Notes on the Cuprates and Superconductivity

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HIGH-TC SUPERCONDUCTIVITY IN CUPRATES

Ever since the discovery of superconductivity in mercury (Hg) with a superconducting transition temperature temperature of $T_c \approx 4.19$K, physicists have never stopped looking for superconductors with higher T_c, in the hope of finding room-temperature superconductors that could be used for lossless power transmission and many other applications. Progress along this road was very slow for the first 75 years after the 1911 discovery; before 1986 the study of superconductivity were mainly limited to the simple metals, which can be understood by the BCS theory as we introduced before. A breakthrough came in 1986, when Bednorz and Müller found superconductivity in $La_{2-x}Ba_xCuO_4$ with $T_c > 30$ K. It was found shortly afterwards that this is just one member of a family of copper-oxide compounds obtained by doping the same parent compound, $La_{2-x}M_xCuO_4$, with the dopant M being Ba, Sr, or Ca. See Fig. 1 for their structures. In the years following this discovery by Bednorz and Müller, more copper-oxide compounds were found, with ever-increasing T_c (and also greater complexity in their structures), including $YBa_2Cu_3O_7$ ($T_c \sim 92$ K), the YBCO family, $Bi_2Sr_2CaCu_2O_8$ ($T_c \sim 89$ K), and the BSCCO family, among others. The record (at the time of writing) at ambient pressure is held by $HgBa_2Ca_2Cu_3O_{8+\delta}$, with $T_c = 135$ K. All of these compounds share a common feature, namely they all contain copper-oxide (CuO_2) planes, which are widely believed to be responsible for the superconductivity as well as many other important properties. These compounds are collectively known as high-temperature cuprate superconductors, or simply cuprates. In the following we analyze the (original) LaMCuO family (in particular LSCO, which is the most studied compound in this family) in some detail due to its relatively simple structure, despite the modest $T_c \sim 39$ K for $x = 0.15$.

As the phase diagrams in Fig. 2 show, the superconducting state emerges near the antiferromagnetic phase. In the yttrium – barium system the regions of antiferromagnetism and superconductivity are adjacent, while in the lanthanum system the two are separated by a region without long-range magnetic order but with strong quantum fluctuations. This region became known as the spin-liquid region. Therefore, the ordinary interrelationship between magnetic order and superconductivity: the two avoid each other. At the same time, experiments in inelastic magnetic scattering of neutrons in the lanthanum and yttrium – barium systems indicate that there are strong magnetic fluctuations for a broad

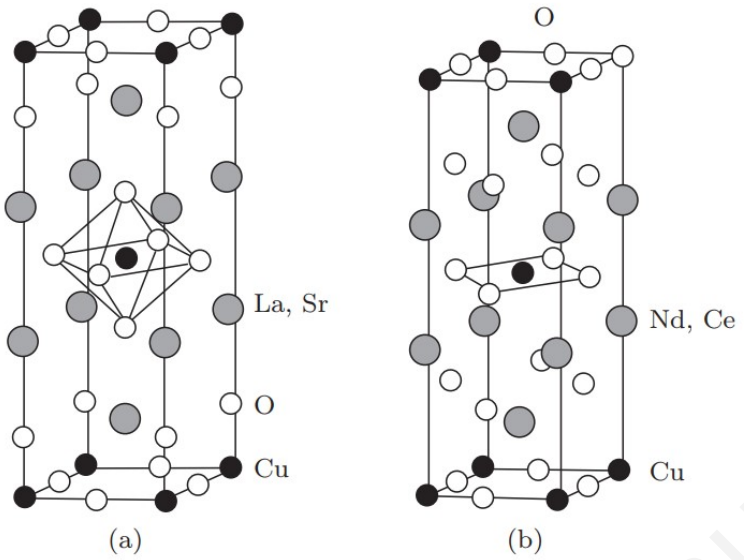

FIG. 1: Crystal structure of cuprate compounds.

range of doping levels outside the antiferromagnetic phase, a range that even penetrates the superconducting-phase region. This, obviously, is an indication of how important antiferromagnetic fluctuations are in the mechanism of high-Tc superconductivity.

Analysis of orbitals

Let us start with the parent compound La_2CuO_4. Compared with other compounds, it already has a fairly complicated structure. We start our analysis with individual atoms (ions). Oxygen's outer-shell electron configuration is $2s^2 2p^4$. As in most cases, here its valence -2 leads to a closed-shell configuration $2s^2 2p^6$ for O^{2-}, which should be familiar from chemistry. Lanthanum's outer-shell electron configuration is $5d^1 6s^2$. It has valence +3, meaning that it loses all of its outer-shell electrons, again resulting in a closed-shell configuration for La^{3+}. Simple electron counting finds that copper must have valence +2 here: Removing two electrons from its $3d^{10}4s^1$ configuration results in $3d^9$ for Cu^{2+}. There is thus a single hole in the copper ion's 3d orbitals, and the system may be magnetic due to its net spin. As we will see shortly, this is indeed the case.

Physical properties of the compound change dramatically when a small fraction of La is replaced by Ba, Sr, or Ca. Let us analyse the effects of such doping. Ba, Sr, and Ca are all alkali earth elements with valence +2. They thus each donate one electron fewer

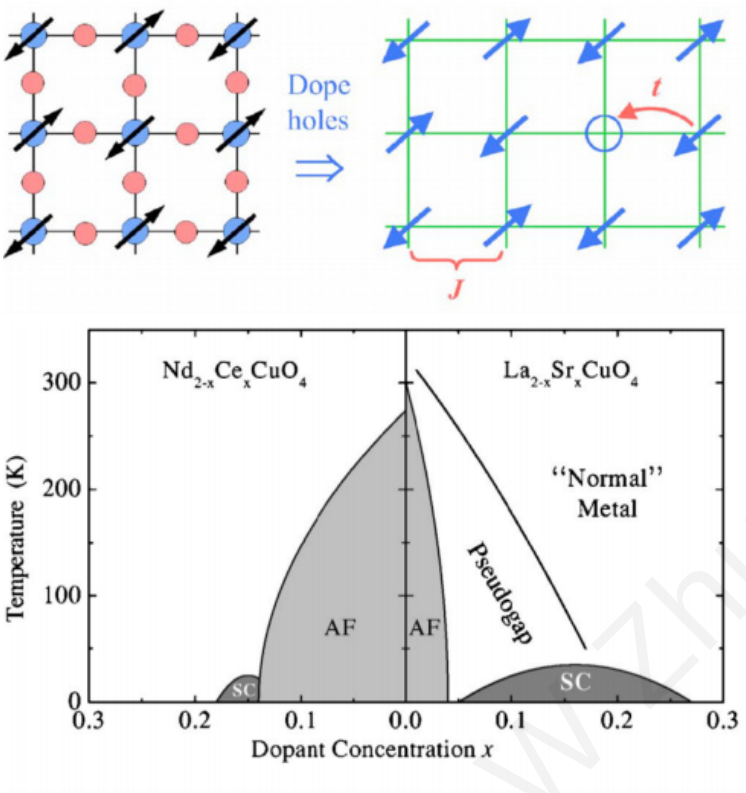

FIG. 2: Top:The blue circles are copper atoms, and red is oxygen. The black arrows indicate the electron in the d orbital. The right part of the figure shows the reduction into a 2D t-J model. Bottom: Phase diagram for hole-doped cuprate; right: Phase diagram for hole-doped and electron-doped cuprate

than La does, and play a role very similar to that of acceptors in a semiconductor. As a result, each such dopant contributes an additional hole to the CuO_2 planes, and dopes them away from half-filling. Most cuprates can be hole-doped, but there are a few that can be electron-doped. One example of such an electron-doped cuprate is $Nd_{2-x}Ce_xCuO_4$. Nd has valence +3; when it is replaced by the dopant Ce with valence +4, an additional electron goes to the CuO_2 planes and annihilates an existing hole. Thus Ce plays a role similar to that of a donor in a semiconductor.

