Cuprate Superconductivity: Boulder Summer School 2014

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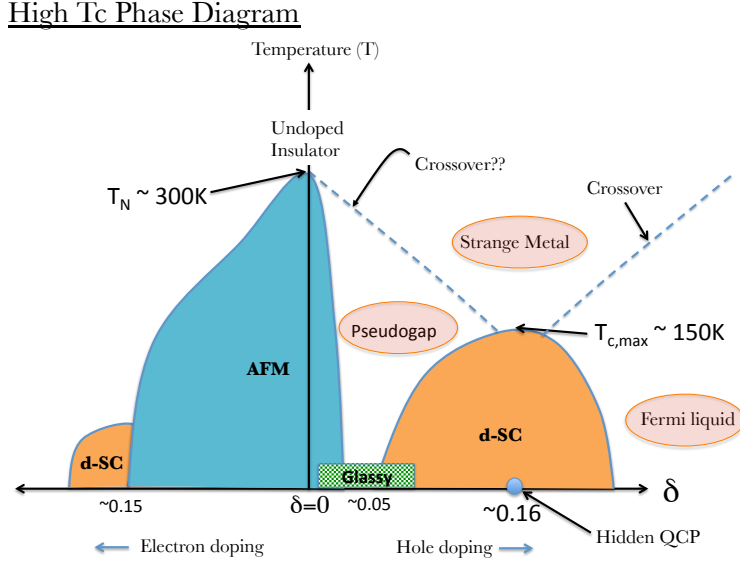
Abstract

High Tc Phase Diagram

FIG. 1. High Tc cuprate superconductor phase diagram

I. BROAD QUESTIONS

- Why is zero doping ($\delta=0$) an insulating antiferromagnet? What sets Néel temperature?
- Why does doping destroy magnetism? Why doping asymmetry?
- Why does doping lead to superconductivity?
- What destroys SC at high/low doping? i.e., why the SC dome?
- What is the pseudogap regime? Is it a new broken symmetry?
- What is the strange non-Fermi liquid metal? Why does the resistivity $\rho \sim T$?
- What sets maximum superconducting T_c? Can we increase it?

II. UNDOPED INSULATOR

A. Local chemistry

Copper ions sit in an approximately octahedral environment of oxygen. In a perfect octahedron, the five degenerate atomic d-orbitals split into a low lying t_{2g} triplet and a high energy e_g doublet, with a typically large splitting $\sim 2\text{eV}$. Deviations from cubic symmetry are also significant due to tetragonal distortion, which splits the t_{2g} multiplet into a higher
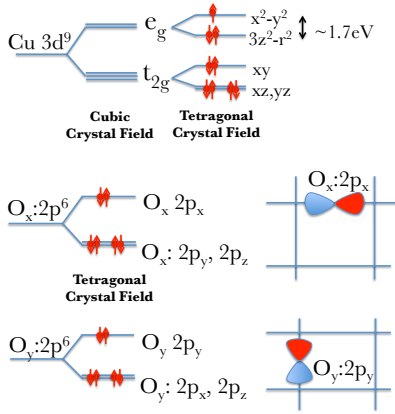
FIG. 2. Crystal field splitting on Cu and O ions

energy xy state and a lower energy xz, yz doublet, this splitting being small $\sim 0.2\text{eV}$. The e_g splitting is however quite big $\sim 1.7\text{eV}$, with a higher energy $d_{x^2-y^2}$ and a lower energy $d_{3z^2-r^2}$. For a recent resonant inelastic x-ray study of orbital Cu-d excitations in various cuprates, see M. M. Sala, *et al*, New J. Phys. **13**, 043026 (2011); related theory work is in L. Hozoi, *et al*, Sci. Rep. **1:65** (2011). The nominal valence Cu^{2+} has a 3d^9 configuration, leading to a single electron (spin-$\uparrow$ or spin-$\downarrow$) in the topmost $d_{x^2-y^2}$ orbital, and all other orbitals being fully occupied. On the x-oxygen ions, the crystal field splitting leads to a low lying $2p_y, 2p_z$ doublet and a high energy $2p_x$ state. All these are fully filled with the nominal valence O^{2-} which leads to a $2p^6$ configuration. Similarly, on the y-oxygen ions, the crystal field splitting leads to a low lying $2p_x, 2p_z$ doublet and a high energy $2p_y$ state. These are also similarly fully filled. These valence assignments are consistent with X-ray studies by J. M. Tranquada, *et al*, PRB **35**, 7187 (1987).

B.   Local excitations in undoped insulator

It is more convenient to think in the hole picture. In the ground state, this leads to one hole in the $d_{x^2-y^2}$ orbital on Cu, and to zero holes on oxygens. There are various classes of local excitations we can make about this ground state.

(i) Hole transfer: We can move a hole from Cu $d_{x^2-y^2}$ to highest orbital on oxygen. This excitation conserves total hole number, and such a neutral excitation is expected to be probed in optics. This is a 'charge transfer' excitation, with energy $\epsilon_p - \epsilon_d \equiv \Delta$. Optical
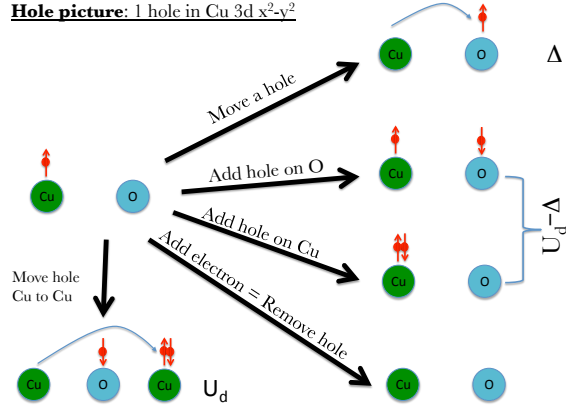
FIG. 3. Some of the local excitations in the undoped insulator

conductivity measurements in the undoped insulator suggest $\Delta \sim 1.5\text{eV}$, see S. L. Cooper, PRB **41**, 11605 (1990). We can also transfer a hole from one Cu to adjacent Cu, this costs energy U_d, which is the local Coulomb repulsion between holes in Cu $3d_{x^2-y^2}$. Materials where $U_d < \Delta$ will be described by an effective model of just Cu sites with local repulsion, such insulators are called Mott-Hubbard insulators. Materials where $U_d > \Delta$ are called Charge Transfer insulators, and the cuprates belong to this category. For a discussion, see J. Zaanen, G. Sawatzky, J. W. Allen, PRL **55**, 418 (1985).

