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)
SC	Superconductor
T_c	Critical temperature

Introduction

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

Chapter 1

Theoretical introduction

[To be continued...]

1.1 Antiferromagnetic ordering in the Hubbard model

Consider the ordinary Hubbard model:

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad t, U > 0 \tag{1.1}$$

The two competing mechanisms are site-hopping of amplitude t and local repulsion of amplitude U. For this model defined **on a bipartite lattice at half filling** and fixed electron number, it is well known [5] that, below a certain critical temperature T_c and above some (small) critical repulsion U_c/t, the ground-state acquires antiferromagnetic (AF) long-range ordering. schematically depicted in Fig. 1.1a. The mechanism for the formation of the AF phase takes advantage of virtual hopping, as described in App. **??**; the Mean-Field Theory treatment of ferromagnetic-antiferromagnetic orderings in 2D Hubbard lattices is rapidly discussed in App. **??**.

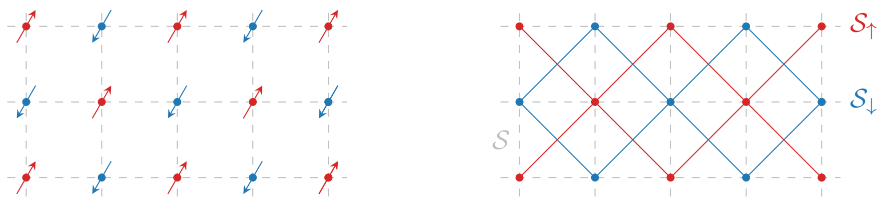
In this chapter the discussion is limited to the two-dimensional square lattice Hubbard model. The lattice considered has N sites per side, N^2 sites in total. All theoretical discussion neglects border effects, thus considering $N \to +\infty$.

1.2 The Extended Fermi-Hubbard model

The Extended Fermi-Hubbard model is defined by:

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - V \sum_{\langle ij \rangle} \sum_{\sigma\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} \tag{1.2}$$

The last term represents an effective attraction between neighboring electrons, of amplitude V. Such an interaction is believed [1] necessary to describe the insurgence of high-T_c superconductivity in cuprate SCs. [To be continued...]



a | Antiferromagnetic phase. b | Polarized sublattices.

Figure 1.1 | Schematic representation of the AF phase. Fig. 1.1a shows a portion of the square lattice with explicit representation of the spin for each site. Fig. 1.1b divides the square lattice $\mathcal{S}$ in two polarized sublattices $\mathcal{S}_\uparrow$, $\mathcal{S}_\downarrow$. The AF phase results from the interaction of two inversely polarized "ferromagnetic" square lattices.

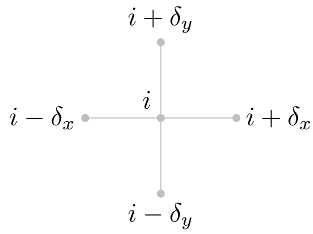


Figure 1.2 | Schematic representation of the four NNs of a given site i for a planar square lattice.

1.2.1 Mean-Field effective hamiltonian

Consider the non-local term,

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

Since the relevant values for V are $\mathcal{O}(t)$, in this model $V \ll U$. The ground-state leading contribution will be the antiferromagnetic state, with the square lattice decomposed in two oppositely polarized square lattices with spacing increased by a factor $\sqrt{2}$. The non-local interaction can be written as a sum of local terms on one of the two sublattices, say, the one up-polarized:

$$\hat{H}_V = \sum_{i \in \mathcal{S}_\uparrow} \hat{h}_V^{(i)} \qquad \hat{h}_V^{(i)} = -V \sum_{\ell = x,y} \left(\hat{n}_{i\uparrow} \hat{n}_{i+\delta_\ell \downarrow} + \hat{n}_{i\uparrow} \hat{n}_{i-\delta_\ell \downarrow} \right)$$

Here the notation of Fig. 1.1b is used. The two-dimensional lattice is regular-square. For each site i, the nearest neighbors sites are four. The notation used is $i \pm \delta_x$, $i \pm \delta_y$ as in Fig. 1.2; all of these sites are part of $\mathcal{S}_\downarrow$. Note finally that, using $i \in \mathcal{S}_\uparrow$, the sum $\sum_{\sigma\sigma'}$ has been omitted: this is because operators resulting from $(\sigma, \sigma') \neq \uparrow\downarrow$ are suppressed in a ground-state with antiferromagnetic leading contribution.