At the local site, due to the symmetry reason, t_{2g} and e_g are splitting. $3d_{xz}$, $3d_{xy}$, $3d_{yz}$ are all filled and below the fermi level. $3d^9$ copper has $3d_{x^2-y^2}$ orbital close to the fermi level. The case of a half-filled band leads to an insulator state with localized magnetic moments ($S = 1/2$) corresponding to the d^9 state of the copper ions in the CuO_2 planes. Upon doping, a fraction of the copper atoms lose one electron each, so that hole type charge carriers are

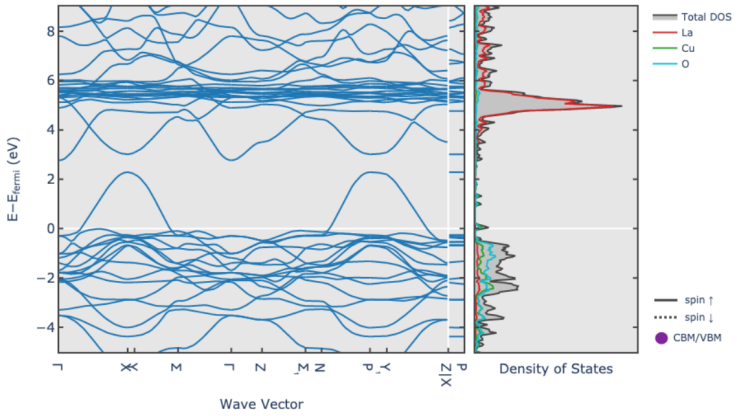

FIG. 3: DFT band structure of $LaCuO_4$. The fermi energy is set to be 0.

created. Strictly speaking, holes are created upon doping not only at copper atoms but also at oxygen atoms. These holes form what is known as Zhang–Rice singlets centered at copper sites.

Hubbard model

The Hubbard model has a relatively long history [J. Hubbard: Electron correlations in narrow energy bands, Proc R. Soc. A, Vol. 276 No. 1365 (1963) 238-257; Proc R. Soc. A, Vol. 277 No. 1369 (1964) 237-259]. Very early (in the 1950s) it was used by Pariser, Pople and Parr for orbital calculations and to describe molecules in quantum chemistry. Variations were used subsequently by P. Anderson and others in difierent contexts. The Hubbard model in its modern form was systematically introduced independently by Gutzwiller, Hubbard and Kanamory in the early 1960s. The aim was to study magnetism in transition metals. This early work initiated a burst of activity in the fleld lasting until today. However, despite its simplistic appearance, the Hubbard model is not fully understood yet. The Hubbard model plays an extremely important role in the fleld of correlated lattice systems. We may call the Hubbard model (with some exaggeration) the Standard Model of solid state physics. The main reason of its popularity is the inclusion of electron correlation, its simplicity and the rich physics contained in the model.

Consider the single-orbital Hubbard model, which introduces an energy cost U for double

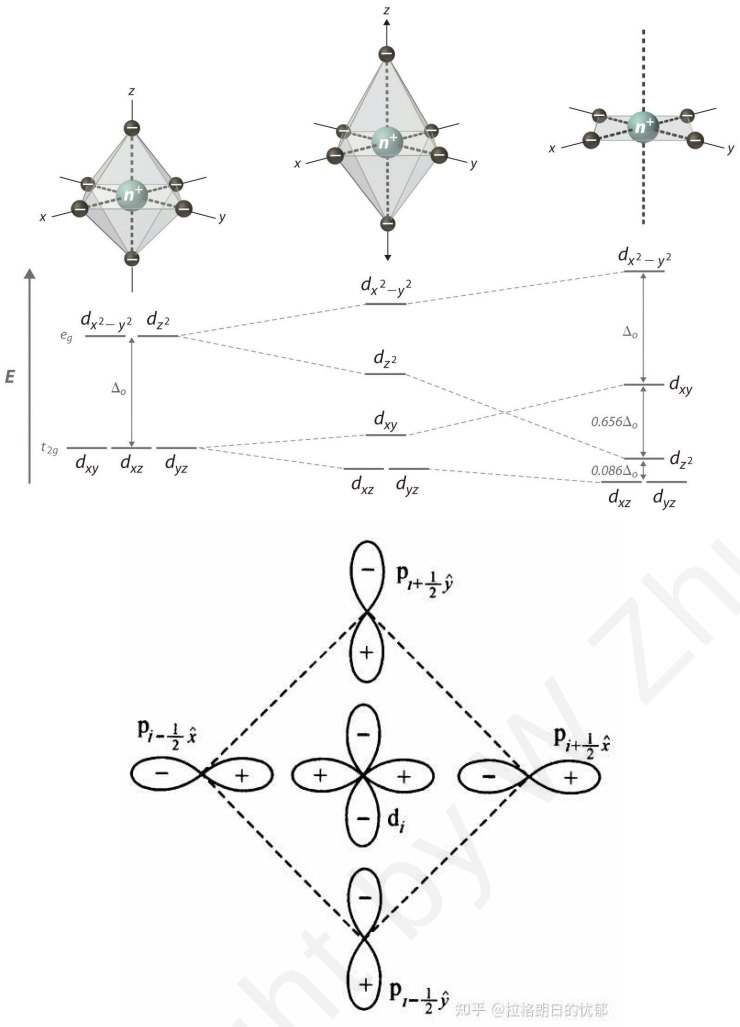

FIG. 4: Local orbitals in the CuO_2 plane.

occupancy on a site, given by

$$H = -t \sum_{\langle i,j \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

where U is the local Coulomb interaction, $c^\dagger_{i,\sigma}$ creates (annihilates) an electron on site i with spin σ. Motivated by the local interaction being a density-density interaction so that particle number is a good quantum number for the interaction.

We see from the above discussion that each term of the Hubbard hamiltonian is very simple: The hopping part has an itinerant electron ground state and the interaction part has a localized ground state. However, the sum of these very simple parts is highly non-trivial and very difficult to understand quantitatively. But we can be sure that the two efiects (localize, delocalize) will compete with each other.

METHODOLOGY OF SLAVE-BOSON

Kotliar-Ruckenstein slave-boson theory introduces bosons to keep track of the occupation of electrons on site i, i.e., it introduces an over-complete description of the states on site i, given by

$$|e_i\rangle \sim \hat{e}_i^\dagger |0_i\rangle \tag{2}$$

$$|\sigma_i\rangle \sim \hat{p}_{i,\sigma}^\dagger |0_i\rangle \tag{3}$$

$$|d_i\rangle \sim \hat{d}_i^\dagger |0_i\rangle \tag{4}$$

where the bosons $\hat{e}_i$, $\hat{p}_{i,\sigma}$, and $\hat{d}_i$ corresponds to an empty site, a site with one electron with spin σ, and a doubly occupied site respectively. Here $|0_i\rangle$ is the vacuum on site i.

Introduction of the bosons enlarges the Hilbert space. The chosen basis that generates the slave-boson Hilbert space is built from tensor products of a (quasi-)fermion Fock state and a boson Fock state. In the enlarged Hilbert space there are nonphysical states that can be eliminated by introducing the constraints

$$1 = \hat{e}_i^\dagger \hat{e}_i + \hat{d}_i^\dagger \hat{d}_i + \hat{p}_{i,\uparrow}^\dagger p_{i,\uparrow} + \hat{p}_{i,\downarrow}^\dagger p_{i,\downarrow} \tag{5}$$

$$\hat{n}_{i,\sigma} = \hat{d}_i^\dagger \hat{d}_i + \hat{p}_{i,\sigma}^\dagger p_{i,\sigma} \tag{6}$$

The first equation is a completeness relation to ensure there is exactly one boson per site, and the second equation ensures that the correct boson corresponds with the (quasi-)fermions. The constraints restrict the enlarged Hilbert space H_{SB} to the physical states in the Hilbert space H. In the enlarged Hilbert space the physical electron has a representation

$$c_{i\sigma} = f_{i\sigma}(\hat{e}_i^\dagger \hat{p}_{i,\sigma} + \hat{p}_{i,-\sigma}^\dagger \hat{d}_i) = f_{i\sigma}\hat{z}_i \tag{7}$$

$\hat{z}_i$ is the renormalization factor that ends up renormalizing the (quasi-)fermion $f_{i\sigma}$ at the mean field level. One can see that this representation is faithful for describing electrons moving between sites i and j.

With the introduction of the slave-bosons, the local part has the representation

$$U n_{i,\uparrow} n_{i,\downarrow} = U \hat{d}_i^\dagger \hat{d}_i \tag{8}$$

Hence, the single orbital Hubbard model in the enlarged Hilbert space HSB is given by

$$H_{SB} = \sum_{ij,\sigma} \hat{z}_i^\dagger z_j f_{i,\sigma}^\dagger f_{j,\sigma} + U\hat{d}_i^\dagger \hat{d}_i + \lambda^1(1 - \hat{e}_i^\dagger \hat{e}_i + \hat{d}_i^\dagger \hat{d}_i + \hat{p}_{i,\uparrow}^\dagger \hat{p}_{i,\uparrow} + \hat{p}_{i,\downarrow}^\dagger \hat{p}_{i,\downarrow})$$
$$+ \sum_\sigma \lambda_\sigma^2 (f_{i,\sigma}^\dagger f_{i,\sigma} - \hat{d}_i^\dagger \hat{d}_i - \hat{p}_{i,\sigma}^\dagger p_{i,\sigma}) \tag{9}$$

where $\lambda^{1,2}$ are Lagrange multipliers used to enforce the constraints.

