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
BCS	Bardeen-Cooper-Schrieffer (theory)
HF	Hartree-Fock
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 [6] 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. A; the Mean-Field Theory treatment of ferromagnetic-antiferromagnetic orderings in 2D Hubbard lattices is rapidly discussed in App. B.

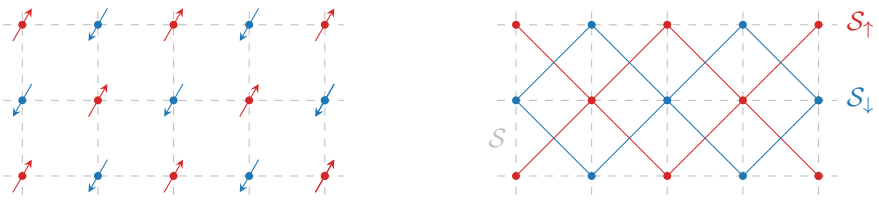
In this chapter the discussion is limited to the two-dimensional square lattice Hubbard model. The lattice considered has N sites per side, N^2 sites in total. All theoretical discussion neglects border effects, thus considering $N \to +\infty$.

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.

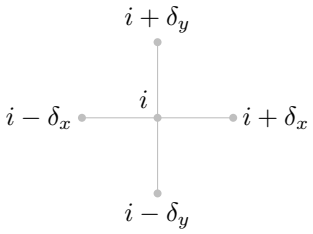


Figure 1.2 | Schematic representation of the four NNs of a given site i for a planar square lattice.

1.2.1 Experimental insight on NN attraction

Todo:

- High T_c SC in cuprates;
- Experimental evidence of topological SC;
- Insertion of the non-local attraction;

1.2.2 Mean-Field effective hamiltonian

This section is devoted to develop a rough mean field approximation of the Extended Hubbard model of Eq. (1.2). First part focuses on the non-local interaction V, expected to be source of superconductivity; the second part on the local interaction U, known to be source of Slater-like anti-ferromagnetism, as described in App. B.

Mean-field treatment of the local term

The mean-field description of the local (on-site) U interaction has been described in detail in App. B, along with a simple numerical analysis of the insurgence of antiferromagnetic ordering in a Hartree-Fock approximation scheme. Here are reported the main results. [To be continued...]

Mean-field treatment of the non-local term

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:

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

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 [4, 5]. This approach leads to the conclusion that the (coherent) ground-state of the system must be an eigenstate of the mean-field effective hamiltonian:

$$\begin{aligned}\hat{H}^{(\mathrm{e})} =& -t\sum_{\langle ij\rangle}\sum_\sigma\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \\ & - V\sum_{i\in\mathcal{S}_\uparrow}\sum_{\ell=x,y}\sum_{\delta=\pm\delta_\ell}\left[\langle\hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i+\delta\downarrow}\rangle\hat{c}_{i+\delta\downarrow}\hat{c}_{i\uparrow} + \text{h.c.}\right]\end{aligned} \tag{1.4}$$

The gap function is defined across each bond as the pairing expectation

$$\Delta_{ij} \equiv V\langle\hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\rangle$$

while the pairing operator is defined as

$$\hat{\phi}_{ij} \equiv \hat{c}_{j\downarrow}\hat{c}_{i\uparrow}$$

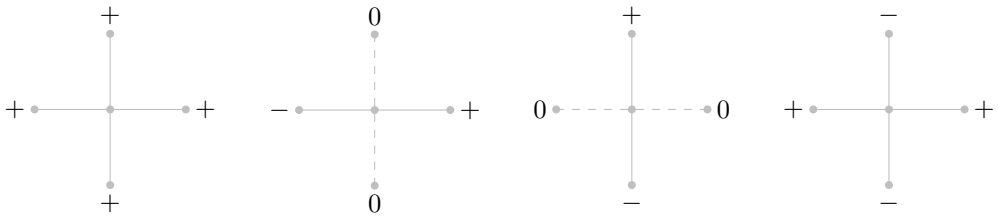
The effective hamiltonian reads:

$$\hat{H}^{(\mathrm{e})} = -t\sum_{\langle ij\rangle}\sum_\sigma\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \sum_{\langle ij\rangle}\left[\Delta_{ij}\hat{\phi}_{ij} + \Delta^*_{ij}\hat{\phi}^\dagger_{ij}\right] \tag{1.5}$$

As in standard BCS theory, this hamiltonian – being quadratic in the electronic operators – can be diagonalized via a Bogoliubov rotation. Superconducting pairing can arise both from the local U term and from the non-local V term. In next sections it is assumed the V term generates dominant superconductivity via its weak non-local pairing.

1.2.3 Topological superconducting parameters over the square lattice

Consider Eq. (1.5). Δ_{ij} is a function of position, specifically it is a function of its variables difference $r \equiv j - i$. Over the square lattice with NN interaction, the latter can assume four values: $\pm\delta_x$, $\pm\delta_y$. For a function of space defined over the four rim sites $i \pm \delta_\ell$ of Fig. 1.2, different symmetry



a | Extended s-wave. b | p_x-wave. c | p_y-wave. d | $d_{x^2-y^2}$-wave.

Figure 1.3 | Different spatial structures of the gap function under planar rotations. The four figures show the first four NN contributions to the spatial structure of Δ_{ij}. Each graph is a different contribution to the expansion of Δ_r. Under each graph, each rim site contributes by a weight given by ± 1 or 0 times a constant, as specified in text.