(ii) We can add an extra hole in the Cu $d_{x^2-y^2}$ orbital, or one hole in the highest oxygen $2p$ orbital. The former will cost energy $U_d + \epsilon_d$, and the latter costs ϵ_p. The relative difference in energy is $U_d - \Delta$. So for $U_d < \Delta$, we will add hole on Cu. For $U_d > \Delta$, we will add hole on O. Experiments by J. M. Tranquada, *et al*, PRB **35**, 7187 (1987) show that the Cu valence is unchanging with doping to fairly large values, suggestive of a charge transfer insulator. This may justify a spin-fermion model of the hole doped cuprates, where the spin is on the Cu site and the fermionic hole resides on O sites.

(iii) We can add an electron, or equivalently remove the Cu $3d_{x^2-y^2}$ hole. This is relevant to electron doped cuprates where the mobile charges live on the Cu sites alone, and the oxygen holes are always absent and so O plays no role in the physics.

C. Insulation and magnetism in the undoped material

Naively, the presence of a single hole in the Cu $d_{x^2-y^2}$ orbital and the absence of any holes on O leads to a single hole per CuO_2 unit cell. This should lead to a metallic state arising from partially filled bands according to band theory. However, the undoped compound is an antiferromagnetic insulator. One route to understanding this result is to appeal to the unit cell doubling arising from Neel order which has antiparallel spins on the two sublattices of the Cu lattice. This leads to 2 holes per unit cell, potentially allowing for an insulator. The energy scale of magnetic interactions is $J \sim 150$meV as seen from neutron scattering measurements of the magnon dispersion; see R. Coldea, *et al*, PRL **86**, 5377 (2001) for data upto high energy over the full Brillouin zone. However, the insulating charge transfer gap observed in optics is nearly 1.5eV, while we expect $U_d \sim 5$eV, both energy scales being much higher than J. Thus, the insulation must arise from interaction effects.

The simplest model for the correlated insulator works in the local site-basis instead of the Bloch basis, and focuses on an effective Hubbard model for Cu spins

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

For $U \gg t$, this leads to an effective tJ model

$$H = -t\mathcal{P}_G \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})\mathcal{P}_G + J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) \tag{2}$$

where P_G is an operator ("Gutzwiller projector") which projects out double occupancy which is energetically costly at large U/t, and $J = 4t^2/U$ is the antiferromagnetic exchange coupling between Cu spin-1/2 moments arising from virtual double occupancy in the intermediate state in second order perturbation theory. See A.H. MacDonald, S.M. Girvin, D. Yoshioka, PRB **37**, 9753 (1988) for a systematic derivation using unitary transformations. At zero doping, the resulting spin Hamiltonian is

$$H_{\text{spin}} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j. \tag{3}$$

On symmetry grounds, we expect the full Hamiltonian to have such a leading order term, although subleading higher order terms will also appear. Nevertheless, this simple Heisenberg Hamiltonian is found to largely capture the spin-wave dispersion in the insulator.

In the full model including oxygen sites, J will have the more complicated expression $J = 4t_{pd}^4(\frac{1}{\Delta^2 U_d} + \frac{1}{2\Delta^3})$ (where repulsion on oxygen has been ignored), but the physics of antiferromagnetism will remain the same.

What do we know about the properties of H_{spin}? In one dimension (1d), this model has been solved by Bethe, and the spin correlations decay as $\sim 1/r$ (upto multiplicative log corrections), so the ground state has no spin order. In 3d, the ground state has long range order which persists to finite temperature, leading to a nonzero Neel temperature T_N. In 2d, there was an early suggestion by Anderson that the ground state might be a quantum spin liquid consisting of resonating valence bonds. However, numerical quantum Monte Carlo methods have unambiguously shown long range order at $T = 0$. See, for example, N. Trivedi and D. M. Ceperley, Phys. Rev. B **41**, 4552 (1990), and A. W. Sandvik, Phys. Rev. B **56**, 11678 (1997). However, for $T > 0$, spin correlations decay exponentially as $\exp(-r/\xi_{2d}(T))$ where the spin correlation length $\xi_{2d}(T) \sim e^{2\pi\rho_s/T}$, with $\rho_s \sim JS^2$ being the spin stiffness; see S. Chakravarty, B. I. Halperin, D. Nelson, PRL **60**, 1057 (1988) and PRB **39**, 2344 (1989) which compares predictions from a non-linear sigma model calculation with neutron experiments which measured the spin correlation length versus temperature.

The cuprate materials are layered systems, with a weak interplane spin coupling $J_\perp/J \sim 10^{-4}$. In this case, 3d Néel order is expected to emerge at T_N, when $J_\perp S^2 \xi_{2d}^2(T_N) \sim T_N$, which leads to an implicit relation

$$T_N \sim \frac{4\pi\rho_s}{\ln(\frac{T_N}{J_\perp S^2})} \tag{4}$$

Plugging in $J \sim 1400K$, $\rho_s = 0.175J$ (renormalized down from $JS^2 = 0.25J$ by fluctuations), and $J_\perp/J \sim 10^{-4}$, we find $T_N \sim 350$K, in good agreement with the experimental result 320K.

III. WHY DOES DOPING DESTROY MAGNETIC ORDER?

A. Static dopant in Mott-Hubbard insulator

Let us begin with the simple case where we consider the dopant charges to be static. In a Mott-Hubbard insulator, the dopant leads to an extra hole or electron on an existing spin-1/2 moment, neutralizing it into a spin singlet, and knocking out one site from the lattice. The four bonds connecting to this site get 'cut', however the antiferromagnetic exchange on

the other bonds still favors a Néel state, i.e., there is no frustration. With doping, this Néel order remains stable all the way to the percolation point $\delta_c \approx 0.4$. Direct experiments of this type have been done by substituting Cu by Zn or Mg, confirming this idea; see O. Vajk, *et al*, Science **295**, 1691 (2002). For theory, see A. W. Sandvik, Phys. Rev. B **66**, 024418 (2002) and N. Bray-Ali, J. Moore, T. Senthil, A. Vishwanath, PRB **73**, 064417 (2006). This may give a qualitative hint that magnetism can persist to high electron doping, but it is clearly not in agreement with the rapid disappearance of magnetism in hole doped cuprates.