Mean field approximation

A mean field approximation is done where the bosons take their average value over all sites and the constraints are only enforced on average, i.e., the lattice is considered homogeneous and the bosonic quantum operators condense to complex numbers (a real number in this case),

$$\langle \hat{e}_i \rangle = e = \tfrac{1}{N} \textstyle\sum_i \langle \hat{e}_i \rangle \tag{10}$$
$$\langle \hat{p}_{i,\sigma} \rangle = p_\sigma = \tfrac{1}{N} \textstyle\sum_i \langle \hat{p}_{i,\sigma} \rangle \tag{11}$$
$$\langle \hat{d}_i \rangle = d = \tfrac{1}{N} \textstyle\sum_i \langle \hat{d}_i \rangle \tag{12}$$

where N is the number of sites on the lattice. Now the slave-bosons give the probability of an electron configuration on the lattice, e.g., $\langle d_i^\dagger d_i \rangle = d^2$ gives the probability of double occupancy on the lattice.

$$H_{SB}^{MF} = \sum_{ij,\sigma} Z_\sigma f_{i,\sigma}^\dagger f_{j,\sigma} + NUd^2 - \mu \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + \lambda^1(1 - e^2 - d^2 - 2p^2) + \sum_\sigma \lambda_\sigma^2 (\hat{f}_{i,\sigma}^\dagger f_{i,\sigma} - d^2 - p^2) \tag{13}$$

Z_σ is renormalization factor (the form will be specified later). Additionally, we have included the chemical potential μ to write H in the grand canonical ensemble.

By Fourier transformation, the mean field Hamiltonian becomes

$$H_{SB}^{MF} = \sum_{k,\sigma} (Z_\sigma \epsilon_k + \lambda_\sigma^2 - \mu) f_{k,\sigma}^\dagger f_{k,\sigma} + N[Ud^2 - 2\lambda^2(d^2 + p^2) + \lambda^1(1 - d^2 - e^2 - 2p^2)] \tag{14}$$

Free-energy functional

Defining the renormalized band of quasiparticles as $\xi_{k,\sigma} = Z_\sigma \epsilon_k + \lambda^2 - \mu$ and remembering $n_{k,\sigma} = f^\dagger_{k,\sigma} f_{k,\sigma}$, the grand canonical partition function is given by

$$Z = Tr[e^{-\beta H^{MF}_{SB}}] = Tr[e^{-\beta \sum_{k,\sigma} \xi_{k,\sigma} n_{k,\sigma}} e^{-\beta(NUd^2 - 2\lambda^2(d^2+p^2) + \lambda^1(1-d^2-e^2-2p^2)}] = Z_f e^{-\beta(NUd^2 - 2\lambda^2(d^2+p^2) + \lambda^1(1-d^2} \tag{15}$$

where

$$Z_f = Tr[e^{-\beta \sum_{k,\sigma} \xi_{k,\sigma} n_{k,\sigma}}] = \prod_{k\sigma} Tr e^{-\beta \xi_{k,\sigma} n_{k,\sigma}} = \prod_{k\sigma} (1 + e^{-\beta \xi_{k,\sigma}}) \tag{16}$$

The corresponding grand potential functional is given by

$$\begin{aligned}\Omega &= -\frac{1}{\beta} \ln Z = -\frac{1}{\beta} \ln[\prod_{k\sigma} (1 + e^{-\beta \xi_{k,\sigma}}) e^{-\beta(N(Ud^2 - 2\lambda^2(d^2+p^2) + \lambda^1(1-d^2-e^2-2p^2))}] \\ &= -\frac{1}{\beta} \sum_{k,\sigma} \ln(1 + e^{-\beta \xi_{k,\sigma}}) + UNd^2 + N[-2\lambda^2(d^2+p^2) + \lambda^1(1-d^2-e^2-2p^2)]\end{aligned}$$

The average energy is

$$\begin{aligned}\langle H \rangle &= -\frac{\partial \ln Z}{\partial \beta} = \frac{\partial(\beta\Omega)}{\partial \beta} \\ &= \sum_{k,\sigma} \xi_{k,\sigma} \frac{1}{1 + e^{\beta \xi_{k,\sigma}}} + UNd^2 + N[-2\lambda^2(d^2+s^2) + \lambda^1(1-d^2-e^2-2p^2)] \\ &= \sum_{k,\sigma} \xi_{k,\sigma} n_F(\xi_{k,\sigma}) + UNd^2 + N[-2\lambda^2(d^2+p^2) + \lambda^1(1-d^2-e^2-2p^2)]\end{aligned}$$

Self-consistent equations

The self-consistent equations are

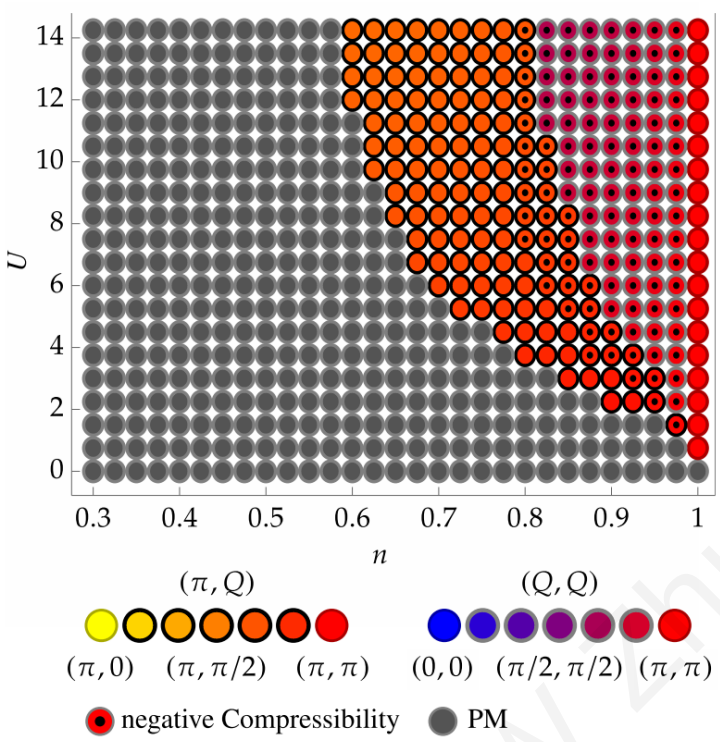

FIG. 5: Slave-boson mean-field solution of the hubbard model.

$$\frac{\partial\langle H\rangle}{\partial\lambda^1} = 0 \to 1 - d^2 - e^2 - 2p^2 = 0 \tag{17}$$

$$\frac{\partial\langle H\rangle}{\partial\lambda^2} = 0 \to \frac{1}{N}\sum_k \langle n_k\rangle = d^2 + p^2 \tag{18}$$

$$\frac{\partial\langle H\rangle}{\partial d} = 0 \to \frac{1}{N}\sum_k \epsilon_k\langle n_k\rangle\frac{\partial Z}{\partial d} + 2Ud - 4\lambda^2 d - 2\lambda^1 d = 0 \tag{19}$$

$$\frac{\partial\langle H\rangle}{\partial e} = 0 \to \frac{1}{N}\sum_k \epsilon_k\langle n_k\rangle\frac{\partial Z}{\partial e} - 2\lambda^1 e = 0 \tag{20}$$

$$\frac{\partial\langle H\rangle}{\partial p} = 0 \to \frac{1}{N}\sum_k \epsilon_k\langle n_k\rangle\frac{\partial Z}{\partial p} - 4\lambda^2 p - 4\lambda^1 p = 0 \tag{21}$$

$$\tag{22}$$

and the constrains that $\sum_k\langle n_k\rangle = n$ to determine the chemical potential μ. The solution are summarized in Figure 5 below. At the half filling case, an insulator appears instead of a metal. Please also see the solution in the hartree-fock section.

