

PSEUDOGAPPED MOTT CRITICALITY: STRETCHING KONDO SCREENING TO BREAKING POINT

HOW A FERMI LIQUID GIVES WAY TO MOTT INSULATOR IN 2D

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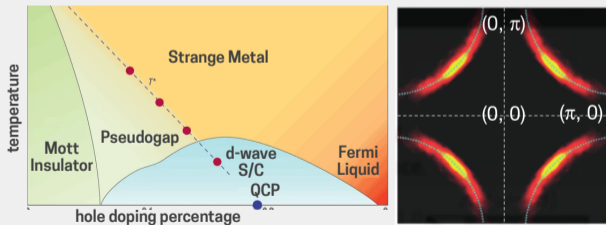


SOME QUESTIONS

The anomalous **pseudogap** (PG) phase exhibits nodal-antinodal dichotomy.

No general consensus yet regarding

- nature of $T = 0$ ground states of the cuprates
- **relation** of PG to Mott insulating and superconducting phases proximate to it
- how pseudogap **evolves** from weak- to strong-coupling
- nature of correlations and entanglement near the transition



Keimer et al. 2015; Proust and Taillefer 2019; Loeser et al. 1996; Norman et al. 1998; Hashimoto et al. 2014; Kyung et al. 2006; Macridin et al. 2006; Wu et al. 2018; Mukherjee and Lal 2020; Hille et al. 2020.

NEW AUXILIARY MODEL APPROACH TO INTERACTING FERMIONS

1. Solve an **impurity model** H_{imp} with certain properties:

- Lattice symmetry
- Impurity phase transition

2. **Construct lattice** model by applying many-body translation operators:

$$H_{\text{latt}} = \sum_{\mathbf{r}} T^{\dagger}(\mathbf{r}) H_{\text{imp}}(\mathbf{r}_0) T(\mathbf{r})$$

3. Relate computables across the models, using many-body Bloch's theorem

Greens functions:

$$\tilde{G}(\mathbf{K}\sigma; \omega) = G^{>}(T_{\mathbf{K}\sigma}^{\dagger}, \omega - \varepsilon_{\mathbf{K}}) + G^{<}(T_{\mathbf{K}\sigma}^{\dagger}, \omega + \varepsilon_{\mathbf{K}})$$

Equal-time **correlation** functions:

$$C_O(\mathbf{k}_1, \mathbf{k}_2) = \sum_{\Delta} \langle \mathbf{r}_c + \Delta | \tilde{O}(\mathbf{k}_2) | \mathbf{r}_c \rangle \langle \mathbf{r}_c | \tilde{O}^{\dagger}(\mathbf{k}_1) | \mathbf{r}_c \rangle$$

where

$$G^{>}(O^{\dagger}, t) = -i \langle O(t) O^{\dagger} \rangle,$$

(imp-bath T-matrix)

$$T_{\mathbf{K}\sigma} = c_{\mathbf{K}\sigma} (\sum_{\sigma'} c_{d\sigma'}^{\dagger} + \text{h.c.}) + c_{\mathbf{K}\sigma} (S_d^{\dagger} + \text{h.c.}),$$

$$\tilde{O}(\mathbf{r}) = O(\mathbf{r}) O^{\dagger}(d)$$

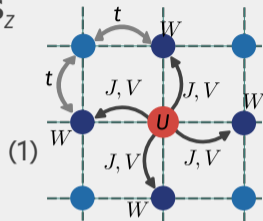
THE CORE INGREDIENT: A LATTICE-EMBEDDED IMPURITY MODEL

$$H_{\text{imp}} = H_{\text{2D-TB-KE}} - \frac{U}{2} (n_{d\uparrow} - n_{d\downarrow})^2 + V \sum_{Z,\sigma} (c_{d\sigma}^\dagger c_{Z\sigma} + \text{h.c.}) + J \sum_Z \mathbf{s}_d \cdot \mathbf{s}_Z$$

$$- \frac{W}{2} \sum_Z (n_{Z\uparrow} - n_{Z\downarrow})^2$$

■ $J_{\mathbf{k},\mathbf{k}'}$ has C_4 -**symmetry**:

$$J_{\mathbf{k},\mathbf{k}'} = \frac{J}{2} [\cos(\mathbf{k}_x - \mathbf{k}'_x) + \cos(\mathbf{k}_y - \mathbf{k}'_y)]$$



