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

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Alessandro Gori*

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Abstract

[To be continued...]

Contents

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*a.gori23@studenti.unipi.it / nepero27178@github.com

List of symbols and abbreviations

AF	Anti-Ferromagnetic
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:

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

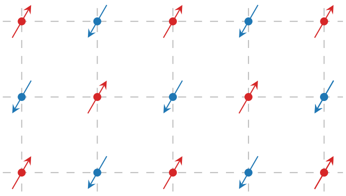
The two competing mechanisms are site-hopping of amplitude t and local repulsion of amplitude U. For this model defined **on a bipartite lattice at half filling** and fixed electron number, it is well known [3] that, below a certain critical temperature T_c and above some (small) critical repulsion U_c/t, 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. **??**.

1.2 The Extended Fermi-Hubbard model

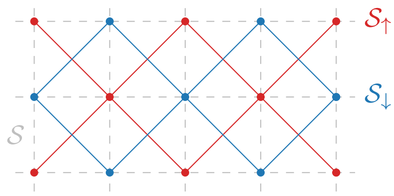
The Extended Fermi-Hubbard model is defined by:

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

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.

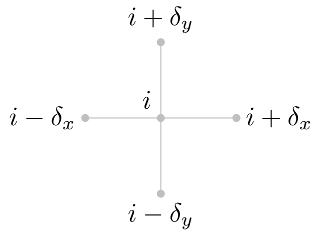


Figure 1.2 | Schematic representation of the four NNs of a given site i for a planar square lattice.

Mean-Field effective hamiltonian

[Why has this subsection no number?]

Consider the non-local term,

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

Since the relevant values for V are $\mathcal{O}(t)$, in this model $V \ll U$. The ground-state leading contribution will be antiferromagnetic, 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.

Consider a single bond, say, the one connecting sites i and $i+\delta_x$. Wick's Theorem states that, if the expectation value is performed onto a coherent state,

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

[To be continued...]

Bibliography

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