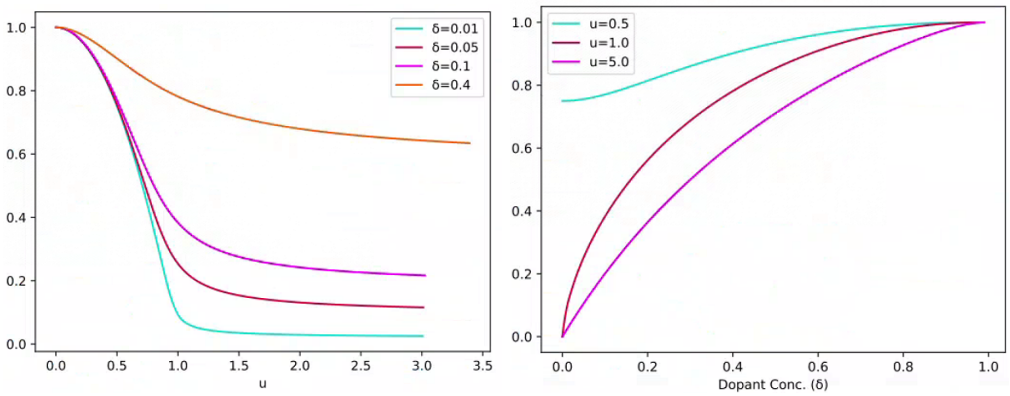

FIG. 6: Renormalization factor as a function of interaction U and doping δ.

T-J MODEL ON SQUARE LATTICE

Derivation of t-J model

The Hubbard model, was devised first to describe the single-band magnetism, particularly to understand the so-called itinerant (Stoner-Wolfharth) ferromagnetism and criterion of its appearance in a microscopic manner. It is represented by the Hamiltonian, which in the second-quantization representation has the form

$$\hat{H} = \sum_{i,j} t_{ij,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{23}$$

One can rewrite the dynamical processes contained in the hopping term as follows

$$c^{\dagger}_{i\sigma} c_{j\sigma} = c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}} + n_{i\bar{\sigma}}) c_{j\sigma}(1 - n_{j\bar{\sigma}} + n_{j\bar{\sigma}}) \tag{24}$$

$$= c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}}) c_{j\sigma}(1 - n_{j\bar{\sigma}}) + c^{\dagger}_{i\sigma} n_{i\bar{\sigma}} c_{j\sigma} n_{j\bar{\sigma}} \tag{25}$$

$$+ c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}}) c_{j\sigma} n_{j\bar{\sigma}} + c^{\dagger}_{i\sigma} n_{i\bar{\sigma}} c_{j\sigma}(1 - n_{j\bar{\sigma}}) \tag{26}$$

The consecutive terms represent the four restricted types of hopping processes: the first hopping from singly occupied site onto an empty one, the second hopping from singly occupied site and formation of a doubly occupied one, etc.

Formally, one can write the full Hamiltonian as operating in four subspaces

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} = P_0 H P_0 + P_0 H P_N + P_N H P_0 + P_N H P_N \tag{27}$$

$$P_0 H P_0 = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}}) c_{j\sigma}(1 - n_{j\bar{\sigma}}) \tag{28}$$

$$P_N H P_N = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} n_{i\bar{\sigma}} c_{j\sigma} n_{j\bar{\sigma}} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} \tag{29}$$

$$P_0 H P_N = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma}(1 - n_{i\bar{\sigma}}) c_{j\sigma} n_{j\bar{\sigma}} \tag{30}$$

$$P_N H P_0 = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} n_{i\bar{\sigma}} c_{j\sigma}(1 - n_{j\bar{\sigma}}) \tag{31}$$

Since every term contains process $-t_{ij}$, it is convenient to define the operator

$$H = H_0 + \epsilon H_1 \tag{32}$$

$$H_0 = P_0 H P_0 + P_N H P_N, \quad H_1 = P_0 H P_N + P_N H P_0 \tag{33}$$

ϵ is to collect the terms of the same order.

The last nontrivial feature is to select the unitary transformation matrix, with the help of which we remove part the hopping processes in the first order and replace them by virtual processes exemplifying physical processes in higher order. For that purpose, we have also proposed the following canonical transformation of the form

$$\tilde{H} = e^{-i\epsilon S} H e^{i\epsilon S} \approx H_0 + \epsilon(H_1 + i[H_0, S]) + \frac{\epsilon^2}{2}(2i[H_1, S] - [[H_0, S], S]) \tag{34}$$

The linear term is absent when

$$H_1 + i[H_0, S] = 0. \tag{35}$$

Under this condition, we obtain

$$\tilde{H} = e^{-i\epsilon S} H e^{i\epsilon S} \approx H_0 + \frac{i\epsilon^2}{2}[H_1, S] \tag{36}$$

has to be solved for S. The main problem is that H_0 is not diagonal. Explicitly, the above vanishing condition gives

$$P_0(H_1 + i[H_0, S])P_N = 0 \tag{37}$$

$$P_0(H_1 + [H_0, S])P_N = P_0[H_0, S]P_N = 0 \tag{38}$$

$$P_N(H_1 + [H_0, S])P_0 = P_N[H_0, S]P_N = 0 \tag{39}$$

Because of the property $P_{0(N)}^2 = P_{0(N)}$, $P_{0(N)}SP_{0(N)} = f(P_{0(N)})$ will satisfy the last two equations and $f(P_{0(N)}) = a + bP_{0(N)}$.

And the first equation becomes

$$-iP_0H_1P_N + P_0H_0P_0P_0SP_N - P_0SP_NP_NH_0P_N = 0 \tag{40}$$

By approximation $\langle P_0H_0P_0\rangle \sim t$ and $\langle P_NH_0P_N\rangle \sim U$, we have

$$P_0SP_N \approx iP_0H_1P_N/(\langle P_0H_0P_0\rangle - \langle P_NH_0P_N\rangle) \approx -iP_0H_1P_N/U \tag{41}$$

Then, we obtain the effective Hamiltonian by projecting into two subspace:

$$\tilde{H} \approx P_0\tilde{H}P_0 + P_N\tilde{H}P_N \tag{42}$$

$$P_0\tilde{H}P_0 = P_0(H_0 - \frac{i}{2}[H_1, S])P_0 = P_0HP_0 - P_0HP_NP_NHP_0/U \tag{43}$$

$$P_N\tilde{H}P_N = P_N(H_0 - \frac{i}{2}[H_1, S])P_N = P_NHP_N + P_NHP_0P_0HP_N/U \tag{44}$$

Finally, we can map out the form explicitly,

$$P_0\tilde{H}P_0 = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{j\sigma}(1-n_{j\overline{\sigma}}) + \sum_{ij}\frac{2t^2_{ij}}{U}[S_i\cdot S_j - \frac{1}{4}n_i n_j] + ... \tag{45}$$

where $S^+_i = c^{\dagger}_{i\uparrow}c_{i\downarrow}$, $S^-_i = c^{\dagger}_{i\downarrow}c_{i\uparrow}$, $S^z_i = (n_{i\uparrow}-n_{i\downarrow})/2$.

When we need to deal with the term $P_0HP_NP_NHP_0$, first we recall $P_0HP_NP_NHP_0 = \sum_{ij\sigma}[c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{j\sigma}n_{j\overline{\sigma}}]\sum_{nm\nu}[c^{\dagger}_{n\nu}n_{n\overline{\nu}}c_{m\nu}(1-n_{m\overline{\nu}})]$ is zero when $i=n, j=m$. Second, $\sum_{ij\sigma}[c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{j\sigma}n_{j\overline{\sigma}}]\sum_{nm\nu}[c^{\dagger}_{n\nu}n_{n\overline{\nu}}c_{m\nu}(1-n_{m\overline{\nu}})]$ can be separated into two terms $\sigma=\nu$ and $\sigma=\overline{\nu}$:

$$\rightarrow (\sigma=\nu)\quad c_{j\sigma}n_{j\overline{\sigma}}c^{\dagger}_{j\sigma}n_{j\overline{\sigma}} = c_{j\sigma}c^{\dagger}_{j\sigma}n_{j\overline{\sigma}}n_{j\overline{\sigma}} = n_{j\overline{\sigma}}(1-n_{j\sigma}) \tag{46}$$

$$\rightarrow (\sigma=\nu)\quad c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{i\sigma}(1-n_{i\overline{\sigma}}) = n_{i\sigma}(1-n_{i\overline{\sigma}}) \tag{47}$$

$$\Rightarrow [c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{j\sigma}n_{j\overline{\sigma}}][c^{\dagger}_{j\nu}n_{j\overline{\nu}}c_{i\nu}(1-n_{i\overline{\nu}})] = n_{i\sigma}(1-n_{i\overline{\sigma}})n_{j\overline{\sigma}}(1-n_{j\sigma}) = n_{i\sigma}n_{j\overline{\sigma}} \tag{48}$$

$$\rightarrow (\sigma=\overline{\nu})\quad c_{j\sigma}n_{j\overline{\sigma}}c^{\dagger}_{j\overline{\sigma}}n_{j\sigma} = c_{j\sigma}c^{\dagger}_{j\overline{\sigma}}(1-n_{j\overline{\sigma}})n_{j\sigma} = -c^{\dagger}_{j\overline{\sigma}}c_{j\sigma} \tag{49}$$

$$\rightarrow (\sigma=\overline{\nu})\quad c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{i\overline{\sigma}}(1-n_{i\sigma}) = c^{\dagger}_{i\sigma}c_{i\overline{\sigma}} \tag{50}$$

$$\Rightarrow [c^{\dagger}_{i\sigma}(1-n_{i\overline{\sigma}})c_{j\sigma}n_{j\overline{\sigma}}][c^{\dagger}_{j\nu}n_{j\overline{\nu}}c_{i\nu}(1-n_{i\overline{\nu}})] = -c^{\dagger}_{i\sigma}c_{i\overline{\sigma}}c^{\dagger}_{j\overline{\sigma}}c_{j\sigma} = -S^+_iS^-_j - S^-_iS^+_j \tag{51}$$

and we need

$$\frac{n_in_j}{2} - 2S^z_iS^z_j = n_{i\uparrow}n_{j\downarrow} + n_{i\downarrow}n_{j\uparrow} \tag{52}$$