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Map to Hubbard-Heisenberg Model

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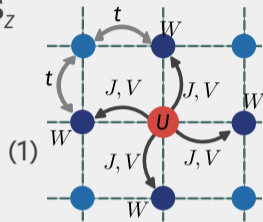
$$= -\frac{\tilde{t}}{\sqrt{Z}} \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle; \sigma} (c_{\mathbf{r}_i, \sigma}^\dagger c_{\mathbf{r}_j, \sigma} + \text{h.c.}) - \tilde{\mu} \sum_{\mathbf{r}} \hat{n}_{\mathbf{r}, \sigma}$$

$$+ \frac{\tilde{J}}{Z} \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle} \mathbf{s}_{\mathbf{r}_i} \cdot \mathbf{s}_{\mathbf{r}_j} - \frac{1}{2} \tilde{U} \sum_{\mathbf{r}} (\hat{n}_{\mathbf{r}, \uparrow} - \hat{n}_{\mathbf{r}, \downarrow})^2$$

$$\tilde{t} = t + 2V$$

$$\tilde{U} = U + W$$

$$\tilde{\mu} = 2\mu + \eta, \quad \tilde{J} = 2J$$



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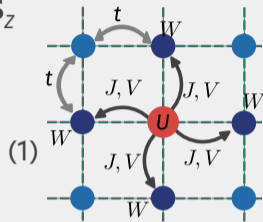
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■ We work in large U limit

■ SW transformation
 \rightarrow **$J - W$ model**

PSEUDOGAPPING TRANSITION FROM KONDO BREAKDOWN

Unitary RG analysis - integrate out high-energy states in the conduction bath:

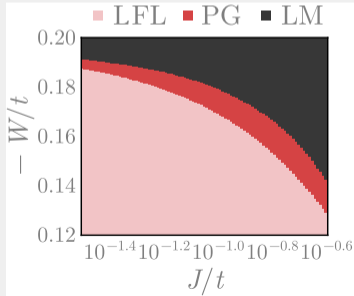
$$\Delta J_{\mathbf{k}_1, \mathbf{k}_2}^{(j)} = - \sum_{\mathbf{q} \in \text{PS}} \frac{J_{\mathbf{k}_2, \mathbf{q}}^{(j)} J_{\mathbf{q}, \mathbf{k}_1}^{(j)} + 4 J_{\mathbf{q}, \bar{\mathbf{q}}}^{(j)} W_{\bar{\mathbf{q}}, \mathbf{k}_2, \mathbf{k}_1, \mathbf{q}}}{\omega - \frac{1}{2} |\varepsilon_j| + J_{\mathbf{q}}^{(j)} / 4 + W_{\mathbf{q}} / 2}$$

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- Contrast with **eSIAM**: $\Delta J \sim J(J + 4W)$

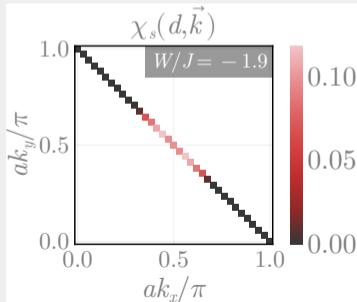
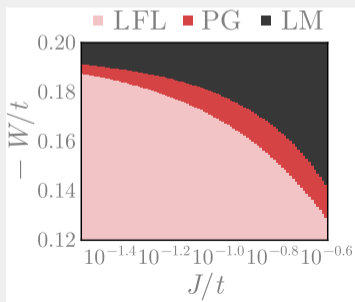


