)*}_{\mathbf{q}'}\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.12}$$

Now, the bare bands $\epsilon_{\mathbf{k}}$ as well as their rigidly renormalized version $\tilde{\epsilon}_{\mathbf{k}}$ are s^*-wave symmetric. The expectation value $\langle\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle=f(\tilde{\epsilon}_{\mathbf{q}};\beta,\tilde{\mu})$ thus exhibits the same symmetry. Then, in Eq. (1.12), due to the presence of the part in square brackets, only $\gamma=s^*$ contributes. Let us define the HFP $w^{(\mathrm{N})}$ as

$$w^{(\mathrm{N})}\equiv\frac{1}{2L_xL_y}\sum_{\mathbf{q}\in\mathrm{BZ}}\left(\cos q_x+\cos q_y\right)f(\tilde{\epsilon}_{\mathbf{q}};\beta,\tilde{\mu})\tag{1.13}$$

which finally gives

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\Big[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\Big]$$
$$\overset{\mathcal{F}}{=}\sum_{\mathbf{q}'}2w^{(\mathrm{N})}V\left(\cos q_x+\cos q_y\right)\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.14}$$

As anticipated, hopping gets shifted by an amount

$$t\to\tilde{t}\equiv t-w^{(\mathrm{N})}V\tag{1.15}$$

with $w^{(\mathrm{N})}$ to be self-consistently determined by iteratively solving Eq. (1.13).

1.2 Free energy density

[To be continued...]

1.3 HF results

[To be continued...]

Chapter 2

Anti-Ferromagnetic instability

This chapter is devoted to an in-depth discussion of the antiferromagnetic (AF) long-range ordering in the EHM by the means of MFT. In the context of the 2D Hubbard model (HM), discussed in App. **??**, AF ordering establishes as an unconventional metallic phase which is only stable at half-filling (as is discussed in Sec. [Missing]). The situation for the EHM is similar: the present analysis is carried out based on the argument that, given the symmetry structure of the non-local NN interaction, the fundamental features of the commensurate AF phase of the HM are effectively preserved, while the parameters are redefined by the interaction itself. The two most relevant effects we discuss in this chapter are the "magnetization boost" (Sec. [Missing]) and the "hopping renormalization" (Sec. [Missing]), the latter being a general feature of the EHM common to all phases preserving (or, at most, weakening without destroying) the translational invariance, discussed in Sec. 1.1.2.

2.1 Sketch and general features of the MFT solution

[To be continued...]

2.1.1 Symmetry considerations for the AF phase

[To be continued...]

2.1.2 Antiferromagnetism in the conventional Hubbard model

Within the Hubbard model, the antiferromagnetic phase (AF) is 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 and reduces the hamiltonian to the form of Eq. (**??**) (ignoring the double-counting terms)

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

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

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

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 $\pm E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}$. The entire system is mapped onto an ensemble of pseudo-spins, each subject to a pseudo-field, as in Fig. 2.1. 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:

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^x\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\theta_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{2.1}$$

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^y\hat{\Psi}_{\mathbf{k}\sigma}\rangle = 0 \tag{2.2}$$

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Psi}_{\mathbf{k}\sigma}\rangle = -\cos(2\theta_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{2.3}$$

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

$$\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle = \frac{1}{2}\left[f\left(-E_{\mathbf{k}};\beta,\mu\right) - f\left(E_{\mathbf{k}};\beta,\mu\right)\right] \tag{2.4}$$

Of these properties, to pseudospin picture is a simple and powerful tool that our MFT discussion should preserve.

2.1.3 Extension to the EHM

Consider now the non-local interaction $\hat{H}_V$: since only translational invariance is partially broken in the AF phase, the only relevant contributions coming from Wick's decomposition are Hartree terms and the same-spin Fock term. The discussion is thus essentially the same as for the normal phase of Chap. 1, with the only relevant difference being the Ansatz we use in Eq. (1.1), substituted by the commensurate oscillatory Ansatz of Eq. (**??**). As for the normal phase, by design the MFT solution to the model for the given phase is described by a redefinition of the various physical quantities and mathematical objects,

$$t \to \tilde{t} \qquad \epsilon_{\mathbf{k}} \to \tilde{\epsilon}_{\mathbf{k}\sigma} \qquad E_{\mathbf{k}} \to \tilde{E}_{\mathbf{k}\sigma} \qquad \Delta_\sigma \to \tilde{\Delta}_{\mathbf{k}\sigma} \qquad \mu \to \tilde{\mu}$$

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 (the *tilde* sign indicates the renormalized quantity):

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^x\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\tilde{\theta}_{\mathbf{k}})\sin(2\tilde{\zeta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{2.5}$$

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^y\hat{\Psi}_{\mathbf{k}\sigma}\rangle = \sin(2\tilde{\theta}_{\mathbf{k}})\cos(2\tilde{\zeta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{2.6}$$

$$\langle\hat{\Psi}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Psi}_{\mathbf{k}\sigma}\rangle = -\cos(2\tilde{\theta}_{\mathbf{k}})\langle\hat{\Gamma}^\dagger_{\mathbf{k}\sigma}\tau^z\hat{\Gamma}_{\mathbf{k}\sigma}\rangle \tag{2.7}$$

with:

$$\sin(2\tilde{\xi}_{\mathbf{k}}) = \frac{\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\}}{|\tilde{\Delta}_{\mathbf{k}}|} \qquad \cos(2\tilde{\xi}_{\mathbf{k}}) = \frac{\mathrm{Im}\{\tilde{\Delta}_{\mathbf{k}}\}}{|\tilde{\Delta}_{\mathbf{k}}|} \qquad \sin(2\tilde{\theta}_{\mathbf{k}}) = \frac{|\tilde{\Delta}_{\mathbf{k}}|}{\tilde{E}_{\mathbf{k}}} \qquad \cos(2\tilde{\theta}_{\mathbf{k}}) = \frac{\tilde{\epsilon}_{\mathbf{k}}}{\tilde{E}_{\mathbf{k}}} \tag{2.8}$$

The physical behavior is the same as for the pure Hubbard model. In terms of MFT discussion, the AF phase is similar enough to the normal phase of Chap. 1: the RWCs are the same of Sec. 1.1, listed in Tabs. **??** and **??**. All three Hartree contractions, responsible in the normal phase of the chemical potential shift, and the s.s. Fock contraction, that originated the hopping renormalization. Let us start by the Hartree terms: due to the "staggered" nature of the commensurate AF phase, their role is here more complex. Then we will move to the Fock term, discussing the MFT approximations effect on bands. Next sections are basically an extension of the calculations of Chap. 1.

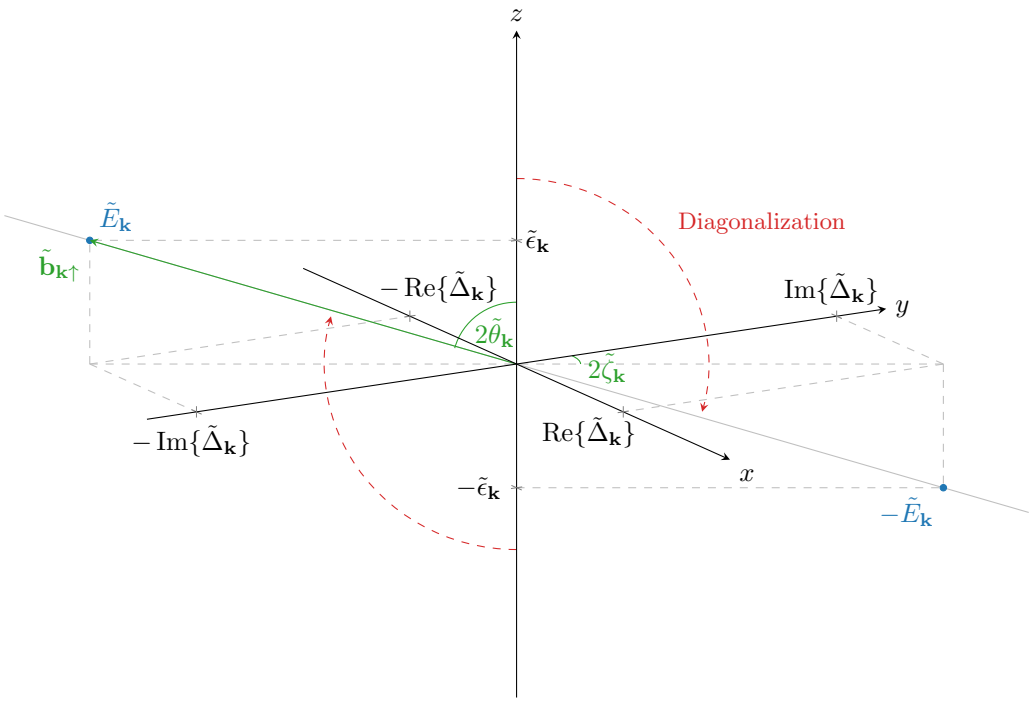


Figure 2.1 | Sketch of the diagonalization of the pseudo-spin problem. The dashed line represents the diagonalization given by the z-axis alignment with the field direction. In the top-right side of the picture are listed the expectation values of the original Nambu spinor.