Finally, let me first summarize the principal features of the so-called t-J model . This model represents a very nontrivial model of strongly correlated fermions because of the following principal reasons:

- It represents a system of strongly inter-correlated itinerant fermions which transform into an antiferromagnetic state of localized particles (the Mott-Hubbard insulator); the classic situation takes place at the concentration of one fermion per single-band state (at the half filling, n = 1). The half-filled state is an antiferromagnetic insulator modeled by the Anderson kinetic exchange.

- The itinerant state is represented by particles called the correlated holes or simply the holes in the Mott-Hubbard insulator, which do not have the ordinary fermion properties (their creation and annihilation operators do not obey the fermionic anticommutation rules). In other words, they cannot be represented by Landau quasiparticles in an exact manner, since they do not represent almost-filled band states.

- Magnetic interaction between the correlated itinerant particles, again the kinetic exchange, is regarded also as the source of real-space pairing as it is represented as taking place between the nearest neighbors. Hence, antiferromagnetism and this new type of paired state must be regarded on equal footing with the paired state (resonance-valence bond state or superconducting state). This is particularly relevant in the context of high- temperature superconductivity near the band filling, i.e. close to the Mott transition.

- Because of the nontrivial character of the kinetic- (or residual-band-) energy (the projected hopping part), it can become comparable or even smaller than the kinetic-exchange-energy part. In effect, magnetic polaron or phase-separated states or new type of spin-paired states can be formed, concomitantly with the transition to a localized state for small carrier concentration of holes. Thus the transition in real systems such as La_{2-x} Sr_x CuO_4 , YBa_2 Cu_3 O_{6+x}, La_{1-x} Sr_x TiO_3 , takes place even for a non-half-filled band configuration. Although, here the role of atomic disorder is probably also very important, if not crucial.

Cuperates are two dimensional, and can also be described by the t-J model. A cuprate is a material that consists of copper-oxygen layers, which possess the property that the copper d orbit is only singly occupied, whereas the oxygen p orbit is doubly occupied. The electronic structure is shown in Figure 1, with to the right the simplification which is exactly the two-dimensional t-J lattice, also called the one-band model. Cuprates are of scientific interest because this group of materials is superconducting at higher temperatures then classic superconducting materials. The driving force behind the phase diagram in figure 1 is the strong correlation, where figure 1 shows the phase diagram of a hole-doped cuprate on the left, the right hand side shows the same, but now for electron-doping. Given the importance of the strong correlation, the t-J model is a natural fit to attempt to describe the dynamics of this class of material. Since the t-J model is in the basis a relatively simple model, there are multiple elaborations to be added, which turn out to be significant and capture some of the interesting physics as already seen in the asymmetry of the phase diagram.

Mean-field calculation

We consider the t-J model on square lattice, with Hamiltonian as

$$H = H_t + H_s - \frac{1}{4}\sum_{<ij>} n_i n_j \tag{53}$$

$$H_t = -t\sum_{\langle ij\rangle,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} \tag{54}$$

$$H_s = \sum_{\langle ij\rangle} J_{ij}\vec{S}^\dagger_i \cdot \vec{S}_j \tag{55}$$

, where the spin operator is defined by

$$\vec{S}_i = (\hat{S}^\dagger_i, \hat{S}^-_i, \hat{S}^z_i) = (c^\dagger_{i,\uparrow}c_{i,\downarrow}, c^\dagger_{i,\downarrow}c_{i,\uparrow}, \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow})) \tag{56}$$

The Fourier transformation is useful in the following calcualtions:

$$c_{i,\sigma} = \frac{1}{\sqrt{N}}\sum_k e^{i\vec{k}\cdot\vec{r}} c_{k,\sigma} \tag{57}$$

$$c_{k,\sigma} = \frac{1}{\sqrt{N}}\sum_r e^{i\vec{k}\cdot\vec{r}} c_{i,\sigma} \tag{58}$$

The hopping term becomes

$$H_t = -t\sum_{\langle ij\rangle,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} = \sum_{k,\sigma} \varepsilon_{k,\sigma} c^\dagger_{k,\sigma} c_{k,\sigma}, \tag{59}$$

where $\varepsilon_{k,\sigma} = -2(t_x \cos k_x + t_y \cos k_y)$ (lattice constant $a = 1$). Here we used the relation

$$\begin{aligned}
&\sum_{\langle ij\rangle,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} = t_x \sum_{\langle ij\rangle,\sigma} \frac{1}{N}\sum_{k,p} e^{-i\vec{k}\cdot\vec{r}_i} c^\dagger_{k,\sigma} e^{i\vec{p}\cdot\vec{r}_j} c_{p,\sigma} + (x \to y) \\
&= t_x \frac{1}{N}\sum_{k,p}\sum_r e^{i\vec{k}\cdot\vec{r} - i\vec{p}\cdot(\vec{r}\pm\hat{x})} c^\dagger_{k,\sigma} c_{p,\sigma} + (x \to y) \\
&= t_x \sum_k e^{i\vec{k}\cdot\hat{x}} c^\dagger_{k,\sigma} c_{k,\sigma} + h.c. + (x \to y) \\
&= t_x \sum_k 2\cos k_x c^\dagger_{k,\sigma} c_{k,\sigma} + (x \to y)
\end{aligned}$$

where the normailzation condition is $\frac{1}{N}\sum_r e^{i(\vec{k}-\vec{p})\cdot\vec{r}} = \delta(\vec{k} - \vec{p})$.

The spin correlation term becomes

$$\begin{aligned}
H_s &= \sum_{\langle ij\rangle} J_{ij}\vec{S}^\dagger_i \cdot \vec{S}_j \\
&= \sum_{\langle ij\rangle} J_{ij}[\frac{1}{2}c^\dagger_{i,\uparrow}c_{i,\downarrow}c^\dagger_{j,\downarrow}c_{j,\uparrow} + \frac{1}{2}c^\dagger_{j,\uparrow}c_{j,\downarrow}c^\dagger_{i,\downarrow}c_{i,\uparrow} + \frac{1}{4}c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{j,\downarrow}c_{j,\downarrow} + \frac{1}{4}c^\dagger_{i,\downarrow}c_{i,\downarrow}c^\dagger_{j,\uparrow}c_{j,\uparrow} + \frac{1}{4}c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{j,\uparrow}c_{j,\uparrow} + \frac{1}{4}c^\dagger_{i,\downarrow}c_{i,}
\end{aligned}$$

The decoupled terms are

$$\langle c^\dagger_{i,\uparrow}c_{i,\downarrow}c^\dagger_{j,\downarrow}c_{j,\uparrow}\rangle = -\langle c^\dagger_{i,\uparrow}c_{j,\uparrow}c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle \simeq -\langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle c^\dagger_{j,\downarrow}c_{i,\downarrow} - c^\dagger_{i,\uparrow}c_{j,\uparrow}\langle c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle + \langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle\langle c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle$$
$$\langle c^\dagger_{i,\uparrow}c_{i,\downarrow}c^\dagger_{j,\downarrow}c_{j,\uparrow}\rangle = -\langle c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}c_{i,\downarrow}c_{j,\uparrow}\rangle \simeq -\langle c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}\rangle c_{i,\downarrow}c_{j,\uparrow} - c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}\langle c_{i,\downarrow}c_{j,\uparrow}\rangle - \langle c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}\rangle\langle c_{i,\downarrow}c_{j,\uparrow}\rangle$$