Structure	Gap function	Graph
Extended s-wave	$\Delta_{ij}^{(s)} = \Delta^{(s)} \left(\delta_{j=i+\delta_x} + \delta_{j=i-\delta_x} + \delta_{j=i+\delta_y} + \delta_{j=i-\delta_y}\right)$	Fig. 1.3a
p_x-wave	$\Delta_{ij}^{(p_x)} = \Delta^{(p_x)} \left(\delta_{j=i+\delta_x} - \delta_{j=i-\delta_x}\right)$	Fig. 1.3b
p_y-wave	$\Delta_{ij}^{(p_y)} = \Delta^{(p_y)} \left(\delta_{j=i+\delta_y} - \delta_{j=i-\delta_y}\right)$	Fig. 1.3c
$d_{x^2-y^2}$-wave	$\Delta_{ij}^{(d_{x^2-y^2})} = \Delta^{(d_{x^2-y^2})} \left(\delta_{j=i+\delta_x} + \delta_{j=i-\delta_x} - \delta_{j=i+\delta_y} - \delta_{j=i-\delta_y}\right)$	Fig. 1.3d

Table 1.1 | First four spatial structures for the gap function Δ_{ij}. In the middle column, all spatial dependence is included in the δs, while $\Delta^{(\ell)} \in \mathbb{C}$. The last column indicates the graph representation of each contribution given in Fig. 1.3.

structure can be defined under the planar rotations group SO(2). In other words, the function Δ_r can be decomposed in planar harmonics (which are simply the sine-cosine basis). Fig. 1.3 show the first four spatial structures for the NN term. For each graph, the relative weight in the decomposition of Δ_r is given by a constant $\Delta^{(\ell)}$ times a sum of signs and zeros as indicated in the various subgraphs of Fig. 1.3. Tab. 1.1 reports said gap function contributions explicitly.

SC is established with a given symmetry – which means, symmetry breaking in the phase transition proceeds in a specific channel. Conventional BCS superconductivity arises from the only possible spatial structure of the local pairing, s-wave – here extended as in Fig. 1.3a. Cuprates exhibit a tendency towards $d_{x^2-y^2}$ SC, while other materials towards p-wave types – eventually with some chirality, as is the case for $p_x \pm ip_y$ SCs.

In this BCS-like approach, a self-consistent equation for the gap function must be retrieved in order to further investigate the model and extract the conditions for the formation of a superconducting phase with a given pairing topology.

1.2.4 Self-consistency equations

[To be continued...]

1.2.5 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...]

Appendix A

Superexchange and virtual hopping in Hubbard lattices

A key mechanism in AF phase formation in Hubbard lattice is superexchange. The AF phase is stabilized by spin fluctuations and second-order virtual hopping. The mechanism becomes clear enough by considering a 2-sites Hubbard toy model.

A.1 Virtual hopping in the 2-sites Hubbard lattice

Consider the toy model:

$$\hat{H} = -t\left\{\hat{c}^{\dagger}_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^{\dagger}_{1\downarrow}\hat{c}_{2\downarrow} + \text{h.c.}\right\} + U\left\{\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right\}$$

with $i = 1, 2$ the site index. The two sites are represented in Fig. A.1. The two competing processes are:

1. electrons inter-sites hopping with amplitude $-t$;

2. local repulsion $+U$, acting when two anti-aligned electrons reside on the same site;

For an half-filled system, the Hilbert space is six-dimensional. I use the notation $|n_{1\uparrow}n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle$ to indicate the six computational basis states:

$$\begin{array}{lll} |\psi_1\rangle \equiv |1010\rangle & |\psi_3\rangle \equiv |1001\rangle & |\psi_5\rangle \equiv |0011\rangle \\ |\psi_2\rangle \equiv |1100\rangle & |\psi_4\rangle \equiv |0110\rangle & |\psi_6\rangle \equiv |0101\rangle \end{array}$$

For example, the top panel of Fig. A.1 shows state $|\psi_2\rangle$.

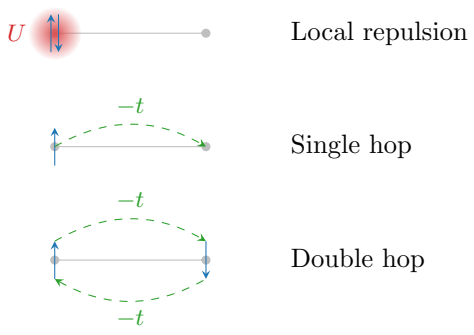


Figure A.1 | Two sites Hubbard model.

Structure	Eigenstate	Energy
Spin-1/2 singlet	$\frac{\lvert\phi_3\rangle - \lvert\phi_4\rangle}{\sqrt{2}}$	$E^- = \frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t^2}$
Spin-1/2 triplet	$\lvert\phi_1\rangle, \frac{\lvert\phi_3\rangle + \lvert\phi_4\rangle}{\sqrt{2}}, \lvert\phi_6\rangle$	0
	$\frac{\lvert\phi_2\rangle - \lvert\phi_5\rangle}{\sqrt{2}}$	U
	$\frac{\lvert\phi_2\rangle + \lvert\phi_5\rangle}{\sqrt{2}}$	$E^+ = \frac{U}{2} + \sqrt{\frac{U^2}{4} + 4t^2}$

Table A.1 | List of exact eigenstates and relative energies for the 2-sites half-filled Hubbard model.

A.1.1 Exact solution of the half-filled model

The hamiltonian matrix is directly evaluated in this basis

$$H_{ij} = \langle\psi_i| \hat{H} |\psi_j\rangle \quad \Longrightarrow \quad H = \begin{bmatrix} 0 & & & & & \\ & U & -t & -t & & \\ & -t & & & -t & \\ & -t & & & -t & \\ & & -t & -t & U & \\ & & & & & 0 \end{bmatrix}$$

Empty slots in the matrix stand for zeros. Evidently the states $|\psi_1\rangle$ (both up) and $|\psi_6\rangle$ (both down) are zero-energy eigenstates. These states cannot realize electrons hopping because of Pauli principle. The internal 4×4 matrix is readily diagonalized by the means of a change of basis V,

$$V \begin{bmatrix} U & -t & -t & \\ -t & & & -t \\ -t & & & -t \\ & -t & -t & U \end{bmatrix} V^\dagger = \begin{bmatrix} E^- & & & \\ & 0 & & \\ & & U & \\ & & & E^+ \end{bmatrix}$$

Tab. A.1 shows the eigenvectors and relative eigenvalues obtained from diagonalization. The ground-state is the singlet state,

$$\frac{|\phi_3\rangle - |\phi_4\rangle}{\sqrt{2}} = \frac{|1010\rangle - |0101\rangle}{\sqrt{2}} = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

of energy

$$E^- = \frac{U}{2} - \sqrt{\frac{U^2}{4} + 4t^2} \simeq -\frac{4t^2}{U}$$

the latter equality being true if $U \gg t$ (strong repulsion limit). The singlet state pairs with a spatially-symmetric (nodeless) wavefunction. The entire triplet (second row of Tab. A.1) remains at zero energy. Excited states are anti-symmetrized and symmetrized version of the polarized states $|\phi_1\rangle$ and $|\phi_6\rangle$.