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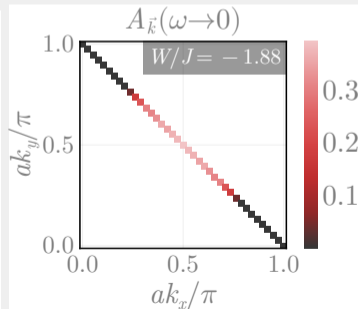
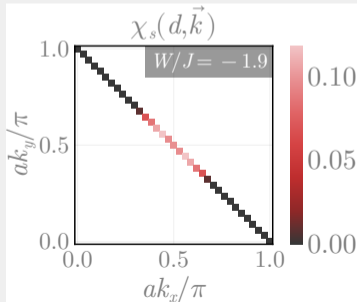
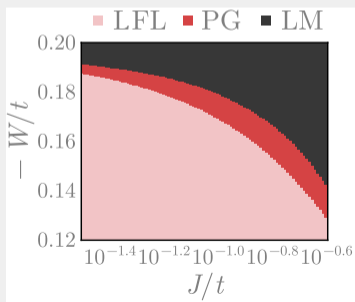


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- Lattice model DOS shows **P-gap**



LOCAL FERMI LIQUID AND LOCAL MOMENT PHASES

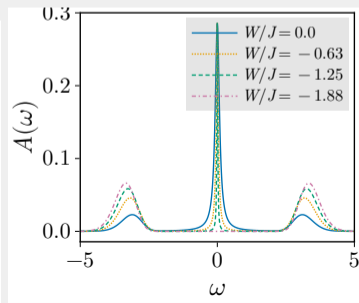
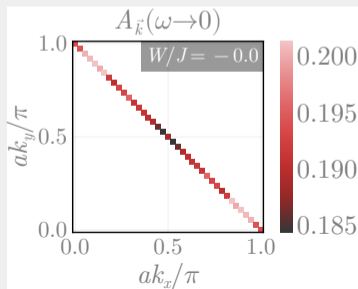
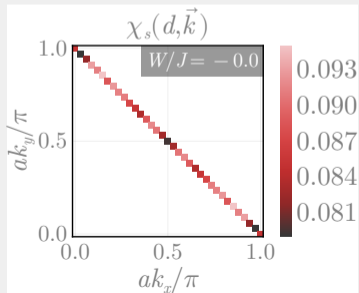
LFL

- Democratic screening in k -space, broad $\omega = 0$ **resonance**
- 1-particle excitations \rightarrow Fermi liquid upon tiling
- $\Sigma'' \sim \omega^2$

LM

- Unscreened moment. Spectral function gapped.
- $\Sigma \sim 1/\omega$
- Irrelevant hopping processes lead to Heisenberg model

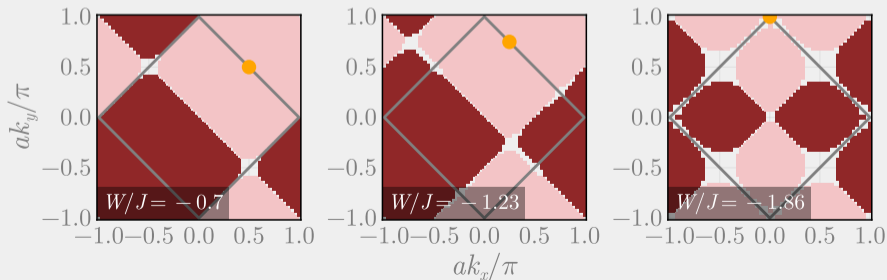
These phases also exist in the **eSIAM**.



UNRAVELLING OF KONDO SCREENING

The Kondo breakdown process can be visualised in terms of **zeros** of $J_{\mathbf{k}_N, \mathbf{k}}$.

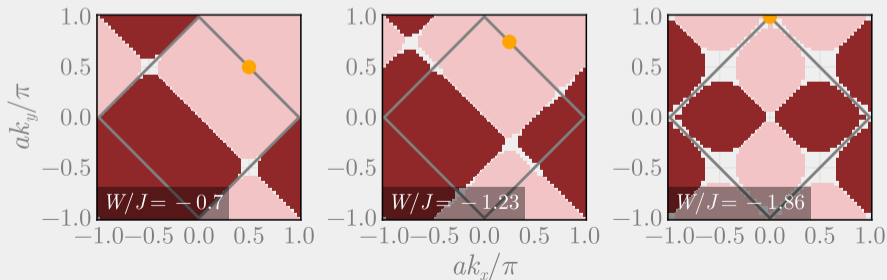
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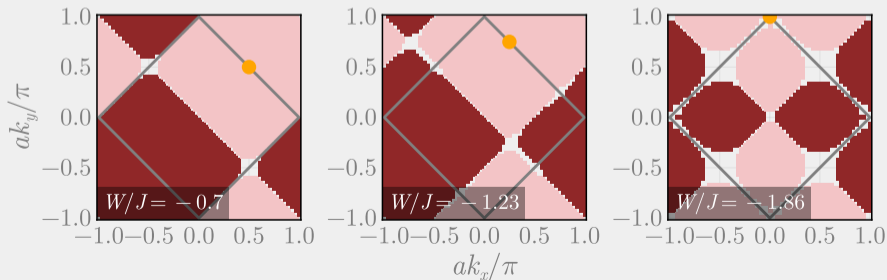
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- Tuning W/J further extends the patch of zeros in $J_{\mathbf{k}_1, \mathbf{k}_2}$ for all \mathbf{k}_1 lying between a given node and the nearest antinodes.