Then

$$\begin{aligned}
H_s \simeq\ & \frac{1}{2}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle c^\dagger_{j,\downarrow}c_{i,\downarrow} - c^\dagger_{i,\uparrow}c_{j,\uparrow}\langle c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle + \langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle\langle c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle - \langle c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}\rangle c_{i,\downarrow}c_{j,\uparrow} - c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow}\langle c_{i,\downarrow}c_{j,\uparrow}\rangle - \\
+\ & \frac{1}{2}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{j,\uparrow}c_{i,\uparrow}\rangle c^\dagger_{i,\downarrow}c_{j,\downarrow} - c^\dagger_{j,\uparrow}c_{i,\uparrow}\langle c^\dagger_{i,\downarrow}c_{j,\downarrow}\rangle + \langle c^\dagger_{j,\uparrow}c_{i,\uparrow}\rangle\langle c^\dagger_{i,\downarrow}c_{j,\downarrow}\rangle - \langle c^\dagger_{j,\uparrow}c^\dagger_{i,\downarrow}\rangle c_{j,\downarrow}c_{i,\uparrow} - c^\dagger_{j,\uparrow}c^\dagger_{i,\downarrow}\langle c_{j,\downarrow}c_{i,\uparrow}\rangle - \\
+\ & \frac{1}{4}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{i,\uparrow}c_{j,\downarrow}\rangle c^\dagger_{j,\downarrow}c_{i,\uparrow} - c^\dagger_{j,\downarrow}c_{i,\uparrow}\langle c^\dagger_{i,\uparrow}c_{j,\downarrow}\rangle + \langle c^\dagger_{i,\uparrow}c_{j,\downarrow}\rangle\langle c^\dagger_{j,\downarrow}c_{i,\uparrow}\rangle - \langle n_{i,\uparrow}\rangle n_{j,\downarrow} - n_{j,\downarrow}\langle n_{i,\uparrow}\rangle + \langle n_{i,\uparrow}\rangle\langle n_{j,\downarrow}\rangle \\
+\ & \frac{1}{4}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{i,\downarrow}c_{j,\uparrow}\rangle c^\dagger_{j,\uparrow}c_{i,\downarrow} - c^\dagger_{j,\uparrow}c_{i,\downarrow}\langle c^\dagger_{i,\downarrow}c_{j,\uparrow}\rangle + \langle c^\dagger_{i,\downarrow}c_{j,\uparrow}\rangle\langle c^\dagger_{j,\uparrow}c_{i,\downarrow}\rangle - \langle n_{i,\downarrow}\rangle n_{j,\uparrow} - n_{j,\uparrow}\langle n_{i,\downarrow}\rangle + \langle n_{i,\downarrow}\rangle\langle n_{j,\uparrow}\rangle \\
+\ & \frac{1}{4}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle c^\dagger_{j,\uparrow}c_{i,\uparrow} - c^\dagger_{j,\uparrow}c_{i,\uparrow}\langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle + \langle c^\dagger_{i,\uparrow}c_{j,\uparrow}\rangle\langle c^\dagger_{j,\uparrow}c_{i,\uparrow}\rangle - \langle n_{i,\uparrow}\rangle n_{j,\uparrow} - n_{j,\uparrow}\langle n_{i,\uparrow}\rangle + \langle n_{i,\uparrow}\rangle\langle n_{j,\uparrow}\rangle \\
+\ & \frac{1}{4}\sum_{\langle ij\rangle} J_{ij}[-\langle c^\dagger_{i,\downarrow}c_{j,\downarrow}\rangle c^\dagger_{j,\downarrow}c_{i,\downarrow} - c^\dagger_{j,\downarrow}c_{i,\downarrow}\langle c^\dagger_{i,\downarrow}c_{j,\downarrow}\rangle + \langle c^\dagger_{i,\downarrow}c_{j,\downarrow}\rangle\langle c^\dagger_{j,\downarrow}c_{i,\downarrow}\rangle - \langle n_{i,\downarrow}\rangle n_{j,\downarrow} - n_{j,\downarrow}\langle n_{i,\downarrow}\rangle + \langle n_{i,\downarrow}\rangle\langle n_{j,\downarrow}\rangle
\end{aligned}$$

If we set

$$\xi_{ij} = \sum_\sigma \langle c^\dagger_{i,\sigma}c_{j,\sigma}\rangle \tag{60}$$
$$\Delta_{ij} = \langle c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow}c^\dagger_{j,\uparrow}\rangle \tag{61}$$
$$\frac{n}{2} = \langle n_{i,\sigma=\uparrow,\downarrow}\rangle \tag{62}$$

We simplify as

$$H_s \simeq -\frac{3}{4}\sum_{\langle ij\rangle,\sigma} J_{ij}(\xi_{ij}c^\dagger_{i,\sigma}c_{j,\sigma} + h.c.) - \frac{3}{4}\sum_{\langle ij\rangle,\sigma} J_{ij}(\Delta_{ij}c^\dagger_{i,\sigma}c_{j,-\sigma} + h.c.) + C_1 \tag{63}$$

where the constant term

$$C_1 = \frac{3}{8}\sum_{\langle ij\rangle,\sigma} J_{ij}(|\xi_{ij}|^2 + |\Delta_{ij}|^2) = \frac{3N}{4}(J_x\xi_x^2 + J_y\xi_y^2) + \frac{3N}{4}(J_x\Delta_x^2 + J_y\Delta_y^2) \tag{64}$$

Within the similar route, we have the n_in_j term:

$$-\frac{1}{4}\sum_{ij} n_in_j \simeq \frac{1}{4}\sum_{\langle ij\rangle,\sigma} J_{ij}(\xi_{ij}c^\dagger_{i,\sigma}c_{j,\sigma} + h.c.) - \frac{1}{4}\sum_{\langle ij\rangle,\sigma} J_{ij}(\Delta^*_{ij}c^\dagger_{i,\sigma}c_{j,-\sigma} + h.c.) - \frac{1}{2}\sum_{\langle ij\rangle}\langle n_i\rangle n_j + C_2 \tag{65}$$

where the constant term

$$C_2 = -\frac{N}{4}(J_x\xi_x^2 + J_y\xi_y^2) + \frac{N}{4}(J_x\Delta_x^2 + J_y\Delta_y^2) + \frac{N}{2}(J_x + J_y)n^2 \tag{66}$$

The mean-field hamiltonian is

$$H_{MF} = \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_k \Delta_k (c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + c_{k,\uparrow} c_{-k,\downarrow}) + C_1 + C_2 \tag{67}$$

To solve this Hamiltonian, we introduce the Bogoliubov transformation.

$$\begin{aligned} H_{MF} &= \sum_{k,\sigma} \xi_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_k \Delta_k (c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + c_{k,\uparrow} c_{-k,\downarrow}) \\ &= \begin{pmatrix} c_{k,\uparrow}^\dagger & c_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \xi_k & \Delta_k \\ \Delta_k & -\xi_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix} \\ &= \sum_k \sum_k E_k (\hat{\gamma}_k^\dagger \hat{\gamma}_k + \hat{\zeta}_k^\dagger \hat{\zeta}_k) \end{aligned}$$

where $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ and

$$c_{k,\uparrow}^\dagger = u_k \hat{\gamma}_k^\dagger + v_k^* \hat{\zeta}_k \tag{68}$$

$$c_{-k,\downarrow}^\dagger = u_k \hat{\zeta}_k^\dagger - v_k^* \hat{\gamma}_k \tag{69}$$

$$|u_k|^2 = \frac{1}{2}(1 + \frac{\xi_k}{E_k}) \tag{70}$$

$$|v_k|^2 = \frac{1}{2}(1 - \frac{\xi_k}{E_k}) \tag{71}$$

$$u_k v_k^* = \frac{\Delta}{2E_k} \tag{72}$$

This choose satisfy the commutation relation:

$$\{c_{k,\uparrow}^\dagger, c_{k,\uparrow}\} = |u_k|^2 \{\hat{\gamma}_k^\dagger, \hat{\gamma}_k\} + |v_k|^2 \{\hat{\zeta}_k^\dagger, \hat{\zeta}_k\} = |u_k|^2 + |v_k|^2 = 1 \tag{73}$$

$$\{\hat{\gamma}_k^\dagger, \hat{\gamma}_k\} = 1, \{\hat{\zeta}_k^\dagger, \hat{\zeta}_k\} = 1 \tag{74}$$