A.1.2 Virtual hopping

The key feature of the singlet state is the one represented in the bottom panel of Fig. A.1: if the two electrons occupy separate sites and are anti-aligned, both "see" the other site as empty, thus free to hop to. [To be continued...]

Appendix B

Mean-Field Theory in Hubbard lattices

In this Appendix the Mean-Field solutions to the Hubbard hamiltonian,

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

are described. The discussion is limited to the two-dimensional square lattice. The two-dimensional square lattice extension of the two-sites model can be studied by the means of Mean Field Theory. We have:

$$\begin{aligned} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} &= \left(\langle \hat{n}_{i\uparrow} \rangle + \delta \hat{n}_{i\uparrow} \right) \left(\langle \hat{n}_{i\downarrow} \rangle + \delta \hat{n}_{i\downarrow} \right) \\ &\simeq \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \delta \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \delta \hat{n}_{i\downarrow} + \mathcal{O}\left(\delta n^2\right) \\ &= - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \mathcal{O}\left(\delta n^2\right) \end{aligned}$$

where $\delta \hat{n}_{i\sigma} \equiv \hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle$ and orders higher than first have been ignored, assuming negligible fluctuations around the equilibrium single-site population. The first term of the above three can be neglected at fixed particles number, being a pure energy shift.

B.1 Ferromagnetic solution

The Mean-Field Theory ferromagnetic solution prescribes an uniformly magnetized lattice,

$$\langle \hat{n}_{i\uparrow} \rangle = n + m \qquad \langle \hat{n}_{i\downarrow} \rangle = n - m$$

where n is the site electron density and m is the density unbalance, leading to a magnetization per site $2m$. The mean-field hamiltonian with these substitutions becomes:

$$\begin{aligned} \hat{H} &\simeq -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \left[\hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} \right] \\ &= -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + nU \sum_{i} \left[\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \right] - mU \sum_{i} \left[\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \right] \end{aligned}$$

Fourier transforming,

$$\begin{aligned} -t \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} &= -2t \sum_{\mathbf{k}\sigma} \left[\cos(k_x) + \cos(k_y) \right] \hat{n}_{\mathbf{k}\sigma} \\ nU \sum_{i} \left[\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \right] &= nU \sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma} \\ mU \sum_{i} \left[\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \right] &= mU \sum_{\mathbf{k}\sigma} \left[\hat{n}_{\mathbf{k}\uparrow} - \hat{n}_{\mathbf{k}\downarrow} \right] \end{aligned}$$

having used adimensional lattice momenta. For a square lattice, the Brillouin Zone is delimited by

$$\mathbf{k} \in [-\pi, \pi] \times [-\pi, \pi]$$

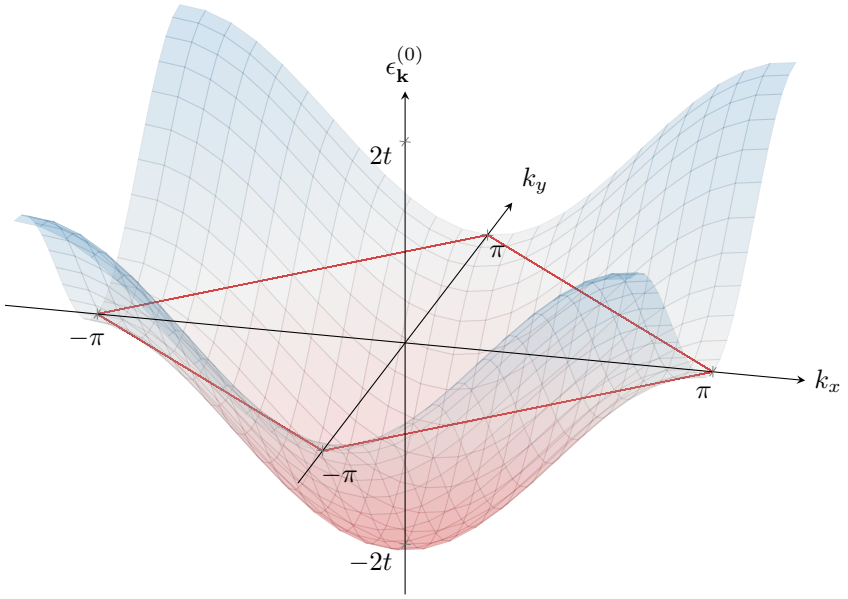


Figure B.1 | Depiction of the Hubbard square lattice hopping band $\epsilon^{(0)}_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)]$. The red lines mark the zero-energy intersection.

The hopping single-state energy is given by

$$\epsilon^{(0)}_{\mathbf{k}} = -2t\left[\cos(k_x) + \cos(k_y)\right]$$

represented as a band in Fig. B.1. At $U = 0$, the mean-field ferromagnetic state fills the band bottom-up. The single-state energy becomes:

$$\epsilon_{\mathbf{k}\uparrow} = U\left(n - m\right) - 2t\left[\cos(k_x) + \cos(k_y)\right]$$
$$\epsilon_{\mathbf{k}\downarrow} = U\left(n + m\right) - 2t\left[\cos(k_x) + \cos(k_y)\right]$$

Now it is a matter of finding the optimal value for m, minimizing the total energy at fixed filling $\rho = 2n$. Notice that said minimization is performed parametrically varying the magnetization m, inside the ferromagnetic-polarized space. As it turns out, for strong local repulsion $U/t \gg 1$, antiferromagnetic ordering is preferred. Comparison is needed in order to assess which magnetic ordering is preferred.