The non-local interaction contribution to energy, as a function of the $T = 0$ full hamiltonian ground-state $|\Psi\rangle$, is given by

$$\begin{aligned} E_V[\Psi] &= \langle \Psi | \hat{H}_V | \Psi \rangle \\ &= -V \sum_{i \in \mathcal{S}_\uparrow} \sum_{\ell = x,y} \langle \hat{n}_{i\uparrow} \hat{n}_{i+\delta_\ell \downarrow} + \hat{n}_{i\uparrow} \hat{n}_{i-\delta_\ell \downarrow} \rangle \end{aligned}$$

Shorthand notation has been used: $\langle \Psi | \cdot | \Psi \rangle = \langle \cdot \rangle$. Consider one specific term, say, $\hat{n}_{i\uparrow} \hat{n}_{i+\delta_x \downarrow}$. Wick's Theorem states that, if the expectation value is performed onto a coherent state,

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

As a first approximation, the theorem is assumed to hold (which, in a BCS-like fashion, is equivalent to assuming for the ground-state to be a coherent state). The last two terms account for single-particle interactions with a background field; they are relevant in the Hartree-Fock scheme, being direct-exchange contributions to single particle energies. The first term accounts for non-local electrons pairing, mimicking the Bogoliubov term of BCS theory. I assume the ground-state to be realized such that the last two terms are suppressed, while the first survives. Energy then is cast to the form

$$E_V[\Psi] = -V \sum_{i \in \mathcal{S}_\uparrow} \sum_{\ell = x,y} \left[\langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i+\delta_\ell \downarrow} \rangle \langle \hat{c}_{i+\delta_\ell \downarrow} \hat{c}_{i\uparrow} \rangle + \langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i-\delta_\ell \downarrow} \rangle \langle \hat{c}_{i-\delta_\ell \downarrow} \hat{c}_{i\uparrow} \rangle \right]$$

The ground-state must realize the condition

$$\frac{\delta}{\delta \langle \Psi |} E[\Psi] = 0$$

being $E[\Psi]$ the total energy (made up of the three terms of couplings t, U and V). [Expand derivation?] The functional derivative must be carried out in a variational fashion including a Lagrange multiplier, the latter accounting for state-norm conservation, as is done normally in deriving the Hartree-Fock approximation for the eigenenergies of the electron liquid [3, 4]. This approach leads to the conclusion that the (coherent) ground-state of the system must be an eigenstate of the mean-field effective hamiltonian:

$$\hat{H}^{(\mathrm{e})} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{1.4}$$

$$- V \sum_{i \in \mathcal{S}_\uparrow} \sum_{\ell = x,y} \sum_{\delta = \pm \delta_\ell} \left[\langle \hat{c}^\dagger_{i\uparrow} \hat{c}^\dagger_{i+\delta\downarrow} \rangle \hat{c}_{i+\delta\downarrow} \hat{c}_{i\uparrow} + \mathrm{h.\ c.} \right] \tag{1.5}$$

[To be continued. . .]

1.2.2 Fourier-transform of the non-local interaction

Let me take a step back and perform explicitly the Fourier-transform of the non-local interaction of Eq. 1.3. Consider a generic bond, say, the one connecting sites j and $j \pm \delta_\ell$ (variable i is here referred to as the imaginary unit to avoid confusion). $\mathbf{x}_j$ is the 2D notation for the position of site j, while $\boldsymbol{\delta}_\ell$ is the 2D notation for the lattice spacing previously indicated as δ_ℓ. Fourier transform it according to the convention

$$\hat{c}_{j\sigma} = \frac{1}{N} \sum_{\mathbf{q} \in \mathrm{BZ}} e^{-i\mathbf{q}\cdot\mathbf{x}_j} \hat{c}_{\mathbf{q}\sigma}$$

Then:

