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

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Abstract

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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
RWC(s)	Relevant Wick's contraction(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,

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

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

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

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,

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

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

$$\mu \to \mu - nU \tag{1.2}$$

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 $\hat{H}_V$,

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

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,

$$\mu \to \mu + 2znV \tag{1.3}$$

Thus, when considering the net shift to μ due to both interactions, we get

$$\tilde{\mu} \equiv \mu + n(2zV - U) \tag{1.4}$$

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 $\hat{H}$:

$$\hat{H}_V \simeq V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma} + \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}\rangle - \langle\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^{\dagger}_{j\sigma}\hat{c}_{i\sigma}\rangle\right] + (\text{all the rest}) \tag{1.5}$$

(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 $w^{(\mathrm{N})}$,

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

The effective diffusive hamiltonian is given by

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

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. (1.5),

$$\begin{aligned}&V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma} + \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle - \langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right]\\ &\quad\stackrel{\mathcal{F}}{=} \frac{2V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\sum_{\sigma}\left[\cos\left(\delta k_x\right) + \cos\left(\delta k_y\right)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma}\rangle\hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma} - E^{(\mathrm{N})}_{\mathrm{F}/V}\end{aligned} \tag{1.6}$$

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

$$E^{(\mathrm{N})}_{\mathrm{F}/V} \equiv \frac{V}{L_xL_y}\sum_{\mathbf{K},\mathbf{k},\mathbf{k}'}\sum_{\sigma}\left[\cos\left(\delta k_x\right) + \cos\left(\delta k_y\right)\right]\langle \hat{c}^\dagger_{\mathbf{K}+\mathbf{k}\sigma}\hat{c}_{\mathbf{K}-\mathbf{k}'\sigma}\rangle\langle \hat{c}^\dagger_{\mathbf{K}-\mathbf{k}\sigma}\hat{c}_{\mathbf{K}+\mathbf{k}'\sigma}\rangle \tag{1.7}$$

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. (1.6) becomes

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

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 Fock	μ shift t shift

Table 1.1

we reduce Eq. (1.6) to

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right]$$
$$\stackrel{\mathcal{F}}{=}\frac{2V}{L_xL_y}\sum_{\mathbf{q},\mathbf{q}'}\sum_{\sigma}\left[\cos\left(\delta q_x\right)+\cos\left(\delta q_y\right)\right]\langle\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.9}$$

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. (1.9) to

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right]$$
$$\stackrel{\mathcal{F}}{=}\sum_{\gamma}\left[\frac{1}{L_xL_y}\sum_{\mathbf{q}}\varphi^{(\gamma)}_{\mathbf{q}}\langle\hat{c}^\dagger_{\mathbf{q}\sigma}\hat{c}_{\mathbf{q}\sigma}\rangle\right]\times V\sum_{\mathbf{q}'}\varphi^{(\gamma)*}_{\mathbf{q}'}\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.10}$$

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. (1.10), due to the presence of the part in square brackets, only $\gamma=s^*$ contributes. Let us define the HFP $w^{(\mathrm{N})}$ as

$$w^{(\mathrm{N})}\equiv\frac{1}{2L_xL_y}\sum_{\mathbf{q}\in\mathrm{BZ}}\left(\cos q_x+\cos q_y\right)f(\tilde{\epsilon}_{\mathbf{q}};\beta,\tilde{\mu})\tag{1.11}$$

which finally gives

$$V\sum_{\langle ij\rangle}\sum_{\sigma}\left[\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}+\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle-\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle\langle\hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma}\rangle\right]$$
$$\stackrel{\mathcal{F}}{=}\sum_{\mathbf{q}'}2w^{(\mathrm{N})}V\left(\cos q_x+\cos q_y\right)\hat{c}^\dagger_{\mathbf{q}'\sigma}\hat{c}_{\mathbf{q}'\sigma}-E^{(\mathrm{N})}_{\mathrm{F}/V}\tag{1.12}$$

As anticipated, hopping gets shifted by an amount

$$t\to\tilde{t}\equiv t-w^{(\mathrm{N})}V\tag{1.13}$$

with $w^{(\mathrm{N})}$ to be self-consistently determined by iteratively solving Eq. (1.11).

1.2 Free energy density

[To be continued. . .]

1.3 HF results

[To be continued. . .]