B.   Static dopant in charge-transfer insulator

In a charge transfer insulator, an added static electron sits on Cu and forms a spin singlet, exactly as in the Mott-Hubbard case. However, an added hole leads to a local spin-1/2 moment on O which couples antiferromagnetically with both neighboring Cu spins with an exchange coupling $J_{\text{CuO}} \gg J_{\text{CuCu}}$. This leads to frustration. One simple classical calculation is to compare the energy of the ferromagnetic state of Cu spins with the Néel state. We have $E_{\text{FM}}/N = 2J_{\text{CuCu}}S^2 - 2J_{\text{CuO}}S^2\delta$ and $E_{\text{Neel}}/N = -2J_{\text{CuCu}}S^2$, so for $\delta > \delta_c = 2J_{\text{CuCu}}/J_{\text{CuO}}$, the antiferromagnetic state is unstable to global ferromagnetism of Cu spins. For $J_{\text{CuO}} \gg J_{\text{CuCu}}$, this can lead to a small δ_c. Clearly, this scenario has the potential to explain the strong doping asymmetry of magnetism. However the above estimate is too simplistic to get at the destruction of Néel order. For an Ising model with antiferromagnetic bond J having probability $1 - \delta$ and ferromagnetic bonds $-J$ having probability δ, the Néel order is lost at the small value $\delta_c \sim 0.09$ as found (numerically) by Vannimenus and Toulouse, J. Phys. C **10**, L537 (1977). If the ferromagnetic bonds have a larger magnitude, as is the case expected for J_{CuO} compared with J_{CuCu}, then we expect an even smaller δ_c. Similar results hold for a Heisenberg model. Further, the existence of both antiferromagnetic Cu-Cu interactions and effective ferromagnetic Cu-Cu interactions induced by the oxygen hole could explain spin glass behavior seen in experiments at low doping. For a discussion, see A. Aharony, *et al*, PRL **60**, 1330 (1988).

C. Mobile holes

Various authors have proposed that the Cu-O model keeping all orbitals is crucial to understand the phase diagram of the cuprate superconductors. See V. J. Emery, PRL **68**, 3794 (1988) and P. B. Littlewood, C. M. Varma, and E. Abrahams, PRL **63**, 2602 (1989) for early work, and C. Weber, T. Giamarchi, and C. M. Varma, PRL **112**, 117001 (2014) for a recent study. With mobile holes, there are various nonsuperconducting states which can get stabilized in doped Mott-Hubbard as well as Charge-Transfer insulators. Such solutions include spin spirals, stripes with spin-density wave and charge order, nematics, etc. In recent work, we have studied the energetics of such solutions within a simplified spin-fermion model with classical Cu spins and mobile oxygen holes. We find that there is quite a close competition between these various ordered states at low doping; see M. Fischer, *et al*, arXiv:1406.2711. For recent work on pairing and pseudogaps in a spin-fermion model, see Y. Wang and A. Chubukov, arXiv:1401.0712.

IV.   DOPED ONE-BAND HUBBARD MODEL

Ignoring subtleties such as glassy order, it has been suggested that the one-band Hubbard model, crucially supplemented by second-neighbor hopping, does capture the essential physics of the cuprates, including the observed particle-hole asymmetry. The argument given by Zhang and Rice, PRB **37**, 3759 (1988) for the adequacy of this model is that the doped hole delocalizes amongst four oxygens surrounding a Cu site, and forms a singlet with the central Cu spin. This effectively removes a spin-1/2 from the Cu lattice, and leads to an extended positively charged object around the Cu site. This effectively looks like a spin-1/2 charged hole centered on the Cu site. Hopping the oxygen hole hops this big object, called a 'Zhang Rice singlet', through the lattice much like a hole in the one-band Hubbard model. We will therefore focus henceforth on the one-band model, although we must keep in mind that certain experimental observations may be more naturally explained in the CuO_2 model. Within this one-band framework, we would like to ask the following questions. How can we understand the effect of doping the Mott insulator? How can we understand the emergence of d-wave superconductivity? Below are partial attempts at answering these questions.

A. Approaching a Mott insulator: Entropy arguments

Consider approaching a metal to Mott insulator transition in 2d by tuning the Hubbard repulsion U at a fixed density of one electron per site. Let us assume that the metal remains a simple Fermi liquid, while the Mott insulator has strictly localized electrons. Let us also be at a small nonzero temperature T. Then, the Fermi liquid entropy $S_{\mathrm{FL}} \sim m^* T$, where m^* is the quasiparticle "effective mass". The fully localized Mott insulator has a spin entropy $S_{\mathrm{loc}} \sim \ln 2$. So the only way to make this match is if $m^* \to \infty$ as we approach the Mott insulator for a continuous transition, or to have a giant entropy jump at a first order transition. This argument goes back to Brinkman and Rice, PRB **2**, 4302 (1970). If we realize that the Mott insulator does not have uncorrelated spins at low temperature, then we should carry out this argument at $T \sim J$ where the spins get decorrelated. This means $m^* J \sim \ln 2$, and the mass divergence is expected to be cutoff. Here, we are using J, the exchange interaction in the vicinity of the Mott transition, as a crude substitute for the spin decorrelation temperature. A very similar argument applies to the (continuous) doping driven Mott transition at $U \gg t$, where $J = 4t^2/U$. Applied to the cuprates, we can compare the renormalized mass to the band mass, and we expect $m^*/m \sim t/J$; optics experiments at low doping roughly confirm this finite mass enhancement. For a review of optics in correlated materials, see D. N. Basov, *et al*, RMP **83**, 471 (2011). Such an entropy argument is also applicable to heavy fermion materials, where we have a thermal crossover from a Fermi liquid to a system with decoupled fermions and local moments; in that case we expect a giant mass $m^* \sim 1/T_K$, where T_K is the (small) Kondo temperature. For a discussion of heavy fermion phenomenology, see C. M. Varma, PRL **55**, 2723 (1985).

