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
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 [Missing] that below a certain critical temperature T_c the ground-state acquires antiferromagnetic (AF) long-range ordering. schematically depicted in Fig. 1.1. The mechanism for the formation of the AF phase takes advantage of virtual hopping, as described in App. A.

App. B describes the Mean-Field Theory description of ferromagnetic-antiferromagnetic orderings in 2D Hubbard lattices.

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] to be a necessary ingredient to describe the insurgence of high-T_c superconductivity in cuprate SCs. [To be continued. . .]

1. Fourier transform and Brillouin zone;

2. Pairing operator;

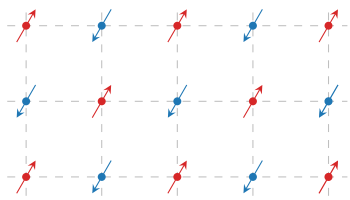

Figure 1.1 | Schematic representation of the AF phase.

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 $|\psi_2\rangle$.

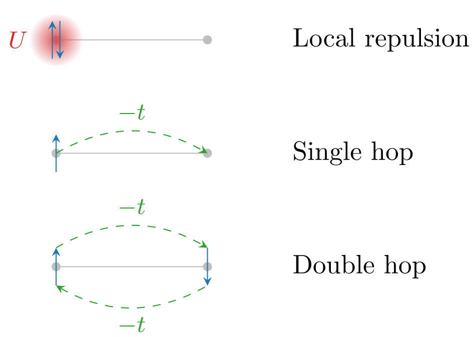

Figure A.1 | Two sites Hubbard model.

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

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

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 $|\phi_6\rangle$.

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 and magnetic ordering

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.

B.1 Ferromagnetic solution

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 magnetization. The first term of the above three can be neglected, being a pure energy shift. 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,

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

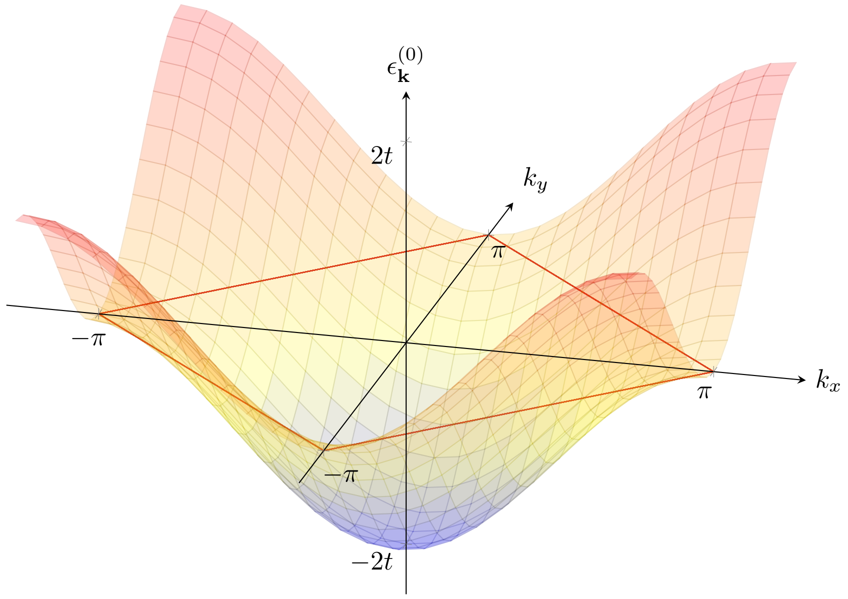

Figure B.1 Depiction of the Hubbard square lattice hopping band $\epsilon_{\mathbf{k}}^{(0)} = -2t[\cos(k_x) + \cos(k_y)]$. The red lines mark the zero-energy intersection.

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

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

The hopping single-state energy is given by

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

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:

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

Now it is a matter of finding the optimal value for m, minimizing the total energy at fixed filling $\rho = 2n$. Consider the half-filling situation. An unpolarized system will have $n = 1/4$, $m = 0$. A perfectly up-ferromagnetic system, $n = 1/4$, $m = 1/4$. [To be continued…]

B.2 Antiferromagnetic solution

Bibliography

[1] Zhangkai Cao et al. *p-wave superconductivity induced by nearest-neighbor attraction in the square-lattice extended Hubbard model*. en. arXiv:2408.01113 [cond-mat]. Jan. 2025. DOI: 10.48550/arXiv.2408.01113. URL: http://arxiv.org/abs/2408.01113 (visited on 03/15/2025).

[2] Piers Coleman. *Introduction to Many-Body Physics*. Cambridge University Press, 2015.