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

It follows,

$$\begin{aligned} \hat{h}^{(j)}_V &= -\frac{V}{N^4} \sum_{\ell=x,y} \sum_{\nu=1}^{4} \sum_{\mathbf{q}_\nu \in \mathrm{BZ}} e^{i[(\mathbf{q}_1+\mathbf{q}_2)-(\mathbf{q}_3+\mathbf{q}_4)]\cdot\mathbf{x}_j} \left(e^{i(\mathbf{q}_2-\mathbf{q}_3)\cdot\boldsymbol{\delta}_\ell} + e^{-i(\mathbf{q}_2-\mathbf{q}_3)\cdot\boldsymbol{\delta}_\ell} \right) \hat{c}^\dagger_{\mathbf{q}_1\uparrow} \hat{c}^\dagger_{\mathbf{q}_2\downarrow} \hat{c}_{\mathbf{q}_3\downarrow} \hat{c}_{\mathbf{q}_4\uparrow} \\ &= -\frac{2V}{N^4} \sum_{\ell=x,y} \sum_{\nu=1}^{4} \sum_{\mathbf{q}_\nu \in \mathrm{BZ}} e^{i[(\mathbf{q}_1+\mathbf{q}_2)-(\mathbf{q}_3+\mathbf{q}_4)]\cdot\mathbf{x}_j} \cos\left[(\mathbf{q}_2-\mathbf{q}_3)\cdot\boldsymbol{\delta}_\ell\right] \hat{c}^\dagger_{\mathbf{q}_1\uparrow} \hat{c}^\dagger_{\mathbf{q}_2\downarrow} \hat{c}_{\mathbf{q}_3\downarrow} \hat{c}_{\mathbf{q}_4\uparrow} \end{aligned}$$

The full non-local interaction is given by summing over all sites of one sublattice. This gives back momentum conservation,

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

Let $\mathbf{q}_1 + \mathbf{q}_2 = \mathbf{q}_3 + \mathbf{q}_4 = \mathbf{Q}$, and define $\mathbf{q}$, $\mathbf{q}'$ such that

$$\mathbf{q}_1 \equiv \mathbf{Q} + \mathbf{q} \qquad \mathbf{q}_2 \equiv \mathbf{Q} - \mathbf{q} \qquad \mathbf{q}_3 \equiv \mathbf{Q} - \mathbf{q}' \qquad \mathbf{q}_4 \equiv \mathbf{Q} + \mathbf{q}' \qquad \Delta\mathbf{q} \equiv \mathbf{q} - \mathbf{q}'$$

Sums over these variable must be intended as over the Brillouin Zone (BZ). Then, finally

$$\begin{aligned} \hat{H}_V &= \sum_{j \in \mathcal{S}_\uparrow} \hat{h}^{(j)}_V \\ &= -\frac{2V}{N^2} \sum_{\ell=x,y} \sum_{\mathbf{Q},\mathbf{q},\mathbf{q}'} \cos\left(\Delta\mathbf{q}\cdot\boldsymbol{\delta}_\ell\right) \hat{c}^\dagger_{\mathbf{Q}+\mathbf{q}\uparrow} \hat{c}^\dagger_{\mathbf{Q}-\mathbf{q}\downarrow} \hat{c}_{\mathbf{Q}-\mathbf{q}'\downarrow} \hat{c}_{\mathbf{Q}+\mathbf{q}'\uparrow} \\ &= -2V \sum_{\ell=x,y} \sum_{\mathbf{q},\mathbf{q}'} \cos\left(\Delta\mathbf{q}\cdot\boldsymbol{\delta}_\ell\right) \hat{c}^\dagger_{\mathbf{q}\uparrow} \hat{c}^\dagger_{-\mathbf{q}\downarrow} \hat{c}_{-\mathbf{q}'\downarrow} \hat{c}_{\mathbf{q}'\uparrow} \\ &= -2V \sum_{\mathbf{q},\mathbf{q}'} \left[\cos\left(\Delta q_x \delta_x\right) + \cos\left(\Delta q_y \delta_y\right)\right] \hat{c}^\dagger_{\mathbf{q}\uparrow} \hat{c}^\dagger_{-\mathbf{q}\downarrow} \hat{c}_{-\mathbf{q}'\downarrow} \hat{c}_{\mathbf{q}'\uparrow} \end{aligned}$$

In the second passage, a sum over $\mathbf{Q}$ has been absorbed recognizing that it generates N^2 identical terms. [To be continued...]

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