2.2 Hartree effects: renormalization of chemical potential and gap

As in Eq. (**??**), the same-spin and opposite-spin non-local Hartree terms are

$$\hat{H}_V \simeq \overbrace{-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\sigma}+\hat{n}_{i\sigma}\langle\hat{n}_{j\sigma}\rangle-\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\sigma}\rangle\right]}^{\text{s.s.}} \underbrace{-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\bar{\sigma}}+\hat{n}_{i\sigma}\langle\hat{n}_{j\bar{\sigma}}\rangle-\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\bar{\sigma}}\rangle\right]}_{\text{o.s.}}+(\text{all the rest})$$

Let $i\to\mathbf{r}=(x,y)$ and $j\to\mathbf{r}'=(x',y')$. The key difference in the present derivation, with respect to the normal phase, is the single-site density Ansatz: instead of Eq. (1.1), we use Eq. (**??**), which describes an oscillatory density for each spin sector,

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

This Ansatz is composed of two parts: the offset n, and the oscillatory part m. The algebraic derivation relative to the n part is, of course, the same as for the normal phase. We now treat separately the "operatorial" part of the braced terms of Eq. (**??**),

$$-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\sigma}+\hat{n}_{i\sigma}\langle\hat{n}_{j\sigma}\rangle\right]-V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{n}_{i\sigma}\rangle\hat{n}_{j\bar{\sigma}}+\hat{n}_{i\sigma}\langle\hat{n}_{j\bar{\sigma}}\rangle\right] \tag{2.9}$$

as well as the its scalar counterpart

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\sigma}\rangle+V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\bar{\sigma}}\rangle \tag{2.10}$$

which accounts for the energy shift to be accounted when performing Wick's contractions.

2.2.1 Operatorial part and mapping on the gapped AF hamiltonian

Let us start from the operator of Expr. (2.9). By inserting the Ansatz of Eq. (**??**), we get

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

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

$$\overbrace{-nV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\sigma}]}^{\text{s.s. (density)}}+\overbrace{mV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}[\hat{n}_{\mathbf{r}\sigma}-\hat{n}_{\mathbf{r}'\sigma}]}^{\text{s.s. (magnetization)}}$$
$$\underbrace{-nV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}]}_{\text{o.s. (density)}}+\underbrace{mV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}]}_{\text{o.s. (magnetization)}} \tag{2.11}$$

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

Density terms. Consider the s.s. and o.s. (density) terms of Expr. (2.11), reintronducing the double counting energy shift

$$-nV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\sigma}]-nV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}] \tag{2.12}$$

The discussion is identical to the one of Sec. 1.1.1 for the normal phase, with the renormalization of μ being the same of Eq. (1.6).

$$\tilde{\mu}\equiv\mu+n(2zV-U) \tag{2.13}$$

Within this equation we are also already implicitly considering the μ shift effect due to $\hat{H}_U$.

Magnetization terms. The s.s. and o.s. (magnetization) terms of Expr. (2.11) are to be reduced to a renormalization of the gap function. Explicitly,

$$mV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}[\hat{n}_{\mathbf{r}\sigma}-\hat{n}_{\mathbf{r}'\sigma}]+mV\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\sum_{\sigma}(-1)^{x+y+\delta_{\sigma=\uparrow}}[\hat{n}_{\mathbf{r}\sigma}+\hat{n}_{\mathbf{r}'\overline{\sigma}}]$$
$$=-2zmV\sum_{\mathbf{r}}(-1)^{x+y}[\hat{n}_{\mathbf{r}\uparrow}-\hat{n}_{\mathbf{r}\downarrow}] \tag{2.14}$$

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

$$\Delta\to\Delta+2zmV+(\text{s.s. contribution}) \tag{2.15}$$

Let us now move to the last part of the Hartree effects on the AF phase originated by $\hat{H}_V$, which is, the energy shift due to double counting terms originated by MFT decomposition of the quartic interactions $\hat{H}_U$ and $\hat{H}_V$.

2.2.2 Double counting terms: energy shift due to contractions

Let us now focus on the scalar Expr. (2.10): it's the sum of two parts, the first coming from s.s. sector, the second from o.s. sector.

s.s. sector double counting energy. For the s.s. part, explicitating the two spin sectors, we get

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\sigma}\rangle = \overbrace{V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\Big[(n-(-1)^{x+y}m)(n-(-1)^{x'+y'}m)\Big]}^{\sigma=\uparrow} + \underbrace{V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\Big[(n+(-1)^{x+y}m)(n+(-1)^{x'+y'}m)\Big]}_{\sigma=\downarrow}$$

Evidently the mixed terms (those of order $\mathcal{O}(n)\times\mathcal{O}(m)$) cancel out, and considering that the sign factor is necessarily alternating on neighboiring site, the remainder is just

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\sigma}\rangle = V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}2(n^2-m^2)$$

o.s. sector double counting energy. Proceeding identically on the o.s. sector, we get

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\bar{\sigma}}\rangle = \overbrace{V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\Big[(n-(-1)^{x+y}m)(n+(-1)^{x'+y'}m)\Big]}^{\sigma=\uparrow} + \underbrace{V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}\Big[(n+(-1)^{x+y}m)(n-(-1)^{x'+y'}m)\Big]}_{\sigma=\downarrow}$$

which gives immediately

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\langle\hat{n}_{i\sigma}\rangle\langle\hat{n}_{j\bar{\sigma}}\rangle = V\sum_{\langle \mathbf{r}\mathbf{r}'\rangle}2(n^2+m^2)$$

Hence, the total "contraction energy", given by the sum of both contributions, is identical to the normal one of Eq. (1.4) indeed:

$$E^{(\mathrm{AF})}_{\mathrm{H}/V} = 2V\sum_{\langle ij\rangle}\sum_{\sigma}n^2 = 4n^2V\times\frac{z}{2}L_xL_y \tag{2.16}$$

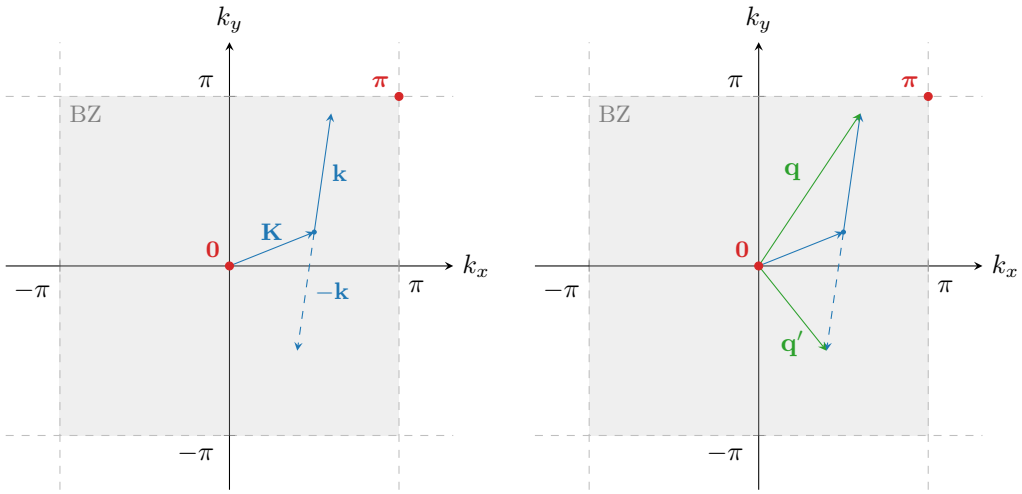
This implies that, when comparing normal and AF phase, we can rule out this energy contribution, being equal for both free energy densities.