Question: If we insist on working at $T = 0$, can we use the *entanglement* entropy S^{en} to reach similar conclusions? The fully localized Mott has $S^{\mathrm{en}}_{\mathrm{loc}} = 0$ while the Fermi liquid has a $S^{\mathrm{en}}_{\mathrm{FL}} \sim L \ln L$ entropy. How can we match unless the $L \ln L$ prefactor contains information about the vanishing quasiparticle residue z or inverse effective mass $1/m^*$? Does the Fermi liquid near the Mott transition have $S^{\mathrm{en}}_{\mathrm{FL}} \sim z L \ln L$ for the Brinkman-Rice transition?

B. Brinkman-Rice theory of the bandwidth-controlled Mott transition

Next, let us formulate a mean field theory of the transition from a Fermi liquid to a Mott insulator with decreasing hole doping. We will do this in the context of the Hubbard model,

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_{\langle ij \rangle} n_{i\uparrow} n_{i\downarrow}. \tag{5}$$

We would like to replace this Hamiltonian by a renormalized hopping Hamiltonian in which interaction induced correlations are ignored but nevertheless double occupancy tends to get suppressed with increasing U. Similarly, we would like replace all operators by renormalized operators such that the correlation functions agree in the two systems. However, since we do not a priori know the true correlations, we have to make some suitable approximation for such renormalization factors. The Gutzwiller approximation amounts to determining these renormalizations using a local statistical argument.

The Hilbert space allows four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$. The table below lists their probabilities and amplitudes assuming no intersite correlations, allowing for a suppression of double occupancy by an unknown factor α in the interacting case.

	Unprojected		Partially projected	
	Probability	Amplitude (A^U)	Probability	Amplitude (A^{PP})
0	$(1-n_{i\uparrow})(1-n_{i\downarrow})$	$\sqrt{(1-n_{i\uparrow})(1-n_{i\downarrow})}$	$1 - n_{i\uparrow} - n_{i\downarrow} + \alpha n_{i\uparrow} n_{i\downarrow}$	$\sqrt{1 - n_{i\uparrow} - n_{i\downarrow} + \alpha n_{i\uparrow} n_{i\downarrow}}$
$\uparrow$	$n_{i\uparrow}(1-n_{i\downarrow})$	$\sqrt{n_{i\uparrow}(1-n_{i\downarrow})}$	$n_{i\uparrow} - \alpha n_{i\uparrow} n_{i\downarrow}$	$\sqrt{n_{i\uparrow} - \alpha n_{i\uparrow} n_{i\downarrow}}$
$\downarrow$	$n_{i\downarrow}(1-n_{i\uparrow})$	$\sqrt{n_{i\downarrow}(1-n_{i\uparrow})}$	$n_{i\downarrow} - \alpha n_{i\uparrow} n_{i\downarrow}$	$\sqrt{n_{i\downarrow} - \alpha n_{i\uparrow} n_{i\downarrow}}$
$\uparrow\downarrow$	$n_{i\uparrow} n_{i\downarrow}$	$\sqrt{n_{i\uparrow} n_{i\downarrow}}$	$\alpha n_{i\uparrow} n_{i\downarrow}$	$\sqrt{\alpha n_{i\uparrow} n_{i\downarrow}}$

Now consider the correlation $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle$. We can relate this to the unprojected correlation via a renormalization factor g_t, where $\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle = \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle_0 \times g_t$.

$$g_t = \frac{(A_j^{PP}(\uparrow) A_j^{PP}(0) + A_j^{PP}(\uparrow\downarrow) A_j^{PP}(\downarrow))(A_i^{PP}(0) A_i^{PP}(\uparrow) + A_i^{PP}(\downarrow) A_i^{PP}(\uparrow\downarrow))}{(A_j^U(\uparrow) A_j^U(0) + A_j^U(\uparrow\downarrow) A_j^U(\downarrow))(A_i^U(0) A_i^U(\uparrow) + A_i^U(\downarrow) A_i^U(\uparrow\downarrow))}. \tag{6}$$

In the uniform half-filled case, we can replace $n_{i\uparrow} = n_{i\downarrow} = 1/2$. This leads to $g_t = 2\alpha(1-\alpha/2)$. Similarly, $\langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} n_{i\downarrow} \rangle_0 \times g_U$, leads to $g_U = \alpha$. The renormalized Hamiltonian is then

$$H_{BR} = -g_t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + g_U U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{7}$$

Making a Fermi sea ansatz for this renormalized Hamiltonian leads to the ground state energy per site (on a 2d square lattice)

$$E(\alpha) = -\frac{16}{\pi^2}\alpha\left(1 - \frac{\alpha}{2}\right)t + \frac{\alpha}{4}U. \tag{8}$$

Since the projection factor α is unknown, we treat it as a variational parameter. Minimizing the energy with respect to α, we find $\alpha = (1 - \frac{\pi^2 U}{64t})$. With increasing U/t, we find α decreases, eventually vanishing at $U_c/t = 64/\pi^2$. This signals the Mott transition at which double occupancy vanishes. This is somewhat smaller than single-site DMFT which yields a (first order) transition at $U_c/t \sim 9.5$. Setting $\alpha = 1 - U/U_c$, we find

$$g_t = 1 - \left(\frac{U}{U_c}\right)^2 \tag{9}$$

The ratio of effective mass to the band mass, $m^*/m = g_t^{-1}$, and it diverges at the Mott transition, consistent with the entropy argument. We can similarly compute the one-body density matrix, whose Fourier transform yields the momentum distribution. Specifically, the off-diagonal density matrix at large distance controls the singular jump in $n(\mathbf{k})$, and it gets renormalized by g_t compared to the free Fermi gas on the lattice. This yields the quasiparticle renormalization factor $z = g_t$, which vanishes upon approaching the Mott transition. Thus, the Brinkman-Rice transition is driven by an increasing localization and mass divergence of the Fermi liquid, while the Fermi surface itself is preserved.