Consider the half-filling situation. An unpolarized system will have $n = 1/4$, $m = 0$: this implies $\langle \hat{n}_{i\uparrow} \rangle = \langle \hat{n}_{i\downarrow} \rangle = 1/4$. A perfectly up-ferromagnetic system, $n = 1/4$, $m = 1/4$: then $\langle \hat{n}_{i\uparrow} \rangle = 1/2$ and $\langle \hat{n}_{i\downarrow} \rangle = 0$. [To be continued...]

Unclear: numerically, it turns out the paramagnetic phase ($m = 0$) is preferred. Let $\Delta \equiv Um$ and ignore the constant contribution to energies Un: graphically, the $\uparrow$ band is shifted by Δ, the $\downarrow$ band by $-\Delta$. At half-filling the Fermi energy remains fixed. For each quadrant (top view of the bands), the DoS is inversion-symmetric with respect to the anti-diagonal (red lines in Fig. B.1), thus filling the bands bottom-up while performing the shifts should leave the total energy unchanged. Why is $m = 0$ preferred?

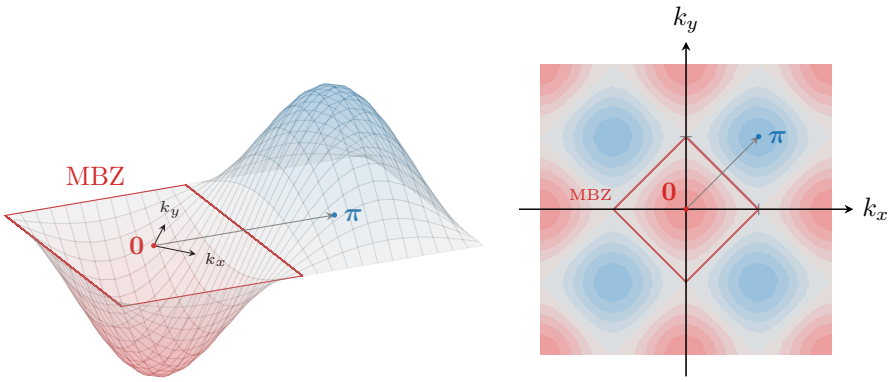
B.2 Antiferromagnetic solution

Consider now an AF mean-field solution. Let me change notation for a brief moment, indicating each site as

$$i \to \mathbf{r} = (x, y) \qquad x, y \in \mathbb{N}$$

The mean-field AF solution at half-filling is the uniform-modulated magnetization

$$m_{\mathbf{r}} = (-1)^{x+y} m \qquad m \in [-1, 1]$$



a | Alternative band. b | Contour plot.

Figure B.2 | Alternative depiction of the Hubbard square lattice hopping band previously reported in Fig. B.1. The Magnetic Brillouin Zone (MBZ) is delimited by the zero-energy contour and is indicated in figure. As it is evident, energy sign flips by taking a (π, π) translation in $\mathbf{k}$ space.

and a mean-field Ansatz

$$\langle \hat{n}_{\mathbf{r}\uparrow} \rangle = n + m_{\mathbf{r}} \qquad \langle \hat{n}_{\mathbf{r}\downarrow} \rangle = n - m_{\mathbf{r}}$$

With respect to the solution presented above, the only detail changing is the last term,

$$\hat{H} = -t \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}'\sigma} + nU \sum_{\mathbf{r}} [\hat{n}_{\mathbf{r}\uparrow} + \hat{n}_{\mathbf{r}\downarrow}] - mU \sum_{\mathbf{r}} (-1)^{x+y} [\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}] \tag{B.1}$$

Fourier-transforming, the phase factor can be absorbed in the destruction operator inside of $\hat{n}_{\mathbf{r}\sigma}$:

$$\begin{aligned}
\sum_{\mathbf{r}} (-1)^{x+y} \hat{n}_{\mathbf{r}\sigma} &= \sum_{\mathbf{r}} (-1)^{x+y} \hat{c}^{\dagger}_{\mathbf{r}\sigma} \hat{c}_{\mathbf{r}\sigma} \\
&= \sum_{\mathbf{r}} e^{i\boldsymbol{\pi}\cdot\mathbf{r}} \frac{1}{N} \sum_{\mathbf{k}\in \mathrm{BZ}} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \frac{1}{N} \sum_{\mathbf{k}'\in \mathrm{BZ}} e^{-i\mathbf{k}'\cdot\mathbf{r}} \hat{c}_{\mathbf{k}'\sigma} \\
&= \sum_{\mathbf{k}\in \mathrm{BZ}} \sum_{\mathbf{k}'\in \mathrm{BZ}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}'\sigma} \frac{1}{N^2} \sum_{\mathbf{r}} e^{-i[\mathbf{k}'-(\mathbf{k}+\boldsymbol{\pi})]\cdot\mathbf{r}} \\
&= \sum_{\mathbf{k}\in \mathrm{BZ}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma}
\end{aligned}$$

where $\boldsymbol{\pi} = (\pi, \pi)$. It follows:

$$mU \sum_{\mathbf{r}} (-1)^{x+y} [\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}] = \Delta \sum_{\mathbf{k}\in \mathrm{BZ}} \left[\hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^{\dagger}_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow} \right] \quad \text{where} \quad \Delta \equiv mU$$

Consider the band of Fig. B.1 at half-filling. As does Fabrizio [3], the area delimited externally by the solid lines at zero energy is denominated "Magnetic Brillouin Zone" (MBZ). The periodicity of $\mathbf{k}$ space guarantees that the full BZ can be taken as well to be the one of Fig. B.2a. Then:

$$\begin{aligned}
\sum_{\mathbf{k}\in \mathrm{BZ}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} &= \sum_{\mathbf{k}\in \mathrm{MBZ}} \left[\hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} + \hat{c}^{\dagger}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} \hat{c}_{\mathbf{k}+2\boldsymbol{\pi}\uparrow} \right] \\
&= \sum_{\mathbf{k}\in \mathrm{MBZ}} \left[\hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} + \hat{c}^{\dagger}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \right]
\end{aligned} \tag{B.2}$$

and the same applies for spin $\downarrow$. Periodicity by shifts $2\boldsymbol{\pi}$ has been used. Now, define the Nambu spinors:

$$\hat{\Psi}_{\mathbf{k}\sigma} \equiv \begin{bmatrix} \hat{c}_{\mathbf{k}\sigma} \\ \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma} \end{bmatrix}$$