2.3 Fock effects: renormalization of the hopping parameter

Let us now move to the effects originated by Fock contractions. We can use the derivation of Sec. 1.1.2 up to Eq. (1.10),

$$\begin{aligned}V\sum_{\langle ij\rangle}\sum_{\sigma}&\Big[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\Big]\\ &\overset{\mathcal{F}}{=}\frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k}}\sum_{\sigma}\left[\cos(2k_x)+\cos(2k_y)\right]\langle\hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}\sigma}\rangle\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}\sigma}-E^{(\mathrm{AF})}_{\mathrm{F}/V}\end{aligned} \tag{2.17}$$

where $E^{(\mathrm{AF})}_{\mathrm{F}/V}$ is defined as in Eq. (1.9), with the expecatation value being computed on the AF (thermal) ground-state. As before, we discuss the operatorial part and the scalar part separately.



a | Generic vectors. b | Change of variables.

Figure 2.2 | Representation of the vectors involved in the diagonal terms of Eq. (**??**). In Fig. 2.2a generic vectors are considered, cycling over all values of $\mathbf{K}, \mathbf{k} \in \mathrm{BZ}$. In Fig. 2.2b is depicted the variables change to the new vectors $\mathbf{q}, \mathbf{q}'$.

2.3.1 Operatorial part and mapping on the gapped AF hamiltonian

In order to proceed from Eq. (2.17), it is 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

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

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 $\mathbf{k} \in \mathrm{MBZ}$, $\sigma \in \{\uparrow, \downarrow\}$. 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. (**??**), this implies only two contributions are non-zero:

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

Then Eq. (2.17) is reduced to:

$$(\cdots) \overset{\mathcal{F}}{=} \frac{2V}{L_x L_y} \sum_{\mathbf{K},\mathbf{k}} \sum_{\sigma} \left[\cos(2k_x) + \cos(2k_y)\right] \left[\underbrace{\langle \hat{c}^{\dagger}_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}\sigma} \rangle \hat{c}^{\dagger}_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}\sigma}}_{\text{Diagonal terms}} - \underbrace{\langle \hat{c}^{\dagger}_{\mathbf{K}+\mathbf{k}\sigma} \hat{c}_{\mathbf{K}+\mathbf{k}+\boldsymbol{\pi}\sigma} \rangle \hat{c}^{\dagger}_{\mathbf{K}-\mathbf{k}\sigma} \hat{c}_{\mathbf{K}-\mathbf{k}-\boldsymbol{\pi}\sigma}}_{\text{Off-diagonal terms}} \right] \tag{2.18}$$

Now, the above equation presents *diagonal* and *off-diagonal* terms.

Diagonal terms. The diagonal terms of Eq. (2.18) are simple density interactions with the mean density field. Consider Fig. 2.2a: 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. 2.2b. Apply in the diagonal part of Eq. (2.18) this variables change (which is the same of Eq. (1.11))

$$\begin{aligned}\frac{2V}{L_x L_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}&\left[\cos\left(2k_x\right)+\cos\left(2k_y\right)\langle\hat{c}^{\dagger}_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}\sigma}\rangle\hat{c}^{\dagger}_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}\sigma}\right.\\ &=\frac{2V}{L_x L_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}\\ &\overset{*}{=}\sum_{\gamma,\sigma}\left[\frac{1}{L_x L_y}\sum_{\mathbf{q}}\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\right]\times V\sum_{\mathbf{q}'}\varphi^{(\gamma)*}_{\mathbf{q}'}\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}\end{aligned}\tag{2.19}$$

where the sign $\overset{*}{=}$ indicates that we have substituted the decomposition of Eq. (**??**). Define the expectation value

$$g_{\mathbf{q}\sigma}\equiv\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle$$

The expression in square brackets of Eq. (2.19) is just its γ component, and is expanded in

$$\begin{aligned}g^{(\gamma)}&=\frac{1}{L_x L_y}\sum_{\mathbf{q}\in\mathrm{BZ}}\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\\ &=\frac{1}{L_x L_y}\sum_{\mathbf{q}\in\mathrm{MBZ}}\left[\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle+\varphi^{(\gamma)}_{\mathbf{q}+\boldsymbol{\pi}}\langle\hat{c}^{\dagger}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\hat{c}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\rangle\right]\\ &=\frac{1}{L_x L_y}\sum_{\mathbf{q}\in\mathrm{MBZ}}\varphi^{(\gamma)}_{\mathbf{q}}\left[\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle-\langle\hat{c}^{\dagger}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\hat{c}_{\mathbf{q}+\boldsymbol{\pi}\sigma}\rangle\right]\\ &=\frac{1}{L_x L_y}\sum_{\mathbf{q}\in\mathrm{MBZ}}\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{\Psi}^{\dagger}_{\mathbf{q}\sigma}\tau^{z}\hat{\Psi}_{\mathbf{q}\sigma}\rangle\\ &=-\frac{1}{2L_x L_y}\sum_{\mathbf{q}\in\mathrm{MBZ}}\varphi^{(\gamma)}_{\mathbf{q}}\frac{\tilde{\epsilon}_{\mathbf{q}}}{\tilde{E}_{\mathbf{q}}}\left[f\left(-\tilde{E}_{\mathbf{q}};\beta,\tilde{\mu}\right)-f\left(\tilde{E}_{\mathbf{q}};\beta,\tilde{\mu}\right)\right]\end{aligned}$$

where, in the last passage, Eqns. (2.3) and (2.4) have been used. Now, the AF phase does not break inversion symmetry: this implies that, whatever the shape of the renormalized bands, it must be

$$\tilde{\epsilon}_{\mathbf{q}}=\tilde{\epsilon}_{-\mathbf{q}}\quad\Longrightarrow\quad g^{(p_\ell)}=0\quad\text{with}\quad\ell\in\{x,y\}$$

The renormalized bands need to be a symmetric function of the moment. Hence for $\gamma\in\{p_x,p_y\}$ the above sum vanishes. Thus, Eq. (2.19) becomes

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

These two factors, together, define the full bands renormalization

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

The s^*-wave component is particularly handy, because if we let:

$$w^{(\mathrm{AF})}\equiv\frac{g^{(s^*)}}{2}\tag{2.20}$$

we can interpret part of the bands renormalization as a rigid hopping shift,

$$\tilde{t}\to t-w^{(\mathrm{AF})}V$$

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. 2.3. 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. (**??**) gives a non-null contribution, reducing the latter to

$$\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle \hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle \hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}$$
$$= \frac{V}{L_xL_y}\sum_{\mathbf{q}'\sigma}\left(\cos q'_x+\cos q'_y\right)\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}\sum_{\mathbf{q}}\left(\cos q_x+\cos q_y\right)\langle \hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle \tag{2.21}$$

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

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

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:

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

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

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

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:

$$\begin{aligned} w^{(\mathbf{0})} &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}}\left(\cos k_x+\cos k_y\right)\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle \\ &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}-\hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\rangle \\ &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow}\tau^z\hat{\Psi}_{\mathbf{k}\uparrow}\rangle \\ &= -\frac{1}{4L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\frac{\tilde{\epsilon}_{\mathbf{k}}}{\tilde{E}_{\mathbf{k}}}\left[f\left(-\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)-f\left(\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)\right] \end{aligned} \tag{2.22}$$

where in the second passage the sign change is due to the presence of the structure factor, and in the fourth passage Eq. (2.7) and the relations (2.8) have been used. It follows, finally, that the hopping parameter gets effectively renormalized:

$$\tilde{t} \equiv t - w^{(\mathbf{0})}V \tag{2.23}$$

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. (**??**). 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. 2.2b, and rewrite

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

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

$$-\frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k}}\sum_{\sigma}\left[\cos\left(2k_x\right)+\cos\left(2k_y\right)\right]\langle\hat{c}^{\dagger}_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}+\boldsymbol{\pi}\sigma}\rangle\hat{c}^{\dagger}_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}-\boldsymbol{\pi}\sigma}$$
$$=-2V\left[\frac{1}{2L_xL_y}\sum_{\mathbf{k}'}\left(\cos k'_x+\cos k'_y\right)\langle\hat{c}^{\dagger}_{\mathbf{k}'\sigma}\hat{c}_{\mathbf{k}'+\boldsymbol{\pi}\sigma}\rangle\right]\sum_{\mathbf{k}\sigma}\left(\cos k_x+\cos k_y\right)\hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma}\qquad(2.24)$$