C. Doping driven metal to Mott insulator transition

Next, let us formulate a mean field theory of the transition from a Fermi liquid to a Mott insulator with decreasing hole doping. We will do this in the context of the tJ model,

$$H = -t\mathcal{P}_G \sum_{\langle ij\rangle\sigma}(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})\mathcal{P}_G + J\sum_{\langle ij\rangle}(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}n_i n_j) \tag{10}$$

where P_G refers to projecting out double occupancy. As before, we would like to replace this Hamiltonian by a renormalized Hamiltonian in which projection is ignored, and similarly replace all operators by renormalized operators, such that the correlation functions agree in the two systems.

In the projected Hilbert space, we are allowed only three states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$ at each site, while the unprojected Hilbert space includes the extra state $|\uparrow\downarrow\rangle$. The table below lists their probabilities and amplitudes assuming no intersite correlations.

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	Unprojected		Projected	
	Probability	Amplitude (A^U)	Probability	Amplitude (A^P)
0	$(1-n_{i\uparrow})(1-n_{i\downarrow})$	$\sqrt{(1-n_{i\uparrow})(1-n_{i\downarrow})}$	$1-n_{i\uparrow}-n_{i\downarrow}$	$\sqrt{1-n_{i\uparrow}-n_{i\downarrow}}$
↑	$n_{i\uparrow}(1-n_{i\downarrow})$	$\sqrt{n_{i\uparrow}(1-n_{i\downarrow})}$	$n_{i\uparrow}$	$\sqrt{n_{i\uparrow}}$
↓	$n_{i\downarrow}(1-n_{i\uparrow})$	$\sqrt{n_{i\downarrow}(1-n_{i\uparrow})}$	$n_{i\downarrow}$	$\sqrt{n_{i\downarrow}}$
↑↓	$n_{i\uparrow}n_{i\downarrow}$	$\sqrt{n_{i\uparrow}n_{i\downarrow}}$	0	0

Now consider the correlation $\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle$. We can relate this to the unprojected correlation via a renormalization factor g_t, where $\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle = \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle_0 \times g_t$. We obtain,

$$g_t = \frac{A_j^P(\uparrow)A_j^P(0)A_i^P(0)A_i^P(\uparrow)}{(A_j^U(\uparrow)A_j^U(0)+A_j^U(\uparrow\downarrow)A_j^U(\downarrow))(A_i^U(0)A_i^U(\uparrow)+A_i^U(\downarrow)A_i^U(\uparrow\downarrow))} = \frac{2\delta}{1+\delta}. \tag{11}$$

Similarly, consider $\langle S_i^+ S_j^-\rangle$. We can relate this to the unprojected correlation via a renormalization factor g_J, where $\langle S_i^+ S_j^-\rangle = \langle S_i^+ S_j^-\rangle_0 \times g_J$, where

$$g_J = \frac{A_j^P(\uparrow)A_j^P(\downarrow)A_i^P(\downarrow)A_i^P(\uparrow)}{A_j^U(\uparrow)A_j^U(\downarrow)A_i^U(\downarrow)A_i^U(\uparrow)} = \frac{4}{(1+\delta)^2}. \tag{12}$$

This leads to the renormalized Hamiltonian

$$H = -g_t t\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + g_J J\sum_{\langle ij\rangle}(\vec{S}_i\cdot\vec{S}_j - \frac{1}{4}n_i n_j) \tag{13}$$

When $\delta\to 1$, we get $g_t\to 1$ and $g_J\to 1$, so that for $J\ll t$, we have a Fermi gas with weak spin-spin interactions. For $\delta\to 0$, since $g_t\to 0$ while $g_J\to 4$, so that $g_J J\gg g_t t$ and interactions become much more important than the kinetic energy. Below, we treat the interactions within mean field theory.

To carry out a mean field analysis of a uniform Fermi liquid, we must make an ansatz for the uniform ground state wavefunction of this Hamiltonian. Equivalently we decouple the interactions within a translationally invariant Hartree-Fock theory, which leads to

$$H_{\text{FL}} = -(g_t t + g_J J\frac{\chi}{2})\sum_{\langle ij\rangle\sigma}(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) \tag{14}$$

with

$$\chi = \frac{1}{2}\sum_\sigma\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle \tag{15}$$

being the self-consistently evaluated nearest-neighbor correlation. For the 2d square lattice, approximating χ by its value at $\delta = 0$, we get $\chi\approx 2/\pi^2$. Further, as the doping $\delta\to 0$,

we get $g_t \to 0$ and $g_J \to 4$, so the effective fermion hopping becomes $2J\chi \sim 4J/\pi^2$. This leads to an effective mass enhancement $m^*/m \sim \frac{\pi^2 t}{4J}$, in rough agreement with the entropy argument. The quasiparticle residue $z \approx 2\delta/(1+\delta)$. For the cuprates, setting $J/t \sim 0.3$ leads to $m^*/m \sim 8$ as $\delta \to 0$. Thus, similar to the bandwidth-tuned Mott transition, the Fermi surface of the metal is preserved but the quasiparticle weight vanishes as we approach the Mott transition. In contrast to the Brinkman-Rice treatment, the mass does not diverge as we approach zero doping. If we realize that the spin-spin interactions will also get generated near the bandwidth-tuned Mott transition, then we should expect the mass divergence gets cutoff in that case as well, which could be captured within a heuristic tUJ model.

D. Superconducting mean field theory of the tJ model

Next, let us consider the renormalized Hamiltonian

$$H = -g_t t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + g_J J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j). \tag{16}$$

For small $g_J J \ll g_t t$, we could carry out an perturbative analysis in terms of "spin fluctuations" to look for pairing instabilities. Alternatively, we can carry out a mean field treatment still assuming translational invariance but allowing for nonzero pairing. The Hartree-Fock-Bogoliubov theory leads to the following mean field equations if we assume d-wave pairing (a more unbiased treatment finds that d-wave pairing wins over other pairing channels for a wide doping range):

$$\frac{1}{g_J J} = \int \frac{d^2 k}{4\pi^2} \frac{(\cos k_x - \cos k_y)^2}{E_{\mathbf{k}}} \tag{17}$$

$$\chi = \int \frac{d^2 k}{4\pi^2} \left(-\frac{\xi_{\mathbf{k}}}{4 E_{\mathbf{k}}} \right) (\cos k_x + \cos k_y) \tag{18}$$

$$1 - \delta = \int \frac{d^2 k}{4\pi^2} \left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right) \tag{19}$$

where

$$\xi_{\mathbf{k}} = -2(g_t t + g_J J \frac{\chi}{2})(\cos k_x + \cos k_y) - \mu \tag{20}$$