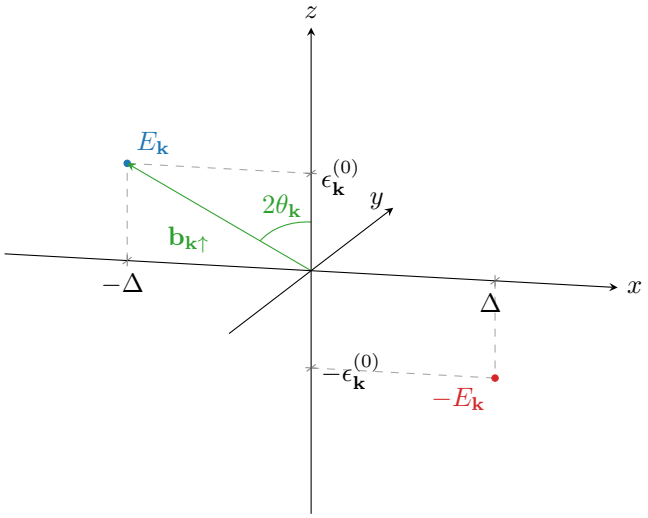


Figure B.3 | Pseudo-magnetic field originating from mean-field treatment of the square Hubbard hamiltonian. Here, only the $\sigma =\uparrow$

and a spin-wise gap,

$$\Delta_\uparrow = \Delta \qquad \Delta_\downarrow = -\Delta$$

At fixed filling, the U term is a pure energy shift, thus will be neglected. The kinetic term transforms as

$$\begin{aligned} -t \sum_{\langle ij \rangle} \sum_\sigma \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} &= \sum_{\mathbf{k}\in \mathrm{BZ}} \sum_\sigma \epsilon^{(0)}_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \\ &= \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_\sigma \left[\epsilon^{(0)}_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \epsilon^{(0)}_{\mathbf{k}+\boldsymbol{\pi}} \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\sigma} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma} \right] \\ &= \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_\sigma \epsilon^{(0)}_{\mathbf{k}} \left[\hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\sigma} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\sigma} \right] \end{aligned}$$

In the second passage, the sum over the full BZ was written considering that the entirety of the zone is given by all the points in the MBZ plus their conjugates obtained by a $\boldsymbol{\pi}$ shift in the flipped band. As depicted in Fig. B.2a, kinetic energy is anti-periodic in $\mathbf{k}$ space by a vector $\boldsymbol{\pi}$. This anti-periodicity accounts for the minus sign arising in the third passage. The hamiltonian is then given by:

$$\hat{H} = \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_\sigma \hat{\Psi}^\dagger_{\mathbf{k}\sigma} h_{\mathbf{k}\sigma} \hat{\Psi}_{\mathbf{k}\sigma} \quad \text{being} \quad h_{\mathbf{k}\sigma} \equiv \begin{bmatrix} \epsilon^{(0)}_{\mathbf{k}} & -\Delta_\sigma \\ -\Delta_\sigma & -\epsilon^{(0)}_{\mathbf{k}} \end{bmatrix} \tag{B.3}$$

Notice: the Nambu hamiltonian is a 2×2 matrix over the MBZ – which is half the full BZ, coherently with a solution which essentially bipartites the lattice giving back a double sized unit cell.

The system ground-state is obtained by the means of a Bogoliubov rotation. The hamiltonian maps onto the simple one of a spin in a magnetic field,

$$h_{\mathbf{k}\sigma} = \epsilon^{(0)}_{\mathbf{k}} \tau^x - \Delta_\sigma \tau^z$$

being τ^α the Pauli matrices. Then, defining

$$\hat{s}^\alpha_{\mathbf{k}\sigma} \equiv \hat{\Psi}^\dagger_{\mathbf{k}\sigma} \tau^\alpha \hat{\Psi}_{\mathbf{k}\sigma} \quad \text{and} \quad \mathbf{b}_{\mathbf{k}\sigma} \equiv \begin{bmatrix} \epsilon^{(0)}_{\mathbf{k}} \\ 0 \\ -\Delta_\sigma \end{bmatrix}$$

one gets:

$$\hat{H} = \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_\sigma \mathbf{b}_{\mathbf{k}\sigma} \cdot \hat{\mathbf{s}}_{\mathbf{k}\sigma} \quad \text{where} \quad \hat{\mathbf{s}}_{\mathbf{k}\sigma} = \begin{bmatrix} \hat{s}^x_{\mathbf{k}\sigma} \\ \hat{s}^y_{\mathbf{k}\sigma} \\ \hat{s}^z_{\mathbf{k}\sigma} \end{bmatrix} \tag{B.4}$$

The hamiltonian represents a system of spins subject to local magnetic fields, each tilted by an angle $\tan(2\theta_{\mathbf{k}\sigma}) = \Delta_\sigma/\epsilon^{(0)}_{\mathbf{k}}$, as sketched in Fig. B.3. At any finite temperature, the ground-state of such a system is well-known. Diagonalization of each $h_{\mathbf{k}\sigma}$ is obtained trivially by a simple rotation around the y axis:

$$d_{\mathbf{k}\sigma} = W_{\mathbf{k}\sigma} h_{\mathbf{k}\sigma} W^\dagger_{\mathbf{k}\sigma}$$

where

$$d_{\mathbf{k}\sigma} = \begin{bmatrix} E_{\mathbf{k}} & \\ & -E_{\mathbf{k}} \end{bmatrix} \quad \text{and} \quad W_{\mathbf{k}\sigma} = e^{i\theta_{\mathbf{k}\sigma}\tau^y} = \begin{bmatrix} \cos\theta_{\mathbf{k}\sigma} & \sin\theta_{\mathbf{k}\sigma} \\ -\sin\theta_{\mathbf{k}\sigma} & \cos\theta_{\mathbf{k}\sigma} \end{bmatrix}$$

Eigenvalues are:

$$E_{\mathbf{k}} \equiv \sqrt{\epsilon^2_{\mathbf{k}} + |\Delta_\sigma|^2}$$

(superscript "(0)" has been dropped momentarily). Notice that the presence of an absolute value makes the eigenvalues independent of the σ index. Eigenvectors are obtained simply as:

$$\hat{\Phi}_{\mathbf{k}\sigma} = W_{\mathbf{k}\sigma} \hat{\Psi}_{\mathbf{k}\sigma}$$

[To be continued...]