Because of this, the x component of the pseudo-magnetic field – the gap already renormalized by Eq. (2.15) when analyzing o.s. terms – takes up another renormalization contribution, finally giving

$$\tilde{\Delta}_{\mathbf{k}\sigma}\equiv m(U+2zV)\times(-1)^{\delta_{\sigma=\uparrow}}+i2Vw^{(\boldsymbol{\pi})}_{\sigma}\left(\cos k_x+\cos k_y\right)\qquad(2.25)$$

where

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

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,

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

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

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

this implies necessarily $|\tilde{\Delta}_{\mathbf{k}\uparrow}|=|\tilde{\Delta}_{\mathbf{k}\downarrow}|$. This is possible either if $w^{(\boldsymbol{\pi})}_{\uparrow}=\pm w^{(\boldsymbol{\pi})}_{\downarrow}$. 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,

$$\tilde{\Delta}_{\mathbf{k}}\equiv m(U+2zV)+2iw^{(\boldsymbol{\pi})}V\left(\cos k_x+\cos k_y\right)\qquad(2.26)$$

This result, together with Eqns. (2.13) and (2.23), concludes the renormalization of all parameters due to the non-local interaction. To calculate $w^{(\boldsymbol{\pi})}$ self consistently, we may use:

$$\begin{aligned}w^{(\boldsymbol{\pi})}&=-\frac{i}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}}\left(\cos k_x+\cos k_y\right)\langle\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\rangle\\&=-\frac{i}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\langle\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}-\hat{c}^{\dagger}_{\mathbf{k}+\boldsymbol{\pi}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\rangle\\&=\frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\langle\hat{\Psi}^{\dagger}_{\mathbf{k}\uparrow}\tau^y\hat{\Psi}_{\mathbf{k}\uparrow}\rangle\\&=\frac{1}{4L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\left(\cos k_x+\cos k_y\right)\frac{\mathrm{Im}\{\tilde{\Delta}_{\mathbf{k}}\}}{\tilde{E}_{\mathbf{k}}}\left[f\left(-\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)-f\left(\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)\right]\end{aligned}\qquad(2.27)$$

Notice that this expression is purely real, as promised, and contributes to the y component of the pseudo-field of Fig. 2.1.

2.3.2 Double counting terms: energy shift due to contractions

[To be continued...]

2.3.3 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:

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

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. (2.22) and (2.27). The self-consistent equation for m comes from Eq. (**??**), and reads

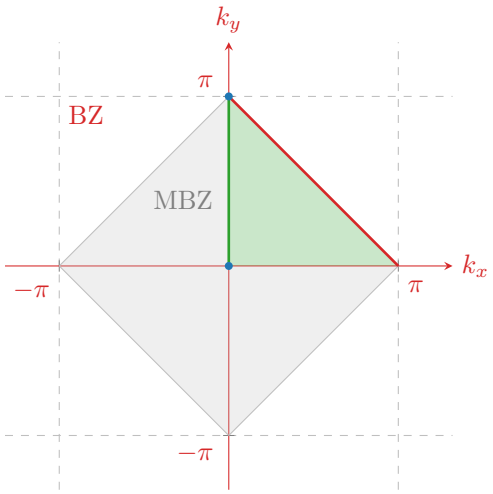
$$\begin{aligned} m &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{BZ}}\langle \hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow}\rangle \\ &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow}\tau^x\hat{\Psi}_{\mathbf{k}\uparrow} - \hat{\Psi}^\dagger_{\mathbf{k}\downarrow}\tau^x\hat{\Psi}_{\mathbf{k}\downarrow}\rangle \\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow}\tau^x\hat{\Psi}_{\mathbf{k}\uparrow}\rangle \\ &= \frac{1}{2L_xL_y}\sum_{\mathbf{k}\in\mathrm{MBZ}}\frac{\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\}}{\tilde{E}_{\mathbf{k}}}\left[f\left(-\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right) - f\left(\tilde{E}_{\mathbf{k}};\beta,\tilde{\mu}\right)\right] \end{aligned} \tag{2.28}$$

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 (2.8) were inserted. The algorithm sketched in Sec. **??** remains essentially identical, with the *caveat* of defining three HF parameters, running for each a convergence analysis.

2.4 Stability of the AF phase

The discussion above is formally correct and self-consistent, thus a HF algorithm can be sketched to extract the HFPs. However we cannot proceed without considering the instability effects of Sec. **??**. As is known (and we would have liked to notice earlier) the AF-SSB at wavevector $\boldsymbol{\pi}$ we are studying here, responsible of halving the BZ down to the MBZ, can produce a stable phase on pure Hubbard lattices only at half filling [**singh1990collective**]. For the EHM the situation is even worse than that: repeating the simple Linear Reponse Theory (LRT) computations of Sec. **??** and mimicking Eq. (**??**), we get a proper response function

$$\tilde{\chi}_{\hat{\mathbf{S}}^-\hat{\mathbf{S}}^+}(\mathbf{k},\omega) = \frac{\chi_{\hat{\mathbf{S}}^-\hat{\mathbf{S}}^+}(\mathbf{k},\omega)}{1 - \left[U - 2V\left(\cos k_x + \cos k_y\right)\right]\chi_{\hat{\mathbf{S}}^-\hat{\mathbf{S}}^+}(\mathbf{k},\omega)} \tag{2.29}$$



Color code	$w(\mathbf{k})$
White	0
Gray	0
Blue	1
Red	2
Green	4

Figure 2.3 Graphic rendition of s^*-wave symmetry over the MBZ employed to optimize calculations. The right-side table indicates, for any point in BZ, the relative weight assigned to calculation.

[Double check the red part and conclude this paragraph...].

As is well documented in literature [**wietek2021stripes**], AF can establish in a wide range of spatial structures with particular shapes, for example stripes. In order to extract the precise AF phase, we should

1. Choose an initializer wavevector, say $\mathbf{k} = \boldsymbol{\pi}$;
2. Solve self-consistently for the HFPs at $\mathbf{k}$;
3. Compute the free energy F as a functional of the wavevector around $\mathbf{k}$;
4. Look for gradient descent of the free energy, $\boldsymbol{\nabla} F < 0$;
5. If the gradient descent is found, update $\mathbf{k} \to \mathbf{k} + \delta\mathbf{k}$ and repeat from step 2, otherwise halt.

Of course the sketched procedure can lead to a lot of complications, first the fact that at incommensurate wavevector $\mathbf{k} \neq \boldsymbol{\pi}$ the unit cell is not as simple as a pair of sites, but can become much larger requiring more refined computational solutions.

In this text we will show the self consistent result for AF-SSB at wavevector $\boldsymbol{\pi}$ even at finite doping as a first step in the above sketched procedure. The presented results are self-consistent, but unfortunately deeply unstable and unphysical at finite doping, a situation where an incommensurate and insulating AF phase is preferred to this commensurate metallic counterpart. Nevertheless we present them anyway.

2.5 HF algorithm, computational strategy and results

This section is devoted to the discussion of the self-consistent results we obtained running an iterative HF algorithm in the parameters space. As said earlier, not all presented results are in fact stable; however we decided to show them as sketch of the first step in a general self-consistent algorithm in search of the stablest AF structure.

2.5.1 Preliminary symmetry considerations

A very important feature when dealing with optimization is recognizing the complete s^* symmetry of the model, and the HFP parameters with relative self-consistency equations. Consider Eqns. (2.28), (2.22) and (2.27): in all of three the term inside the sum exhibits s^*-wave symmetry and is summed over the MBZ. Then there is no need of sweeping the entirety of the MBZ, it suffices to sweep just one fourth and just multiply coherently the result.

A little care is necessary when dealing with borders, due to MBZ nesting. Consider in fact the MBZ rhombus, sketched in gray in Fig. 2.3: due to periodicity, two of its four boundaries must be excluded from computation in order to avoid redundancy. Let those be the lower boundaries,

$$k_y = |k_x| - \pi$$

Due to periodicity, the remaining upper boundaries lead to identical results, thus we may compute just one of them and multiply the result by 2. In doing this, we need to avoid the edges: due to nesting of the MBZ, the three points

$$(0, \pi) \qquad (-\pi, 0) \qquad (\pi, 0)$$

are the same point. Thus these need to be considered once. Looking to the bulk of the rhombus, due to s^* periodicity it suffices to integrate over one quarter (considering just one internal border) and multiply by 4. In doing this, the origin $(0, 0)$ must be counted only once. Fig. 2.3 summarizes this argument: if we assign to any given point $\mathbf{k} \in \mathrm{BZ}$ a weight function $w(\mathbf{k})$ defined as in figure, in particular avoiding computations over white and gray points, we get an optimized integral over the entire MBZ saving *circa* 75% of runtime.