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_d^2 \frac{(\cos k_x - \cos k_y)^2}{4}}. \tag{21}$$

What are some basic features of the solution? At large doping, $\delta \sim 1$, the Fermi surface is small and almost circular, and as the Fermi surface shrinks, we have $\chi \sim 0$. Further

$g_t, g_J \sim 1$. This leads to a gap $\Delta_d \sim \mathrm{e}^{-\alpha \frac{t}{J(1-\delta)^2}}$, vanishing rapidly as $\delta \to 1$. At small $\delta \sim 0$, we have $g_t \to 0$, while $\chi \sim \mathcal{O}(1)$. Now, since the dispersion and the interactions both scale as J, the pairing gap $\Delta_d \sim J$. The pairing scale in this ansatz thus starts off at J and vanishes with increasing doping. What about the superconducting order parameter? For this we need to consider the off-diagonal two-particle density matrix operator $O_2 = c_{i\uparrow}^\dagger c_{i+\delta\downarrow}^\dagger c_{j\downarrow} c_{j+\delta'\uparrow}$. For large $|i - j| \to \infty$ goes as $\langle O_2 \rangle \to \Phi_d^2 \eta_\delta \eta_{\delta'}$, where Φ_d is the SC order parameter, with $\eta_{\pm x} = 1$ and $\eta_{\pm y} = -1$. In RMFT, we can replace $O_2 \to g_{\mathrm{sc}} O_2$, where

$$g_{\mathrm{sc}} = \frac{N}{D} \tag{22}$$

$$N = A_j^P(\downarrow) A_j^P(0) A_{j+\delta'}^P(\uparrow) A_{j+\delta'}^P(0) A_i^P(0) A_i^P(\uparrow) A_{i+\delta}^P(0) A_{i+\delta}^P(\downarrow) \tag{23}$$

$$D = (A_j^U(\downarrow) A_j^U(0) + A_j^U(\uparrow\downarrow) A_j^U(\uparrow)) \times (A_{j+\delta'}^U(\uparrow) A_{j+\delta'}^U(0) + A_{j+\delta'}^U(\uparrow\downarrow) A_{j+\delta'}^U(\downarrow))$$
$$\times (A_i^U(0) A_i^U(\uparrow) + A_i^U(\downarrow) A_i^U(\uparrow\downarrow)) \times (A_{i+\delta}^U(0) A_{i+\delta}^U(\downarrow) + A_{i+\delta}^U(\uparrow) A_{i+\delta}^U(\uparrow\downarrow)) \tag{24}$$

This yields $g_{\mathrm{sc}} = g_t^2$, so that the SC order parameter is $g_t \Phi_d^0$, where Φ_d^0 is the unrenormalized order parameter. Thus, projection leads to $\Phi_d \sim 2\delta$ for $\delta \ll 1$. Then we get a SC dome, with a maximal order parameter at intermediate dopings where both pairing is strong and projection physics does not suppress the order parameter. Similarly, $g_t \sim 2\delta$ also suppresses the superfluid stiffness $\rho_s(T = 0)$ which sets the scale of the low doping thermal transition.

When is this mean field theory possibly reliable? The effective interaction exceeds the effective bandwidth when $g_J J \sim 8 g_t t$. For $J/t = 0.25\text{-}0.3$, we find $\delta_c \sim 0.06\text{-}0.08$ below which we definitely cannot trust a simple mean field analysis of interactions. For instance, the magnetic instability at low doping should result from fluctuations beyond mean field theory. Above this doping, mean field theory may provide a useful guide.

In summary, the renormalized mean field theory predicts a d-wave superconducting dome. Pairing occurs due to antiferromagnetic exchange interactions. At low doping, projection kills superconductivity, while at high doping the pairing itself is weak. Turning to experiments, we expect disorder to strongly suppress superconductivity when the pairing gets very weak. Furthermore, in this 'dirty limit', we also expect the superfluid stiffness $\rho_s \sim \Delta_d$, which should lead to dome in $\rho_s(T = 0)$ versus doping. Finally, at low doping, the separation of scales between pairing scale ($\sim J$) and the order parameter (vanishing as $\sim \delta$), suggests the emergence of a pseudogap in the normal state electron spectral function. A full inhomogeneous mean field treatment, following recent work by Sachdev and collaborators, appears to find charge ordering tendencies in the underdoped regime. However, the

RMFT completely misses the strong antiferromagnetic correlations which develop with underdoping, with $\xi_{2d}^{\text{spin}}(T = 0) \sim 1/\sqrt{\delta}$, and which cause the undoped insulator to have a Néel ordered ground state. Furthermore, RMFT does not present a route to incorporating beyond-mean-field effects of projection. Finally, any translational symmetry breaking state will also have *inhomogeneous* projection factors g_t, g_J which needs to be taken into account in computing energetics of candidate instabilities.

V. PARTON THEORIES

One of the key points which the RMFT treatment raises is the very different renormalizations of spin operators and operators which change particle number locally, the former surviving into the insulator while the latter get suppressed as we approach zero doping. This motivates a treatment which tries to explicitly write the electron in terms of separate spin and charge degrees of freedom. This class of theories are referred to as 'slave particle' or 'parton' theories. We here review the slave-rotor description introduced by S. Florens and A. Georges, Phys. Rev. B 70, 035114 (2004), which has the advantage of being applicable also to systems like the organic superconductors. The electron Hilbert space at a single lattice site has four states, $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$. That is, it could be empty, or be occupied by a spin up electron, or a spin down electron, or be doubly occupied. In the slave rotor representation, the electron charge degree of freedom is described by a charged rotor and the spin degree of freedom is described by a spin-1/2 spinon (fermion). Each of the four physical states then corresponds to a direct product of the rotor state and the spinon state,

$$|0\rangle \equiv |1\rangle|0\rangle$$
$$|\uparrow\rangle \equiv |0\rangle|\uparrow\rangle$$
$$|\downarrow\rangle \equiv |0\rangle|\downarrow\rangle$$
$$|\uparrow\downarrow\rangle \equiv |-1\rangle|\uparrow\downarrow\rangle$$