SUPERCONDUCTIVITY IN A TWO-BAND MODEL

The two-band model on a square lattice is

$$H = H_c + H_f + H_{hyb} + H_J \tag{75}$$

$$H_c = t_c \sum_{\langle ij\rangle} c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. = \sum_{\mathbf{k},\sigma} \epsilon^c_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{76}$$

$$H_f = t_f \sum_{\langle ij\rangle} f^\dagger_{i,\sigma} f_{j,\sigma} + h.c. + U \sum_i f^\dagger_{i\uparrow} f_{i,\uparrow} f^\dagger_{i,\downarrow} f_{i,\downarrow} = \sum_{\mathbf{k},\sigma} \epsilon^f_{\mathbf{k}} f^\dagger_{\mathbf{k},\sigma} f_{\mathbf{k},\sigma} + U \sum_i f^\dagger_{i\uparrow} f_{i,\uparrow} f^\dagger_{i,\downarrow} f_{i,\downarrow} \tag{77}$$

$$H_{hyb} = V \sum_{i,\sigma} c^\dagger_{i,\sigma} f_{i,\sigma} + h.c = V \sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k},\sigma} f_{\mathbf{k},\sigma} + h.c. \tag{78}$$

$$H_J = J \sum_{\langle i,j\rangle,\sigma} f^\dagger_{j,\sigma} f_{j,-\sigma} f^\dagger_{i,-\sigma} f_{i,\sigma} = J \sum_{\langle i,j\rangle} S^+_j S^-_i + S^+_i S^-_j \tag{79}$$

The two bands are descibed by the dispersion relaitons ϵ^c_k and ϵ^f_k for c-electrons and f-electrons. There is a onsite repulsive interaction on $f-$electrons. H_{hyb} describes the hybridization between c- and f-electrons. The last term H_J describes an effective exchange interaction between f-electrons in neighboring sites and it is responsible for superconductivity.

Pairing term

The mean-field treatment of pairing term is the same as that in t-J model. Here we neglect the $S^z_i S^z_j$ terms and only consider the xy exchange terms.

$$\textstyle\sum_{\langle ij\rangle} J_{ij}(S^+_i S^-_j + S^-_j S^+_i) = J \sum_i (S^+_i S^-_{i+\hat{x}} + S^+_i S^-_{i+\hat{y}} + S^+_i S^-_{i-\hat{x}} + S^+_i S^-_{i-\hat{y}}) \tag{80}$$

and the spin operators are

$$\vec{S}_i = (\hat{S}^\dagger_i, \hat{S}^-_i, \hat{S}^z_i) = (c^\dagger_{i,\uparrow} c_{i,\downarrow}, c^\dagger_{i,\downarrow} c_{i,\uparrow}, \frac{1}{2}(n_{i,\uparrow} - n_{i,\downarrow})) \tag{81}$$

In the mean-field level,

$$\begin{aligned} S^+_i S^-_j &= c^\dagger_{i,\uparrow} c_{i,\downarrow} c^\dagger_{j,\downarrow} c_{j,\uparrow} = -c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} c_{i,\downarrow} c_{j,\uparrow} \\ &= -\langle c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}\rangle c_{i,\downarrow} c_{j,\uparrow} - c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} \langle c_{i,\downarrow} c_{j,\uparrow}\rangle + \langle c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}\rangle \langle c_{i,\downarrow} c_{j,\uparrow}\rangle \\ &= -(-\frac{\Delta^{s*}_{ij}}{2}) c_{i,\downarrow} c_{j,\uparrow} - (-\frac{\Delta^s_{ji}}{2}) c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + (-\frac{\Delta^{s*}_{ij}}{2})(-\frac{\Delta^s_{ji}}{2}) \end{aligned} \tag{82}$$

The singlet pairing potential is defined as

$$\Delta^s_{ij} = \langle c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}\rangle \tag{83}$$

$$(\Delta^s_{ij})^* = \langle c^+_{j\downarrow}c^+_{i\uparrow} - c^+_{j\uparrow}c^+_{i\downarrow}\rangle \tag{84}$$

If the triplet pairing is zero, $\langle c_{i\uparrow}c_{j\downarrow}\rangle = \langle c_{j\uparrow}c_{i\downarrow}\rangle = \frac{\Delta^s_{ij}}{2}$.

Next we further assume the s-wave pairing, i.e. all pairing terms are identical $\Delta^s_{ij} = \Delta^s$. We have

$$\begin{aligned}\sum_i S^+_i S^-_{i+x} &= \sum_i \frac{\Delta^{s*}}{2}c_{i,\downarrow}c_{i+x,\uparrow} + \frac{\Delta^s}{2}c^\dagger_{i,\uparrow}c^\dagger_{i+x,\downarrow} + \frac{\Delta^{s*}\Delta^s}{4} \\ &= \frac{\Delta^{s*}}{2}\sum_i \frac{1}{N}\sum_{k,p} e^{-ikr_i}c_{k,\downarrow}e^{-ipr_{i+x}}c_{p,\uparrow} + \frac{\Delta^s}{2}\sum_i \frac{1}{N}\sum_{k,p} e^{ikr_i}c^\dagger_{k,\uparrow}e^{ipr_{i+x}}c^\dagger_{p,\downarrow} + N\frac{\Delta^{s*}\Delta^s}{4} \\ &= \frac{\Delta^{s*}}{2}\sum_k e^{ik\hat{x}}c_{k,\downarrow}c_{-k,\uparrow} + \frac{\Delta^s}{2}\sum_k c^\dagger_{k,\uparrow}e^{-ik\hat{x}}c^\dagger_{-k,\downarrow} + N\frac{\Delta^{s*}\Delta^s}{4}\end{aligned} \tag{85}$$

Thus we have

$$\begin{aligned}&\sum_i (S^+_i S^-_{i+\hat{x}} + S^+_i S^-_{i+\hat{y}} + S^+_i S^-_{i-\hat{x}} + S^+_i S^-_{i-\hat{y}}) = \\ &\frac{\Delta^{s*}}{2}\sum_k (\sum_\delta e^{ik\hat{\delta}})c_{k,\downarrow}c_{-k,\uparrow} + \frac{\Delta^s}{2}\sum_k (\sum_\delta e^{-ik\hat{\delta}})c^\dagger_{k,\uparrow}c^\dagger_{-k,\downarrow} + 4N\frac{\Delta^{s*}\Delta^s}{4}\end{aligned} \tag{86}$$

Order parameter can be re-expressed as

$$\begin{aligned}\Delta_{i,i+\delta} = \langle c_{i\uparrow}c_{i+\delta\downarrow}\rangle &= \frac{1}{N}\sum_i \langle c_{i\uparrow}c_{i+\delta\downarrow}\rangle \\ &= \frac{1}{N}\sum_i \frac{1}{N}\langle \sum_{k,p} e^{-ikr_i}c_{k,\downarrow}e^{-ipr_{i+\delta}}c_{p,\uparrow}\rangle \\ &= \frac{1}{N}\sum_k \langle c_{k,\uparrow}c_{-k,\downarrow}\rangle e^{ik\delta}\end{aligned} \tag{87}$$

Since we have four nearest-neighbor on square lattice,

$$\begin{aligned}\Delta^s = 2\langle c_{i\uparrow}c_{j\downarrow}\rangle &= 2\frac{1}{4}[\Delta_{i,i+\hat{x}} + \Delta_{i,i+\hat{y}} + \Delta_{i,i-\hat{x}} + \Delta_{i,i-\hat{y}}] \\ &= \frac{1}{2}\frac{1}{N}\sum_k \langle c_{k,\uparrow}c_{-k,\downarrow}\rangle \sum_\delta e^{ik\delta}\end{aligned} \tag{88}$$

We see this order parameter is consistent with the self-consistent equation from Eq. 86 (by varitional method):

$$N\Delta^s + \frac{1}{2}\sum_k (\sum_\delta e^{ik\hat{\delta}})\langle c_{k,\downarrow}c_{-k,\uparrow}\rangle = 0 \tag{89}$$

Slave-boson mean-field

We introduce four bosons to the various states that f-electrons can occupy. The boson d,d are associated with empty and doubly occupied sites, respectively, and p_σ with a singly occupied site with spin component σ. There is an enlargement of the Hilbert space and restrictions must be implemented at each site $e_i^\dagger e_i + d_i^\dagger d_i + p_{i,\uparrow}^\dagger p_{i,\uparrow} + p_{i,\downarrow}^\dagger p_{i,\downarrow} = 1$, and $f_{i,\sigma}^\dagger f_{i,\sigma} = p_{i,\uparrow}^\dagger p_{i,\uparrow} + d_i^\dagger d_i$. In the physical space, the operators $f_{i,\sigma}$ is replaced by $f_{i,\sigma} Z_{i,\sigma}$, where $Z_{i\sigma} = (1 - d_i^\dagger d_i - p_{i,\uparrow}^\dagger p_{i,\uparrow})^{-1/2}(e_i^\dagger p_{i,\sigma} + p_{i,-\sigma} d_i)(1 - e_i^\dagger e_i - p_{i,\uparrow}^\dagger p_{i,\uparrow})^{-1/2}$. The usual procedure consists in taking a mean-field approach where we assume the slave bosons to be condensed. In the solution of paramagnet or ferromagnet solutions, we take $\langle Z_{i,\sigma} \rangle = Z_\sigma$, $\langle e_i \rangle = e$.