2.5.2 Results of the HF algorithm at generic doping

Within this section we will ignore stability considerations. The first set of simulations was run keeping the local repulsion fixed at a *not-so-strong* coupling value, $U/t = 4$, and letting V vary up to a comparable value, $0 \leq V/t \leq 3$, for various fillings. The temperature is kept to a finite large value $\beta = 100$ to avoid Fermi surface discontinuities, while lattice size is kept to a reasonably high value $L_x = L_y = 256$ to suppress finite-size effects while keeping runtime low enough. The HF has been set with the following parameters:

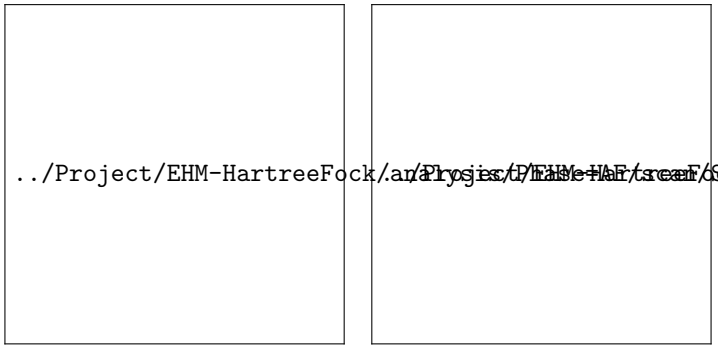
```
p::Int64 = 100                          # Maximum number of iterations
dv::Dict{String,Float64} = Dict([       # Relative tolerance on each HFP
    "m" => 1e-4,
    "w0" => 1e-4,
    "wp" => 1e-4
])
dn::Float64 = 1e-2                      # Relative tolerance on density
g::Float64 = 0.5                        # Mixing parameter
```

First HFP: m (magnetization). Consider first Fig. 2.4a. As is to be expected from Eq. (2.28), being it dependent on

$$\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\} = m(U + 2zV) \quad \text{with } z = 4$$

in this renormalized antiferromagnetic phase the non-local attraction acts as a magnetization boost, essentially reproducing the same behavior of m with U for the conventional Hubbard model plotted in Fig. **??**. The non-local attraction also enlarges the AF phase when considering various dopings, as is seen in Fig. 2.4. The magnetized region is largely extended with respect to the low-doped segment that magnetizes at $V = 0$. These effects are not particularly interesting or surprising. However, something more interesting arises when looking to Fig. 2.5, a couple of heatmaps in UV and $V\delta$ planes obtained respectively at $\delta = 0.2$ and $U = 4.0$, with L_x halved down to 128 for computational reasons. Fig. 2.5 expresses again the boost to magnetization given by V, with a magnetized region separated by a linear boundary approximately tilted as $-1/2z$, coherently with the renormalization of $\mathrm{Re}\{\tilde{\Delta}_{\mathbf{k}}\}$. Fig. 2.5b in particular is interesting: a sort of shallow "phase boundary" appears to follow a regular sub-linear curve.

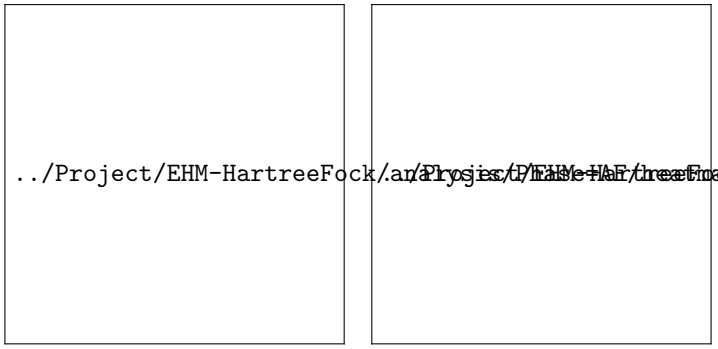
Second HFP: $w^{(0)}$ (hopping renormalization coefficient). Moving to the second HFP, things get interesting. Fig. 2.6 is set up as Fig. 2.4, while Fig. 2.7 as Fig. 2.5. When considering the behavior of the parameter at fixed U, thus looking to Fig. 2.6a, a series of *plateaus* later interrupted by a continuous change in derivative are present at each doping. This is clearly evident also in



a Non-local attraction V/t dependence.

b Doping $\delta = n - 0.5$ dependence.

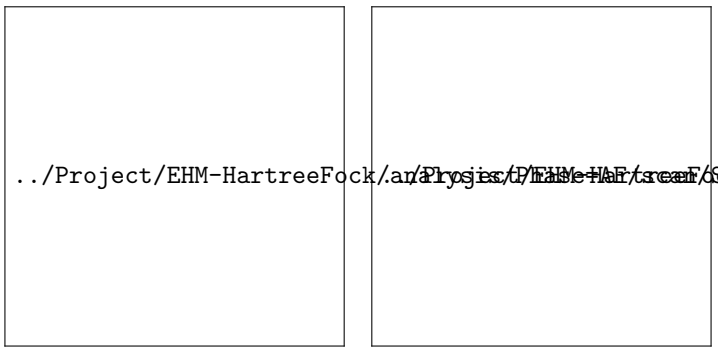
Figure 2.4 Plots of the magnetization m in the antiferromagnetic phase as a function of both the non-local attraction V/t (Fig. 2.4a) and the doping $\delta = n - 1/2$ (Fig. 2.4b), at fixed local repulsion $U/t = 4$. As discussed in text, actually only $\delta = 0$ simulations are stable.



a Magnetization in the UV plane.

b Magnetization in the $V\delta$ plane.

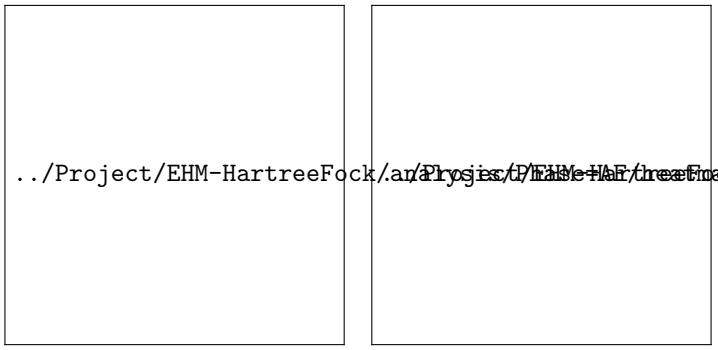
Figure 2.5 Heatmaps of the magnetization m in the antiferromagnetic phase in the UV plane (Fig. 2.5a) and the $V\delta$ plane (Fig. 2.5b).



a Non-local attraction V/t dependence.

b Doping $\delta = n - 0.5$ dependence.

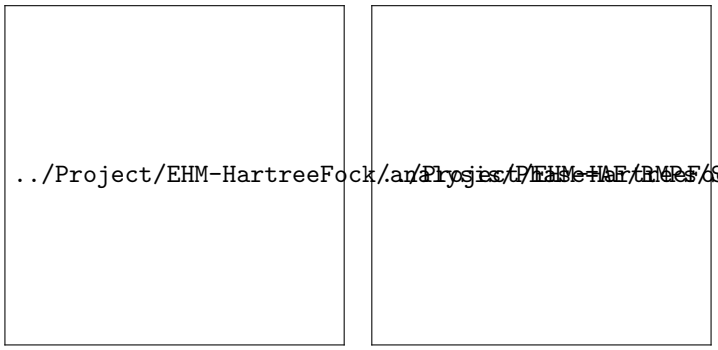
Figure 2.6 Plots of the parameter $w^{(\mathbf{0})}$ in the antiferromagnetic phase as a function of both the non-local attraction V/t (Fig. 2.6a) and the doping $\delta = n - 1/2$ (Fig. 2.6b), at fixed local repulsion $U/t = 4$.



a Magnetization in the UV plane.

b Magnetization in the $V\delta$ plane.

Figure 2.7 Heatmaps of the parameter $w^{(\mathbf{0})}$ in the antiferromagnetic phase in the UV plane (Fig. 2.7a) and the $V\delta$ plane (Fig. 2.7b).



a Effective hopping in the UV plane.

b Effective hopping in the $V\delta$ plane.