Here on the r.h.s., the first ket $|n^\theta\rangle$ is the eigenstate of rotor charge with eigenvalue $n^\theta = 0, \pm 1$, and the second ket is eigenstate of spinon occupation number, $n_{f,\sigma} = 0, 1$ for $\sigma = \uparrow, \downarrow$. Notice we have chosen a background charge 0 for the state with one electron, and each doped hole sends $n^\theta \to n^\theta + 1$. The enlarged rotor-spinon Hilbert space contains unphysical states

such as $|1\rangle|\uparrow\rangle$. These unphysical states are avoided by imposing the operator constraint

$$n_i^\theta + n_{i,\uparrow}^f + n_{i,\downarrow}^f = 1. \tag{25}$$

In the slave rotor representation, the electron number is equal to the spinon number, i.e.,

$$n_{i\sigma}^{\mathrm{e}} = n_{i\sigma}^f. \tag{26}$$

The electron creation (annihilation) operator

$$c_{i,\sigma}^\dagger = f_{i,\sigma}^\dagger \mathrm{e}^{-i\theta_i}, \tag{27}$$

$$c_{i,\sigma} = f_{i,\sigma} \mathrm{e}^{+i\theta_i}, \tag{28}$$

where f_σ is the spinon annihilation operator, and the rotor creation and annihilation operators are given by $\mathrm{e}^{+i\theta_i}$ and $\mathrm{e}^{-i\theta_i}$ respectively, where we define by

$$\mathrm{e}^{\pm i\theta_i}|n_i^\theta\rangle = |n_i^\theta \pm 1\rangle. \tag{29}$$

We will use a heuristic tUJ Hamiltonian, and write it in terms of the spinon and rotor field operator as

$$H_{\mathrm{SR}} = -\sum_{i,j,\sigma} t_{ij} f_{i\sigma}^\dagger f_{j\sigma} \mathrm{e}^{-i\theta_i} \mathrm{e}^{+i\theta_j} + \frac{U}{2} \sum_i (n_i^\theta)^2 + J \sum_{\langle i,j \rangle} \mathbf{S}_i^f \cdot \mathbf{S}_j^f. \tag{30}$$

Here we have expressed the Hubbard repulsion between electron charges in terms of the rotors since only the rotors carry charge. Similarly, the antiferromagnetic exchange interaction is expressed in terms of the spinons, with $\mathbf{S}_i^f \equiv f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta}$ since only the spinons have a spin quantum number. Finally, the electron density is determined via the spinon density since $\langle n^f \rangle = \langle n^{\mathrm{e}} \rangle$ as mentioned earlier.

In the spirit of mean field theory, we approximate the electron wavefunction by the direct product of appropriate spinon and rotor wavefunctions, with the constraint equation satisfied on average in the resulting mean field state, $\langle n_i^\theta \rangle + \langle n_{i,\uparrow}^f \rangle + \langle n_{i,\downarrow}^f \rangle = 1$. Together with $\langle n^{\mathrm{e}} \rangle = \langle n^f \rangle$, this leads to two mean field constraints,

$$\sum_\sigma \langle n_{i,\sigma}^f \rangle = \langle n^{\mathrm{e}} \rangle \equiv 1 - \delta, \tag{31}$$

$$\langle n_i^\theta \rangle = 1 - \langle n^{\mathrm{e}} \rangle \equiv \delta, \tag{32}$$

where we have defined the doping δ, with $\delta > 0$ ($\delta < 0$) representing hole (electron) doping. For example, the electron ground state $|\Psi\rangle = |\Psi_\theta\rangle|\Psi_f\rangle$, and our task reduces to find the

normalized wavefunctions $|\Psi_\theta\rangle, |\Psi_f\rangle$ subject to the constraint that $\langle\Psi_\theta|n_i^\theta|\Psi_\theta\rangle = \delta$ and $\langle\Psi_f|n_i^f|\Psi_f\rangle = 1 - \delta$.

We define reduced spinon and rotor Hamiltonian as

$$
\begin{aligned}
\tilde{H}_f &= \langle\Psi_\theta|H_{\mathrm{SR}}|\Psi_\theta\rangle \\
&= -\sum_{i,j,\sigma} t_{ij} f_{i\sigma}^\dagger f_{j\sigma} B_{ij} + \frac{U}{2}\sum_i \langle(n_i^\theta)^2\rangle_\theta + J\sum_{\langle i,j\rangle} \mathbf{S}_i^f \cdot \mathbf{S}_j^f
\end{aligned}
\tag{33}
$$

$$
\begin{aligned}
\tilde{H}_\theta &= \langle\Psi_f|H_{\mathrm{SR}}|\Psi_f\rangle \\
&= -\sum_{i,j,\sigma} t_{ij}\chi_{ij}\mathrm{e}^{-i\theta_i}\mathrm{e}^{+i\theta_j} + \frac{U}{2}\sum_i (n_i^\theta)^2 + J\sum_{\langle i,j\rangle}\langle\mathbf{S}_i^f \cdot \mathbf{S}_j^f\rangle_f.
\end{aligned}
\tag{34}
$$

Here we have used the notation, $\langle\ldots\rangle_f \equiv \langle\Psi_f|\ldots|\Psi_f\rangle$ and $\langle\ldots\rangle_\theta \equiv \langle\Psi_\theta|\ldots|\Psi_\theta\rangle$, and also defined

$$
B_{ij} = \langle\mathrm{e}^{-i\theta_i}\mathrm{e}^{+i\theta_j}\rangle_\theta,
\tag{35}
$$

$$
\chi_{ij} = \langle f_{i\sigma}^\dagger f_{j\sigma}\rangle_f.
\tag{36}
$$

Note that there is no implicit summation over spin σ in defining χ_{ij}, and we have assumed χ_{ij} is spin-independent.