B.2.1 Theoretical mean-field solution

A convergence algorithm can be designed to find the Hartree-Fock solution to the model. Ultimately, we aim to extract m self-consistently. Since

$$\begin{aligned} m &= \frac{1}{2L^2} \sum_{\mathbf{r}} (-1)^{x+y} \langle \hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow} \rangle \\ &= \frac{1}{2L^2} \sum_{\mathbf{k}\in \mathrm{BZ}} \left\langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow} \right\rangle \\ &= \frac{1}{2L^2} \sum_{\mathbf{k}\in \mathrm{MBZ}} \left\langle \left(\hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\uparrow} + \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \right) - \left(\hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}+\boldsymbol{\pi}\downarrow} + \hat{c}^\dagger_{\mathbf{k}+\boldsymbol{\pi}\downarrow} \hat{c}_{\mathbf{k}\downarrow} \right) \right\rangle \end{aligned}$$

In the last passage, Eq. (B.2) has been used. Then magnetization can be computed simply as

$$m = \frac{1}{2L^2} \sum_{\mathbf{k}\in \mathrm{MBZ}} \left[\left\langle \hat{\Psi}^\dagger_{\mathbf{k}\uparrow} \tau^x \hat{\Psi}_{\mathbf{k}\uparrow} \right\rangle - \left\langle \hat{\Psi}^\dagger_{\mathbf{k}\downarrow} \tau^x \hat{\Psi}_{\mathbf{k}\downarrow} \right\rangle \right] \tag{B.5}$$

In this equation, spin expectation values appear:

$$\left\langle \hat{\Psi}^\dagger_{\mathbf{k}\sigma} \tau^x \hat{\Psi}_{\mathbf{k}\sigma} \right\rangle = \langle \hat{s}^x_{\mathbf{k}\sigma} \rangle$$

Now discussion is divided in two parts: zero temperature and finite temperature.

Zero temperature solution

For a spin system at zero temperature, the spin operator expectation value anti-aligns with the external field,

$$\langle \hat{s}^x_{\mathbf{k}\sigma} \rangle = \sin(2\theta_{\mathbf{k}\sigma})$$

(see Fig. B.3). Now, since $\Delta_\downarrow = -\Delta_\uparrow$, it follows

$$\theta_{\mathbf{k}\downarrow} = -\theta_{\mathbf{k}\uparrow} \equiv \theta_{\mathbf{k}}$$

Then, from Eq. (B.5)

$$\begin{aligned} m &= \frac{1}{L^2} \sum_{\mathbf{k}\in \mathrm{MBZ}} \sin(2\theta_{\mathbf{k}}) \\ &= \frac{1}{2L^2} \sum_{\mathbf{k}\in \mathrm{BZ}} \sin(2\theta_{\mathbf{k}}) \end{aligned}$$

The last passage is due to the fact that the sum over the MBZ can be performed identically over $\mathrm{BZ} \setminus \mathrm{MBZ}$ and yield the same result. This is because of the lattice periodicity in reciprocal space. Then, finally:

$$m = \frac{1}{L^2} \sum_{\mathbf{k} \in \mathrm{BZ}} [W_{\mathbf{k}\uparrow}]_{11} [W^\dagger_{\mathbf{k}\uparrow}]_{21} \tag{B.6}$$

where $\sin(2\theta_{\mathbf{k}}) = 2 \sin\theta_{\mathbf{k}} \cos\theta_{\mathbf{k}}$ has been used. As will become clear in next section, the sudden appearance of matrix elements of W is not casual.

Finite temperature solution

At finite temperature β, discussion is analogous to the section above. Here will be treated somewhat more theoretically. Define the generic order parameter:

$$\Delta_{ij}(\mathbf{k}\sigma) \equiv \left\langle [\hat{\Psi}^\dagger_{\mathbf{k}\sigma}]_i [\hat{\Psi}_{\mathbf{k}\sigma}]_j \right\rangle$$

In last section, the relevant indices (i, j) were $(1, 2)$ and $(2, 1)$. Transform this order parameter,

$$\begin{aligned}
\Delta_{ij}(\mathbf{k}\sigma) &= \sum_{i'j'} \left\langle [\hat{\Phi}^\dagger_{\mathbf{k}\sigma}]_{i'} [W_{\mathbf{k}\sigma}]_{i'i} [W^\dagger_{\mathbf{k}\sigma}]_{jj'} [\hat{\Phi}_{\mathbf{k}\sigma}]_{j'} \right\rangle \\
&= \sum_{i'j'} [W_{\mathbf{k}\sigma}]_{i'i} [W^\dagger_{\mathbf{k}\sigma}]_{jj'} \left\langle [\hat{\Phi}^\dagger_{\mathbf{k}\sigma}]_{i'} [\hat{\Phi}_{\mathbf{k}\sigma}]_{j'} \right\rangle \\
&= \sum_{i'j'} [W_{\mathbf{k}\sigma}]_{i'i} [W^\dagger_{\mathbf{k}\sigma}]_{jj'} \delta_{i'j'} f\left([d_{\mathbf{k}\sigma}]_{i'i'}; \beta, \mu\right) \\
&= \sum_{\ell=1}^{2} [W_{\mathbf{k}\sigma}]_{\ell i} [W^\dagger_{\mathbf{k}\sigma}]_{j\ell} f\left((-1)^{\ell+1} E_{\mathbf{k}\sigma}; \beta, \mu\right) \\
&= [W_{\mathbf{k}\sigma}]_{1i} [W^\dagger_{\mathbf{k}\sigma}]_{j1} f\left(-E_{\mathbf{k}\sigma}; \beta, \mu\right) + [W_{\mathbf{k}\sigma}]_{2i} [W^\dagger_{\mathbf{k}\sigma}]_{j2} f\left(E_{\mathbf{k}\sigma}; \beta, \mu\right)
\end{aligned} \tag{B.7}$$

being f be the Fermi-Dirac distribution at inverse temperature β and chemical potential μ,