Figure 2.8 Plots of the effective hopping $\tilde{t}$ in the antiferromagnetic phase in the UV plane (Fig. 2.8a) and the $V\delta$ plane (Fig. 2.8b).

Fig. 2.5b, with the parameter staying constant when approaching from left the maximum situated at the position of the "phase boundary" of Fig. 2.5b. The fact that there exists a geometric region of the $V\delta$ plane where are located both the phase transition and the maximum of this parameter, which controls hopping renormalization, is particularly interesting, suggesting the possibility of finding a maximally localized system by following the path extrapolated by maximizing $w^{(\mathbf{0})}$ around the phase transition.

Interestingly enough, the highly doped region, $\delta > 0.4$, presents seemingly no dependency on V in Fig. 2.7b (at least for thus value of U), as is also evident from the asymptotic behavior at increasing V visible in Fig. 2.7b. Moreover, Fig. 2.5a and 2.7a appear almost reciprocal: where one parameter grows, the other is suppressed. In terms of hopping renormalization, this tells us that antiferromagnetic ordering tends to maintain t non-renormalized.

Fig. 2.8 reports in its subplots the renormalized hopping as a function of the model parameters, in the same setups as in the aforementioned heatmaps. As is depicted, the NN interaction V tends to reduce effective hopping amplitude down to a significant fraction of the starting value: t is damped of a 30% factor or so. As is evident from Fig. 2.8b, for a small local repulsion $U = 4$ the value of $\tilde{t}$ lowers as the doping grows, reaching a maximum approximately on the position of the maxima of $w^{(\mathbf{0})}$ in Fig. 2.7b, which was expected considering Eq. (2.23).

Third HFP: $w^{(\boldsymbol{\pi})}$ (imaginary gap coefficient). Unsurprisingly, the third HFP turns out to be essentially zero in all parameters space, considering also numerical fluctuations. This was expected: when deriving the MF solution to the model within AF phase, we essentially reduced it to the already known solution of Sec. **??**. The gap there was a real parameter, thus by purely

renormalizing the parameters obtained within such solution there is no need for the present gap to acquire a non-zero imaginary part.

2.5.3 Role of hopping renormalization: switching off $w^{(0)}$

[To be continued...]

Chapter 3

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.]

3.1 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. 3.1.

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

3.2 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 3.1 | 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,

$$\hat{H}_U \simeq \sum_{\mathbf{k}}\Big[\mathcal{U}_{\mathbf{k}}\hat{\phi}_{\mathbf{k}} + \mathcal{U}^*_{\mathbf{k}}\hat{\phi}^\dagger_{\mathbf{k}}\Big] \tag{3.1}$$

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

$$\mathcal{U}_{\mathbf{k}} \equiv \frac{U}{L_xL_y}\sum_{\mathbf{k}}\langle \hat{\phi}^\dagger_{\mathbf{k}}\rangle \tag{3.2}$$

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

$$\mathcal{V}_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \langle \hat{\phi}_{\mathbf{k}'}^\dagger \rangle \tag{3.3}$$

one gets immediately

$$\hat{H}_V \simeq -\sum_{\mathbf{k}} \left[\mathcal{V}_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k}}^* \hat{\phi}_{\mathbf{k}}^\dagger \right] \tag{3.4}$$

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. (3.3) 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

$$\forall \gamma \in \{s^*, p_x, p_y, d_{x^2-y^2}\} \qquad \mathcal{V}_{\mathbf{k}}\big|_\gamma \equiv \frac{V}{2L_x L_y} \sum_{\mathbf{k}} \varphi_{\mathbf{k}}^{(\gamma)} \langle \hat{\phi}_{\mathbf{k}}^\dagger \rangle \tag{3.5}$$

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

3.2.1 Full gap function and self-consistency equations

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

$$\Delta_{\mathbf{k}} \equiv \mathcal{V}_{\mathbf{k}} - \mathcal{U}_{\mathbf{k}} \tag{3.6}$$

The full self-consistency equation is given by the simple combination of Eqns. (3.2) and (3.5),

$$\Delta_{\mathbf{k}} \equiv \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'} \right] \langle \hat{\phi}_{\mathbf{k}'}^\dagger \rangle \quad \text{with} \quad V^{(s)} = -\frac{U}{2L_x L_y} \tag{3.7}$$

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 3.2 | Symmetry resolved self-consistency equations for the MFT parameters $\Delta^{(\gamma)}$, based on Eq. (3.7) and (3.8). 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. (3.7),

$$\begin{aligned}\Delta^{(\gamma)} &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\Delta_{\mathbf{k}}\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\sum_{\mathbf{k}'}\left[V^{(s)}+V_{\mathbf{k}\mathbf{k}'}\right]\langle\hat{\phi}^\dagger_{\mathbf{k}'}\rangle\\ &= \frac{1}{L_xL_y}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\sum_{\mathbf{k}'\gamma'}V^{(\gamma')}\varphi^{(\gamma')}_{\mathbf{k}}\varphi^{(\gamma')*}_{\mathbf{k}'}\langle\hat{\phi}^\dagger_{\mathbf{k}'}\rangle\\ &= V^{(\gamma)}\sum_{\mathbf{k}}\varphi^{(\gamma)*}_{\mathbf{k}}\langle\hat{\phi}^\dagger_{\mathbf{k}}\rangle\end{aligned} \tag{3.8}$$

This result provides a set of self-consistency equations for each symmetry channel, listed in Tab. 3.2. 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.

3.2.2 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. (2.23), 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. (??),

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

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. (??)

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}+\text{h.c.}\right]=\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle\hat{c}^{\dagger}_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\hat{c}^{\dagger}_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma} \tag{3.9}$$

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.

3.3 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,

$$\phi_{\mathbf{k}}=\hat{\Psi}^{\dagger}_{\mathbf{k}}\begin{bmatrix}0&1\\0&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}}\qquad\phi^{\dagger}_{\mathbf{k}}=\hat{\Psi}^{\dagger}_{\mathbf{k}}\begin{bmatrix}0&0\\1&0\end{bmatrix}\hat{\Psi}_{\mathbf{k}} \tag{3.10}$$

The full hamiltonian is then given by:

$$\hat{H}=\sum_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}h_{\mathbf{k}}\hat{\Psi}_{\mathbf{k}}\qquad h_{\mathbf{k}}\equiv\begin{bmatrix}\epsilon_{\mathbf{k}}&-\Delta^{*}_{\mathbf{k}}\\-\Delta_{\mathbf{k}}&-\epsilon_{\mathbf{k}}\end{bmatrix} \tag{3.11}$$

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

3.3.1 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

$$\begin{aligned}\hat{n}_{\mathbf{k}\uparrow}+\hat{n}_{-\mathbf{k}\downarrow}&=\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}+\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow}\\&=\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}-\hat{c}_{-\mathbf{k}\downarrow}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}+\mathbb{I}\\&=\hat{\Psi}^{\dagger}_{\mathbf{k}}\tau^{z}\hat{\Psi}_{\mathbf{k}}+\mathbb{I}\end{aligned} \tag{3.12}$$

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

$$\mathbf{b}_{\mathbf{k}}\equiv\begin{bmatrix}-\text{Re}\{\Delta_{\mathbf{k}}\}\\-\text{Im}\{\Delta_{\mathbf{k}}\}\\\epsilon_{\mathbf{k}}-\mu\end{bmatrix} \tag{3.13}$$

[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. (??),

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}\in \mathrm{BZ}} \mathbf{b}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}} = \begin{bmatrix} \hat{s}^x_{\mathbf{k}} \\ \hat{s}^y_{\mathbf{k}} \\ \hat{s}^z_{\mathbf{k}} \end{bmatrix} \tag{3.14}$$

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

$$\begin{aligned} W_{\mathbf{k}} &= e^{i\left(\theta_{\mathbf{k}} - \frac{\pi}{2}\right)\tau^y} e^{i\zeta_{\mathbf{k}}\tau^z} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} & -\cos\theta_{\mathbf{k}} \\ \cos\theta_{\mathbf{k}} & -\sin\theta_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} e^{i\zeta_{\mathbf{k}}} & \\ & e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \\ &= \begin{bmatrix} -\sin\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\cos\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \\ \cos\theta_{\mathbf{k}} e^{i\zeta_{\mathbf{k}}} & -\sin\theta_{\mathbf{k}} e^{-i\zeta_{\mathbf{k}}} \end{bmatrix} \end{aligned} \tag{3.15}$$

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.