The ground state energy in mean field theory is $E_0 = \langle\Psi_f|\tilde{H}_f|\Psi_f\rangle = \langle\Psi_\theta|\tilde{H}_\theta|\Psi_\theta\rangle$. Thus, in order to minimize E_0, we must choose $|\Psi_f\rangle$ to be the ground state of $\tilde{H}_f$, and $|\Psi_\theta\rangle$ to be the ground state of $\tilde{H}_\theta$. This means we must self consistently solve for the ground state of the two coupled Hamiltonians

$$
H_f = -\sum_{i,j,\sigma} t_{ij} B_{ij} f_{i\sigma}^\dagger f_{j\sigma} + J\sum_{\langle i,j\rangle} \mathbf{S}_i^f \cdot \mathbf{S}_j^f - \mu_f\sum_{i\sigma} n_{i\sigma}^f,
\tag{37}
$$

$$
H_\theta = -2\sum_{i,j} t_{ij}\chi_{ij}\mathrm{e}^{-i\theta_i}\mathrm{e}^{+i\theta_j} + \frac{U}{2}\sum_i (n_i^\theta)^2 - \mu_\theta\sum_{i\sigma} n_i^\theta,
\tag{38}
$$

where we have introduced chemical potentials for the spinons (μ_f) and rotors (μ_θ) as Lagrange multipliers to impose the mean field number constraints Eq.(31) and (32). The main qualitative similarity with RMFT is the very different spin and charge physics which becomes evident at low doping close to the Mott insulator. Note that the two decoupled Hamiltonians H_f, H_θ are, at this stage, still strongly interacting models, and we have to use further approximations in the spinon and rotor sectors to make progress. However, note that if we develop better techniques to solve these independent spinon and rotor Hamiltonians, we can obtain better results within this self-consistent mean field approach. Finally, the ground

state energy of the electronic model is given by the expectation value of the Hamiltonian $H_{\rm SR}$ of Eq.(30), which leads to

$$E_{\rm e}^0 = -\sum_{i,j,\sigma} t_{ij}\chi_{ij}B_{ij} + \frac{U}{2}\sum_i \langle (n_i^\theta)^2\rangle_\theta + J\sum_{\langle i,j\rangle}\langle \mathbf{S}_i^f\cdot\mathbf{S}_j^f\rangle_f. \tag{39}$$

The details of this method and some applications are discussed in E. Zhao and A. Paramekanti, Phys. Rev. B **76**, 195101 (2007).

A. Spinon Sector

The spinon sector corresponds to a Hamiltonian with kinetic energy and an antiferromagnetic exchange interaction. In principle, the spinon sector can be treated using diagrammatic techniques, especially when the spin interaction strength is small compared to the spinon kinetic energy. Away from this regime, for larger spin interactions, the diagrammatic methods may not be adequate. Here we adopt a simpler mean field approach to the spinon sector which has the advantage that we can describe the normal state, various broken symmetry states, and singlet pairing states of spinons. Upto constant terms, following the RMFT prescription, this yields

$$\mathbf{S}_i^f\cdot\mathbf{S}_j^f \rightarrow -\frac{3}{4}\chi_{ij}\sum_\sigma\left(f_{i\sigma}^\dagger f_{j\sigma} + \text{h.c.}\right) - \frac{3}{4}\Delta_{ij}\left(f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger + \text{h.c.}\right). \tag{40}$$

Here we assume χ_{ij} is real, and $|\Delta_{ij}| \equiv |\langle f_{i\downarrow}f_{j\uparrow}\rangle|$ is magnitude of the d-wave pairing, with Δ_{ij} being positive on x-bonds and negative on y-bonds of the square lattice.

B. Rotor Sector

The rotor Hamiltonian can be solved by using methods for correlated bosons. One option is a cluster mean field theory which is a straightforward extension of the single-site mean field theory used to describe the boson Mott transition. This focuses on a cluster of sites and treats the influence of the sites outside the cluster (the "bath") using a mean field order parameter. The hopping terms that couple sites within the cluster to sites outside the cluster are decoupled using $e^{-i\theta_i}e^{i\theta_j} \rightarrow e^{-i\theta_i}\Phi$, $i \in$ cluster, $j \in$ bath, where the mean field superfluid order parameter $\Phi \equiv \langle e^{i\theta_i}\rangle$ has to be determined self-consistently. In the superfluid phase, $\Phi \neq 0$. The Mott insulator phase, on the other hand, is characterized by
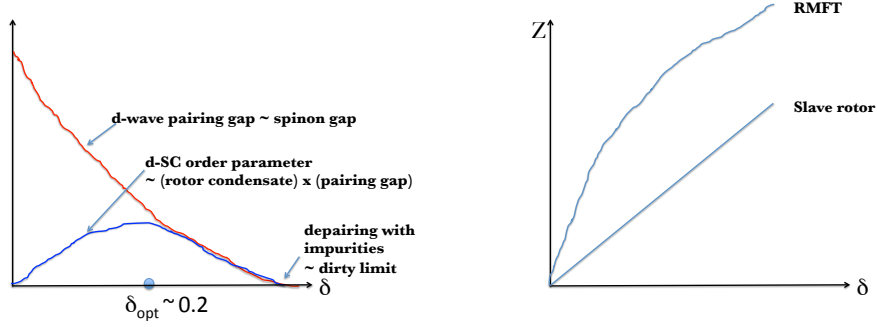
FIG. 4. Order parameter, pairing gap, and nodal quasiparticle weight z

$\Phi = 0$. All terms within the cluster, including the onsite U and intra-cluster hopping, are retained completely. This cluster mean field Hamiltonian is diagonalized exactly to obtain the eigen-energies and the ground state rotor wave function. Going to larger clusters, we can obtain a better description of the bosonic excitations of the rotor sector.

C. Some results

Results from slave rotor theory are in line with the RMFT results. For example, the SC pairing gap and d-wave SC order parameter are in reasonable agreement with RMFT. The most important quantitative difference is that while the quasiparticle residue $z \sim g_t \sim 2\delta$ in RMFT, the slave rotor theory leads to $z \sim \delta$ at low doping. Again, antiferromagnetism is not captured in the spinon mean field theory. Crucially, in addition to solving the spinon and rotor Hamiltonians, we have also to worry about other fluctuations - although the spinon and rotor may appear to be separate degrees of freedom at low energy, they must bind (confine) into electrons at high energy, which needs additional gauge fluctuations. We will not pursue this, instead just noting recent work by M. A. Metlitski, D. F. Mross, S. Sachdev, and T. Senthil (arXiv:1403.3694) which discusses this issue in the context of spinon pairing.