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

In the second passage this distribution appeared because an expectation value over a gas of free Φ fermions was taken. Such an expectation value admits no off-diagonal values, hence the $\delta_{i'j'}$. The diagonal entries are precisely the definition of the Fermi-Dirac distribution for the given energy. At zero temperature and half-filling, the lower band $-E_{\mathbf{k}}$ is completely filled while the upper band $E_{\mathbf{k}}$ is empty. Substituting $f = 1$ in the first term of line (B.7), $f = 0$ in the second and summing Δ_{12} and Δ_{21} as done in Eq. (B.5), it's easy to derive the result of Eq. (B.6). At finite temperature, following the lead of the above paragraph, the antiferromagnetic instability order parameter m will be given simply by

$$m = \frac{1}{2L^2} \sum_{\mathbf{k} \in \mathrm{BZ}} \sum_{\ell=1}^{2} [W_{\mathbf{k}\uparrow}]_{\ell 1} [W^\dagger_{\mathbf{k}\uparrow}]_{2\ell} f\left((-1)^{\ell+1} E_{\mathbf{k}\sigma}; \beta, \mu\right) \tag{B.8}$$

Then: mean-field approximations yield an estimate for the magnetization at a given temperature and chemical potential just by carefully combining the elements of the diagonalizing matrix W of each Bogoliubov matrix $h_{\mathbf{k}\sigma}$.

B.2.2 Hartree-Fock algorithm in k space

The above sections offers a self-consistency equation for the magnetization m; W is determined by m indeed. Then a self-consistent algorithm to search for a self consistent estimate for m may be sketched:

0. Algorithm setup: initialize a counter $i = 1$ and choose:

- the coarse-graining of the BZ, which is, fix L_x and L_y. Then

$$k_x = 2\pi n_x/L_x \qquad k_y = 2\pi n_y/L_y$$

  where $-L_j/2 \leq n_j \leq L_j/2$, $n_j \in \mathbb{Z}$;
- the desired density n;
- the number of iterations $p \in \mathbb{N}$;
- the mixing parameter $g \in [0, 1]$;
- the tolerance parameters $\delta_m, \delta_n \in \mathbb{R}$ (respectively for magnetization and density);

1. Select a random starting value $m_0 \in [-(1-n), 1-n]$;
2. For each slot of the BZ, initialize the appropriate 2×2 matrix $h_{\mathbf{k}\sigma}$;
3. For the given hamiltonian, find the optimal chemical potential μ as follows:
   a) Define the generic matrix $A[m_0, \mu]$ dependent on m_0 and μ;
   b) Define the density as a function of the chemical potential μ,

   ...

4. Diagonalize the matrix $h_{\mathbf{k}\sigma} - \mu n_{\mathbf{k}\sigma}$;
5. Compute m using Eq. (B.8) and update the counter, $i \to i + 1$;
6. Check if $|m - m_0| \leq \delta_m$:
   - If yes, halt;
   - If not: check if $i > p$
     - If yes, halt and consider choosing better tolerance and model parameters;
     - If not, define

$$m_0 = gm + (1-g)m_0$$

       (logical assignment notation used) and repeat from step 2.

[To be continued...]

B.2.3 An alternative (less efficient) real-space approach

The theoretical derivation of the above paragraphs offers a simple description of the system anti-ferromagnetic instability as the instauration of a ground-state of quasiparticles. Here a self-consistent algorithmic extraction of the expected magnetization is presented, following [7]. Note that this algorithm is by far the least efficient, being performed in real space with dimensional exponential scaling in terms of computational time. It is here presented just for completeness as an alternative derivation. Consider a square lattice of $L_x \times L_y$ sites: the hamiltonian will be a matrix of dimension $2L_xL_y \times 2L_xL_y$,

$$[\hat{H}]_{(\mathbf{r}\sigma)(\mathbf{r}'\sigma')} = \langle\Omega|\hat{c}_{\mathbf{r}\sigma}\hat{H}\hat{c}^\dagger_{\mathbf{r}'\sigma'}|\Omega\rangle$$

For simplicity, in the following $D \equiv 2L_xL_y$. In this context, the following convention is used: the rows/column index entry $\alpha = (\mathbf{r}\sigma)$ is associated to a specific site $\mathbf{r} = (x, y)$ and spin σ through the relation

$$\alpha = 2j_{\mathbf{r}} - \delta_{\sigma=\uparrow} \quad \text{where} \quad j_{\mathbf{r}} = x + (y-1)L_x$$

Let me break this through. For each site $\mathbf{r}$, two sequential indices are provided ($2j_{\mathbf{r}} - 1$, hosting spin $\uparrow$, and $2j_{\mathbf{r}}$, hosting spin $\downarrow$). $j_{\mathbf{r}}$ just orders the site rows-wise. This way, $(x, 1)$ is assigned to $j_{(x,1)} = x$, while its NN one site above $(x, 2)$ is assigned to an entry shifted by L_x, $j_{(x,2)} = x + L_x$. This is just a way of counting the site of a finite square lattice by sweeping along a row and then moving to the row above. Fig. B.4 reports a scheme of the used site ordering.