3.3.2 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 $i = 1$, $j = 2$

$$\langle \hat{\phi}^\dagger_{\mathbf{k}} \rangle = [W_{\mathbf{k}}]_{11}[W^\dagger_{\mathbf{k}}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21}[W^\dagger_{\mathbf{k}}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.16}$$

$$= \frac{1}{2}\sin\left(2\theta_{\mathbf{k}}\right) e^{i2\zeta_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{3.17}$$

The last passage has been obtained by computing the matrix element from the explicit form of $W_{\mathbf{k}}$ of Eq. (3.15) 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 $i = 1$, $j = 1$

$$\langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \rangle = [W_{\mathbf{k}}]_{11} [W^\dagger_{\mathbf{k}}]_{11} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{21} [W^\dagger_{\mathbf{k}}]_{12} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.18}$$

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

$$= \sin^2\theta_{\mathbf{k}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) + f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.19}$$

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

$$\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} \rangle = [W_{\mathbf{k}}]_{12} [W^\dagger_{\mathbf{k}}]_{21} f\left(-E_{\mathbf{k}}; \beta, 0\right) + [W_{\mathbf{k}}]_{22} [W^\dagger_{\mathbf{k}}]_{22} f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.20}$$

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

$$= \cos^2\theta_{\mathbf{k}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) + f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.21}$$

Gap function. Eqns. (3.16), (3.17) 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

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

$$= \frac{1}{2} \sum_{\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'}\right] \frac{\Delta_{\mathbf{k}'}}{\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}} \tanh\left(\frac{\beta}{2}\sqrt{\xi^2_{\mathbf{k}'} + |\Delta_{\mathbf{k}'}|^2}\right) \tag{3.22}$$

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. 3.2.

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. (3.12),

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

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

$$+ \left(|[W_{\mathbf{k}}]_{21}|^2 - |[W_{\mathbf{k}}]_{22}|^2 \right) f\left(E_{\mathbf{k}}; \beta, 0\right) \tag{3.23}$$

$$= 1 - \cos\left(2\theta_{\mathbf{k}}\right) \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) \tag{3.24}$$

coherently with Eqns. (3.19) and (3.21). 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. (3.23) 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. (3.11),

$$|\mathrm{BCS}\rangle = \bigotimes_{\mathbf{k}} |2\theta_{\mathbf{k}}\rangle \tag{3.25}$$

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. 2.1). 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...],

$$|2\theta_{\mathbf{k}}\rangle = \cos\theta_{\mathbf{k}}\,|\Downarrow_{\mathbf{k}}\rangle - \sin\theta_{\mathbf{k}}\,|\Uparrow_{\mathbf{k}}\rangle \tag{3.26}$$

Due to Eq. (3.12) it holds

$$\begin{aligned}\left[\hat{\Psi}^{\dagger}_{\mathbf{k}}\tau^{z}\hat{\Psi}_{\mathbf{k}} + \mathbb{I}\right]|\Uparrow_{\mathbf{k}}\rangle = 2\,|\Uparrow_{\mathbf{k}}\rangle \quad &\Longrightarrow \quad |\Uparrow_{\mathbf{k}}\rangle = -\hat{\phi}^{\dagger}_{\mathbf{k}}\,|\Omega_{\mathbf{k}}\rangle \\ \left[\hat{\Psi}^{\dagger}_{\mathbf{k}}\tau^{z}\hat{\Psi}_{\mathbf{k}} + \mathbb{I}\right]|\Downarrow_{\mathbf{k}}\rangle = 0 \quad &\Longrightarrow \quad |\Downarrow_{\mathbf{k}}\rangle = |\Omega_{\mathbf{k}}\rangle\end{aligned}$$

being $|\Omega_{\mathbf{k}}\rangle$ the local electron vacuum,

$$|\Omega\rangle = \bigotimes_{\mathbf{k}} |\Omega_{\mathbf{k}}\rangle$$

Taking Eq. (3.25), combined with Eq. (3.26), we get

$$\begin{aligned}|\mathrm{BCS}\rangle &= \bigotimes_{\mathbf{k}} \left[\cos\theta_{\mathbf{k}}\,|\Downarrow_{\mathbf{k}}\rangle - \sin\theta_{\mathbf{k}}\,|\Uparrow_{\mathbf{k}}\rangle\right] \\ &= \bigotimes_{\mathbf{k}} \left[\cos\theta_{\mathbf{k}} + \sin\theta_{\mathbf{k}}\hat{\phi}^{\dagger}_{\mathbf{k}}\right]|\Omega_{\mathbf{k}}\rangle\end{aligned} \tag{3.27}$$

which is the well-known coherent BCS state.

3.3.3 Renormalization of the bare bands

We now deal with the renormalization of bare bands anticipated in Sec. 3.2.2. Taking together Eqns. (3.9), (3.16) and (3.17) we get:

$$\begin{aligned}V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} + \mathrm{h.c.}\right] &= \frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\left[\cos\left(\delta q_x\right) + \cos\left(\delta q_y\right)\right] \\ &\times\left[\left(\sin^2\theta_{\mathbf{q}}\tanh\left(\frac{\beta E_{\mathbf{q}}}{2}\right) + f\left(E_{\mathbf{q}};\beta,0\right)\right)\hat{c}^{\dagger}_{\mathbf{q}'\uparrow}\hat{c}_{\mathbf{q}'\uparrow}\right. \\ &\left. + \left(1-\cos^2\theta_{-\mathbf{q}}\tanh\left(\frac{\beta E_{-\mathbf{q}}}{2}\right) - f\left(E_{-\mathbf{q}};\beta,0\right)\right)\hat{c}^{\dagger}_{\mathbf{q}'\downarrow}\hat{c}_{\mathbf{q}'\downarrow}\right]\end{aligned} \tag{3.28}$$

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

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

Use now:

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

and let:

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

which further simplifies to

$$g_{\mathbf{q}} \equiv \frac{1}{2} - \frac{\xi_{\mathbf{q}}}{2\sqrt{\xi_{\mathbf{q}}^2 + |\Delta_{\mathbf{q}}|^2}} \tanh\left(\frac{\beta}{2}\sqrt{\xi_{\mathbf{q}}^2 + |\Delta_{\mathbf{q}}|^2}\right) \tag{3.29}$$

Thus, the original o.s. Fock term retrieved from Wick's theorem on the EHM reduces to

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

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

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

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

$$\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos(\delta q_x) + \cos(\delta q_y)\right] g_{\mathbf{q}}\hat{c}_{\mathbf{q}'\sigma}^{\dagger}\hat{c}_{\mathbf{q}'\sigma} = \frac{V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma,\gamma}\varphi_{\mathbf{q}}^{(\gamma)}\varphi_{\mathbf{q}'}^{(\gamma)*} g_{\mathbf{q}}\hat{c}_{\mathbf{q}'\sigma}^{\dagger}\hat{c}_{\mathbf{q}'\sigma} \tag{3.30}$$

Evidently from Eq. (3.29), $g_{\mathbf{q}}$ is an even function of the momentum, a feature that ensures

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

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

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

and from Eq. (3.30) we get the final form

$$\begin{aligned}\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}&\left[\cos(\delta q_x) + \cos(\delta q_y)\right] g_{\mathbf{q}}\hat{c}_{\mathbf{q}'\sigma}^{\dagger}\hat{c}_{\mathbf{q}'\sigma} \\ &= V\sum_{\mathbf{q}\sigma}\left[g^{(s^*)}(\cos q_x + \cos q_y) + g^{(d)}(\cos q_x - \cos q_y)\right]\hat{c}_{\mathbf{q}\sigma}^{\dagger}\hat{c}_{\mathbf{q}\sigma}\end{aligned} \tag{3.31}$$

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,

$$\tilde{\epsilon}_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} + V\left[g^{(s^*)}(\cos k_x + \cos k_y) + g^{(d)}(\cos k_x - \cos k_y)\right] \tag{3.32}$$

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. (3.32)

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

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:

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

The only remainder of Eq. (3.32) is its s^* part

$$\tilde{\epsilon}_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} + V g^{(s^*)} (\cos k_x + \cos k_y) \tag{3.33}$$

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. (2.23). Indeed, let $w \equiv g^{(s^*)}/2$ be the new HF parameter, we get

$$\tilde{t} \equiv t - wV \tag{3.34}$$

Once again the hopping parameter shift is rigid and controlled directly by V. As done for the AF phase, we will denote the new bands as:

$$\xi_{\mathbf{k}} \to \tilde{\xi}_{\mathbf{k}} \qquad E_{\mathbf{k}} \to \tilde{E}_{\mathbf{k}}$$