The mean-field hamiltonian is

$$\begin{aligned} H_{MF} = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}}^c - \mu) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}}^f + \lambda' - \mu) f_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + V \sum_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + h.c. \\ + UNd^2 + N\lambda(e^2 + d^2 + 2p^2 - 1) + \lambda' N 2(p^2 + d^2) \\ + Z^2 \Delta \sum_k (\eta_k f_{k\uparrow}^\dagger f_{-k\downarrow}^\dagger + \eta_k f_{-k,\downarrow} f_{k,\uparrow}) + N \frac{\Delta^2}{J} \end{aligned} \tag{90}$$

where $\eta_k = \cos k_x + \cos k_y$ for s-wave pairing.

Reduce the variational parameters

We consider the constrains

$$e^2 + d^2 + 2p^2 = 1 \tag{91}$$

$$n_f = 2(p^2 + d^2) \tag{92}$$

we have $p = \sqrt{n_f/2 - d^2}$ and $e = \sqrt{1 - d^2 - 2p^2}$. So

$$Z = \frac{p(e+d)}{\sqrt{(p^2+e^2)(p^2+d^2)}} = \frac{\sqrt{n_f/2 - d^2}(\sqrt{1 + d^2 - n} + d)}{\sqrt{(1 - n/2)n/2}} \tag{93}$$

and

$$\frac{\partial Z}{\partial d} = \frac{-d(n_f/2 - d^2)^{-1/2}(\sqrt{1 + d^2 - n} + d) + (n_f/2 - d^2)^{1/2}(1 + d(1 + d^2 - n_f)^{-1/2})}{\sqrt{(1 - n/2)n/2}} \tag{94}$$

Then the energy reduces to the form with three parameters: d, Δ, μ

$$H_{MF} = \sum_{\mathbf{k},\sigma}(\epsilon^c_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma}(\epsilon^f_{\mathbf{k}} - \mu)f^\dagger_{\mathbf{k},\sigma}f_{\mathbf{k},\sigma} + V\sum_{\mathbf{k},\sigma}c^\dagger_{\mathbf{k},\sigma}f_{\mathbf{k},\sigma} + h.c.$$
$$+UNd^2 + +Z^2\Delta\sum_k(\eta_k f^\dagger_{k\uparrow}f^\dagger_{-k\downarrow} + \eta_k f_{-k,\downarrow}f_{k,\uparrow}) + N\frac{\Delta^2}{J} \tag{95}$$

Bogoliubov-de Gennes equations

BdG equations can then be written as

$$\mathcal{H}\psi_n = E_n\psi_n \tag{96}$$

$$\mathcal{H} = \begin{bmatrix} (\epsilon^c_{\mathbf{k}} - \mu) & VZ & 0 & 0 \\ VZ & \epsilon^f_{\mathbf{k}} - \mu & 0 & Z^2\Delta\eta_k \\ 0 & 0 & -(\epsilon^c_{\mathbf{k}} - \mu) & -VZ \\ 0 & Z^2\Delta\eta_k & -VZ & -(\epsilon^f_{\mathbf{k}} - \mu) \end{bmatrix} \tag{97}$$

where $\psi^T_n = (u^c_n(k,\uparrow), u^f_n(k,\downarrow), v^c_n(k,\downarrow), v^f_n(k,\downarrow))$.

$$\begin{aligned}
\langle f^\dagger_{k\uparrow}f^\dagger_{-k,\downarrow}\rangle &= \langle{\sum_n}'[u^f_n(k,\uparrow)\gamma^\dagger_n - v^f_n(k,\uparrow)\gamma_n]{\sum_m}'[u^f_m(-k,\downarrow)\gamma^\dagger_m - v^f_m(-k,\downarrow)\gamma_m]\rangle \\
&= {\sum_n}' u^f_n(k,\uparrow)v^f_n(-k,\downarrow)\langle\gamma^\dagger_n\gamma_n\rangle - v^f_n(k,\uparrow)u^f_n(-k,\downarrow)\langle\gamma_n\gamma^\dagger_n\rangle \\
&= \sum_{E_n>0} u^f_n(k,\uparrow)v^f_n(-k,\downarrow)n_F(E_n) - \sum_{E_n>0} v^f_n(k,\uparrow)u^f_n(-k,\downarrow)n_F(-E_n) \\
&= \sum_{E_n>0} u^f_n(k,\uparrow)v^f_n(-k,\downarrow)n_F(E_n) - \sum_{E_n<0} -u^f_n(k,\uparrow)v^f_n(-k,\downarrow)n_F(E_n) \\
&= \sum_{E_n} u^f_n(k,\uparrow)v^f_n(-k,\downarrow)n_F(E_n)
\end{aligned} \tag{98}$$

and alternatively

$$-\langle f^\dagger_{-k\downarrow}f^\dagger_{k,\uparrow}\rangle = -\sum_{E_n} u^f_n(k,\uparrow)v^f_n(-k,\downarrow)n_F(-E_n) \tag{99}$$

$$n_f(E_n) - n_F(-E_n) = n_F(E_n) - (1 - n_F(E_n)) = 2n_F(E_n) - 1 \tag{100}$$

One may have another equivalent form of pairing term

$$\langle f^{\dagger}_{k\uparrow} f^{\dagger}_{-k,\downarrow}\rangle = \sum_{E_n} u^f_n(k,\uparrow) v^f_n(-k,\downarrow)[n_f(E_n) - n_F(-E_n)]/2 = \sum_{E_n} u^f_n(k,\uparrow) v^f_n(-k,\downarrow)[2n_F(E_n) - 1]/2 \tag{101}$$

$$\begin{aligned}
\langle f^{\dagger}_{k\uparrow} f_{k,\uparrow}\rangle &= \langle \sum_n{}' [u^f_n(k,\uparrow)\gamma^{\dagger}_n - v^f_n(k,\uparrow)\gamma_n] \sum_m{}' [u^f_m(k,\uparrow)\gamma_m - v^f_m(k,\uparrow)\gamma^{\dagger}_m]\rangle \\
&= \sum_n{}' u^f_n(k,\uparrow) u^f_n(k,\uparrow)\langle\gamma^{\dagger}_n\gamma_n\rangle + v^f_n(k,\uparrow) v^f_n(k,\uparrow)\langle\gamma_n\gamma^{\dagger}_n\rangle \\
&= \sum_{E_n>0} u^f_n(k,\uparrow) u^f_n(k,\uparrow) n_F(E_n) + \sum_{E_n>0} v^f_n(k,\uparrow) v^f_n(k,\uparrow) n_F(-E_n) \\
&= \sum_{E_n>0} u^f_n(k,\uparrow) u^f_n(k,\uparrow) n_F(E_n) + \sum_{E_n<0} (-u^f_n(k,\uparrow))(-u^f_n(k,\uparrow)) n_F(E_n) \\
&= \sum_{E_n} u^f_n(k,\uparrow) u^f_n(k,\uparrow) n_F(E_n)
\end{aligned} \tag{102}$$

and

$$\langle f^{\dagger}_{k\downarrow} f_{k,\downarrow}\rangle = \sum_{E_n} v^f_n(k,\downarrow) v^f_n(k,\downarrow) n_F(-E_n) \tag{103}$$

Homework: 1. Compared to the s-wave pairing in BCS theory, one can assume the d-wave pairing in the cuprate system which has been confirmed by experiments. The only change is in the mean-field self-consistent equation for the order parameter Δ is not a constant any more. Instead, we set

$$\Delta(\mathbf{k}) = \Delta\cos(2\phi), \phi = arctan(k_y/k_x) \tag{104}$$

and the attractive interaction is not constant:

$$V(k,k') = V(k\cdot k') = -V_d\cos(2(\phi-\phi')) \tag{105}$$

Then please solve the following self-consistent gap equation:

$$\Delta\cos(2\phi) = V_d\cos(2\phi)\sum_{k'}\frac{\cos^2(2\phi')\tanh(\frac{\beta\xi_{k'}}{2})}{2\xi_{k'}} \tag{106}$$

[1] J. G. Bednorz and K. A. Muller, Z. Phys. B64, 189 (1986)

[2] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).