Within this convention, matrix elements $H_{\alpha\beta}$ are defined by:

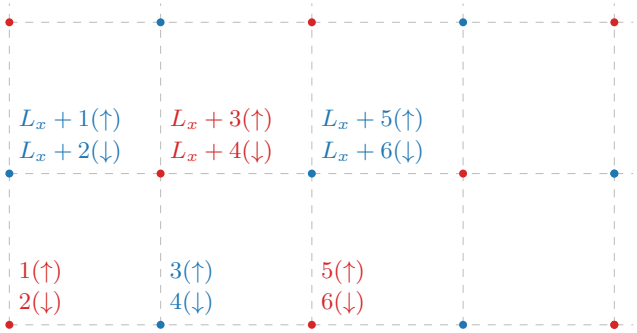


Figure B.4 Schematics of the site ordering on a square lattice performed by sweeping along rows. Left-bottom side is one corner of the lattice. Red sites are characterized by $x+y$ being odd, blue sites by being even. The number reported near to each site is the α entry in the matrix representation for a finite square lattice.

- If $\sigma = \sigma'$ and $\mathbf{r}$, $\mathbf{r}'$ are NN, the matrix entry is $-t$. In terms of the used greek indices, α and β satisfy said requirement if $|\alpha - \beta| = 2$ (horizontal hopping) or $|\alpha - \beta| = 2L_x$ (vertical hopping). Along column α of the hamiltonian matrix, the elements $-t$ appear at positions

$$(\alpha \pm 2L_x) \mod D \quad \text{and} \quad (\alpha \pm 2) \mod D$$

- If $\mathbf{r} = \mathbf{r}'$ and $\sigma = \sigma'$ (along the diagonal), the local interaction with the mean field is given by the matrix element

$$-mU \times (-1)^{x+y} \times (-1)^{\delta_{\sigma=\downarrow}}$$

Starting from a given entry α, $j_{\mathbf{r}}$ is retrieved simply by $j_{\mathbf{r}} = \lfloor \alpha/2 \rfloor$, and then

$$x + y = (j_{\mathbf{r}} + 1) - \left\lfloor \frac{j_{\mathbf{r}}}{L_x} \right\rfloor (L_x - 1)$$

Then the $j_{\mathbf{r}}$-th 2×2 block along the diagonal will be given by

$$(-1)^{x+y} \underbrace{\begin{bmatrix} -mU & \\ & mU \end{bmatrix}}_{\mathcal{B}}$$

Note that the resulting block diagonal contribution to the hamiltonian is shaped like follows (assume L_x to be even):

$$\begin{array}{c} \\ 1 \\ 2 \\ \vdots \\ L_x - 1 \\ L_x \\ L_x + 1 \\ L_x + 2 \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & \cdots & L_x - 1 & L_x & L_x + 1 & L_x + 2 & \cdots \end{array} \\ \begin{bmatrix} \mathcal{B} & & & & & & & \\ & -\mathcal{B} & & & & & & \\ & & \ddots & & & & & \\ & & & \mathcal{B} & & & & \\ & & & & -\mathcal{B} & & & \\ & & & & & -\mathcal{B} & & \\ & & & & & & \mathcal{B} & \\ & & & & & & & \ddots \end{bmatrix} \end{array}$$

Along the same row, on the diagonal the 2×2 blocks $\mathcal{B}$ alternate signs; changing row (in the example above, at positions $L_x, L_x + 1$), due to the anti-ferromagnetic configuration of local mean-fields, an additional -1 is included. If L_x is taken to be odd, the diagonal blocks just alternate signs all the way.

These prescriptions allow to build from scratch the hamiltonian matrix. After that, diagonalization provides D orthonormal eigenvectors $\mathbf{v}^\ell \in \mathbb{C}^{D \times D}$ with $\ell = 1, \cdots, D$, each associated to a precise

eigenvalue $\epsilon^\ell \in \mathbb{R}$. At equilibrium, electrons will fill up the energy eigenstates according to,

$$\langle \hat{n}_{\mathbf{r}\sigma} \rangle = \sum_{\ell=1}^{D} \left| v_\alpha^\ell \right|^2 f(\epsilon^\ell; \beta, \mu) \quad \text{where} \quad \alpha = (\mathbf{r}\sigma)$$

For a fixed filling $n = N/D$, the chemical potential must satisfy

$$\begin{aligned} n &= \frac{1}{D} \sum_{\mathbf{r}\sigma} \langle \hat{n}_{\mathbf{r}\sigma} \rangle \\ &= \frac{1}{D} \sum_{\mathbf{r}\sigma} \sum_{\ell=1}^{D} \left| v_\alpha^\ell \right|^2 f(\epsilon^\ell; \beta, \mu) \\ &= \frac{1}{D} \sum_{\ell=1}^{D} f(\epsilon^\ell; \beta, \mu) \end{aligned}$$

since the $\mathbf{v}^\ell$ eigenvectors are orthonormal. The chemical potential for the half-filled model is already known to be

$$\mu\big|_{n=1/2} = -\frac{U}{2}$$

as evident from Eq. (B.1). Average magnetization is then given by

$$\begin{aligned} m &= \frac{1}{D} \sum_{\mathbf{r}} (-1)^{x+y} \left[\langle \hat{n}_{\mathbf{r}\uparrow} \rangle - \langle \hat{n}_{\mathbf{r}\downarrow} \rangle \right] \\ &= \frac{1}{D} \sum_{\lambda=1}^{D/2} (-1)^{(\lambda+1)-\lfloor \lambda/L_x \rfloor (L_x-1)} \sum_{\ell=1}^{D} \left[\left| v_{2\lambda-1}^\ell \right|^2 - \left| v_{2\lambda}^\ell \right|^2 \right] f(\epsilon^\ell; \beta, \mu) \end{aligned} \tag{B.9}$$

since $\mathbf{r} \uparrow$ is associated to an odd index entry, while $\mathbf{r} \downarrow$ to the following even entry. The associated HF algorithm is identical to the one presented in Sec. B.2.2, with the following substitutions:

2. Initialize the hamiltonian matrix $H_{\alpha\beta}$ matrix according to the initialized m_0 and the site indexing rules of Fig. B.4;
4. Diagonalize the matrix associated to the operator $\hat{H}_{\alpha\beta} - \mu \hat{N}$ collecting the $\mathbf{v}^\ell$ eigenvectors;
5. Compute m using Eq. (B.9) and update the counter, $i \to i + 1$;

Results

[To be continued...]

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