3.3.4 Ground state energy and BCS condensation

BCS essentially relies on the insurgence of an effective free fermionic field, described by the Bogoliubov bands, and the condensation of Cooper pairs. Superconducting state is favored by the lowering of free energy granted by the shifting of much of the spectral weight to a lower-energy maximum [**zhou1992density**]. "Condensation energy" is simply the energy difference between the superconducting state and the normal state, and its negativity indicates instability towards superconducting order. It's pretty straightforward to derive the ground state energy for the standard BCS state. When performing Wick's contractions,

$$\begin{aligned} \langle \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\gamma \hat{c}_\delta \rangle \sim{}& \langle \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \rangle \hat{c}_\gamma \hat{c}_\delta + \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \langle \hat{c}_\gamma \hat{c}_\delta \rangle - \langle \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \rangle \langle \hat{c}_\gamma \hat{c}_\delta \rangle \quad \text{Cooper terms} \\ & - \langle \hat{c}_\alpha^\dagger \hat{c}_\gamma \rangle \hat{c}_\beta^\dagger \hat{c}_\delta - \hat{c}_\alpha^\dagger \hat{c}_\gamma \langle \hat{c}_\beta^\dagger \hat{c}_\delta \rangle + \langle \hat{c}_\alpha^\dagger \hat{c}_\gamma \rangle \langle \hat{c}_\beta^\dagger \hat{c}_\delta \rangle \quad \text{Fock terms} \\ & + \langle \hat{c}_\alpha^\dagger \hat{c}_\delta \rangle \hat{c}_\beta^\dagger \hat{c}_\gamma + \hat{c}_\alpha^\dagger \hat{c}_\delta \langle \hat{c}_\beta^\dagger \hat{c}_\gamma \rangle - \langle \hat{c}_\alpha^\dagger \hat{c}_\delta \rangle \langle \hat{c}_\beta^\dagger \hat{c}_\gamma \rangle \quad \text{Hartree terms} \end{aligned}$$

Form each of the three rows above, the last term is the "leftover" part which shifts energy. Thus it can be ignored in derivation, but becomes important when considering the energy in the end. The EHM hamiltonian can be written as:

$$\begin{aligned} \hat{H} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} \left[\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{\mathbf{k}\uparrow} + \mathbb{I} - \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}\downarrow}^\dagger \right] - \sum_{\mathbf{k},\mathbf{k}'} \left[V^{(s)} + V_{\mathbf{k}\mathbf{k}'} \right] \hat{\phi}_{\mathbf{k}}^\dagger \hat{\phi}_{\mathbf{k}'} \\ - \frac{2V}{L_x L_y} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma} \left[\cos(\delta k_x) + \cos(\delta k_y) \right] \hat{n}_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}'\sigma} \end{aligned} \tag{3.35}$$

as in Eq. (3.7). Following the scheme above, the "leftovers" of the MFT hamiltonian are just

$$\sum_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k}} \langle \hat{\phi}_{\mathbf{k}'} \rangle - \frac{2V}{L_x L_y} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma} \left[\cos(\delta k_x) + \cos(\delta k_y) \right] g_{\mathbf{k}} g_{\mathbf{k}'}$$

Further developing this result and applying Eqns. (3.17), (**??**), these last terms can be written as:

$$\sum_{\mathbf{k}} \frac{|\Delta_{\mathbf{k}}|^2}{2\tilde{E}_{\mathbf{k}}} \tanh\left(\frac{\beta \tilde{E}_{\mathbf{k}}}{2} \right) - 2V L_x L_y \sum_{\gamma} \left| g^{(\gamma)} \right|^2 \qquad \gamma \in \{s^*, d_{x^2-y^2}\} \tag{3.36}$$

as for Eq. (3.31). Notice the presence of a volume factor in the $\mathcal{O}\left(g^2\right)$ correction.

Now, we retrieve the expression for the MFT free energy density [**hutchinson2021mixed**] simply by adding four contributions:

1. Bogoliubov free quasiparticles thermal ground state energy density,
$$\frac{1}{L_xL_y}\sum_{\mathbf{k}}\tilde{E}_{\mathbf{k}}\left[f(\tilde{E}_{\mathbf{k}};\beta,0)-f(-\tilde{E}_{\mathbf{k}};\beta,0)\right]=\frac{1}{L_xL_y}\sum_{\mathbf{k}}\tilde{E}_{\mathbf{k}}\left[f(\tilde{E}_{\mathbf{k}};\beta,0)-\Big(1-f(\tilde{E}_{\mathbf{k}};\beta,0)\Big)\right]$$
$$=\frac{2}{L_xL_y}\sum_{\mathbf{k}}\tilde{E}_{\mathbf{k}}f(\tilde{E}_{\mathbf{k}};\beta,0)-\frac{1}{L_xL_y}\sum_{\mathbf{k}}\tilde{E}_{\mathbf{k}}$$
having used the simple property of the Fermi-Dirac distribution $f(-x;\beta,0)=1-f(-x;\beta,0)$.
2. The term originated by the identity produced by fermionic anticommutation rules in Eq. (3.35),
$$\frac{1}{L_xL_y}\sum_{\mathbf{k}}\tilde{\xi}_{\mathbf{k}}$$
averaged on the lattice.
3. The "leftovers" of Eq. (3.36), divided by L_xL_y.
4. The entropic free energy
$$-Ts$$
with $T=1/k_B\beta$ and s the free Fermi gas entropy density for the Bogoliubov quasiparticles,
$$s=-\frac{2k_B}{L_xL_y}\sum_{\mathbf{k}}\left[\Big(1-f(\tilde{E}_{\mathbf{k}};\beta,0)\Big)\ln\Big(1-f(\tilde{E}_{\mathbf{k}};\beta,0)\Big)+f(\tilde{E}_{\mathbf{k}};\beta,0)\ln f(\tilde{E}_{\mathbf{k}};\beta,0)\right]$$
We use the identity:
$$\ln\left(1-\frac{1}{e^x+1}\right)=x+\ln\left(\frac{1}{e^x+1}\right)$$
and reduce the above expression to:
$$s=-\frac{2k_B}{L_xL_y}\sum_{\mathbf{k}}\Big[\ln\Big(1-f(\tilde{E}_{\mathbf{k}};\beta,0)\Big)+f(\tilde{E}_{\mathbf{k}};\beta,0)\ln f(\tilde{E}_{\mathbf{k}};\beta,0)$$
$$-\beta\tilde{E}_{\mathbf{k}}f(\tilde{E}_{\mathbf{k}};\beta,0)-f(\tilde{E}_{\mathbf{k}};\beta,0)\ln f(\tilde{E}_{\mathbf{k}};\beta,0)\Big]$$
Second and fourth terms cancel out, while the third compensates the first one of contribution 1.

All together, the MFT averaged free energy looks like this:
$$f_{\mathrm{MFT}}[\Delta_{\mathbf{k}},g_{\mathbf{k}}]=\frac{1}{L_xL_y}\sum_{\mathbf{k}}\left[\tilde{\xi}_{\mathbf{k}}-\tilde{E}_{\mathbf{k}}+\frac{|\Delta_{\mathbf{k}}|^2}{2\tilde{E}_{\mathbf{k}}}\tanh\left(\frac{\beta\tilde{E}_{\mathbf{k}}}{2}\right)\right]$$
$$-2V\sum_{\gamma\in\{s^*,d\}}\left|g^{(\gamma)}\right|^2+\frac{2}{\beta L_xL_y}\sum_{\mathbf{k}}\ln\Big(1-f(\tilde{E}_{\mathbf{k}};\beta,0)\Big)\tag{3.37}$$

The two main differences with the commonly known expressions for f_{MFT} [**hutchinson2021mixed**, **senarath2025mixed**] are the presence of bands renormalization , the absence of $-\mu n$ [Why?], and the $\mathcal{O}\left(g^2\right)$ correction. The latter, not only is negative for attractive V, a feature that can lead to superconducting phase energy lowering and stabilisation, but also it depends explicitly on the spectral amplitude of the s^* and d-wave components of $g_{\mathbf{k}}$. Since as seen the d-wave part of $g_{\mathbf{k}}$ arises for mixed symmetries, this details seems to indicate an energetic preference for multi-symmetry phases.

3.4 Results of the HF algorihtm

[To be continued...]