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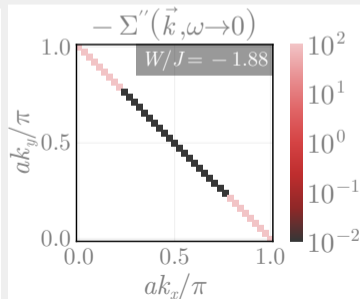
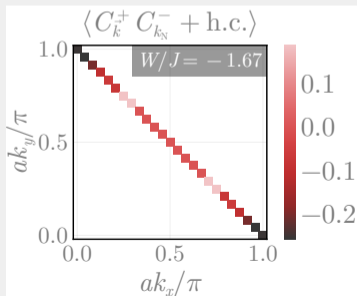
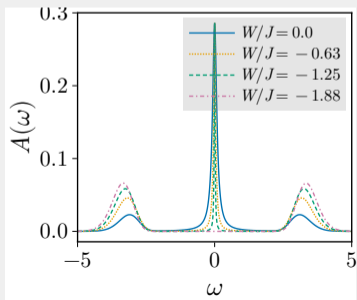
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- Tuning W/J further extends the patch of zeros in $J_{\mathbf{k}_1, \mathbf{k}_2}$ for all \mathbf{k}_1 lying between a given node and the nearest antinodes.
- At $W = W_{\text{PG}}$, the **antinode** joins this connected region of zeros in $J_{\mathbf{k}_1, \mathbf{k}_2}$, marking the onset of the PG. The antinode **decouples** from all Fermi points.



DYNAMICAL SPECTRAL WEIGHT TRANSFER

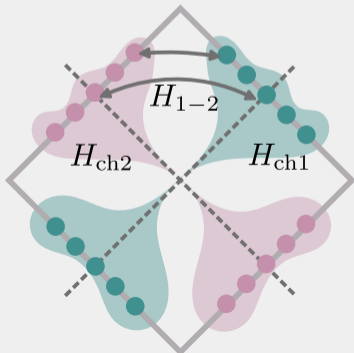
- strong fluctuations observed in **charge correlations** between the gapless nodal and gapped antinodal regions in PG regime
- PG results from **selective transfer** of spectral weight from low to high energies
- **Differs from eSIAM** (spectral weight transferred from entire FS at once)
- PG coincides with the appearance of poles of the lattice self-energy $\Sigma(\mathbf{k}, \omega = 0)$ near the antinodes



NON-FERMI LIQUID NATURE OF THE PSEUDOGAP

Kondo scattering processes can be divided into two classes

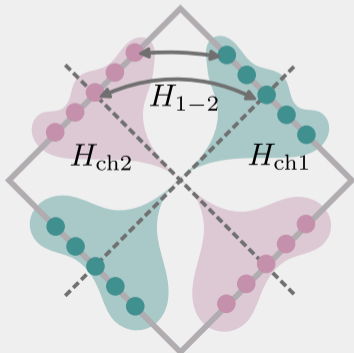
- $H_{\text{ch1}}, H_{\text{ch2}}$: **Within** the green/pink regions
- H_{1-2} : **Connecting** the green and pink regions
- Fermi liquid: $H_{\text{ch1}} = H_{\text{ch2}} \approx H_{1-2}$



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- Pseudogap: H_{1-2} **irrelevant**:

$$H = H_{\text{ch1}} + H_{\text{ch2}}$$

- Effective **two-channel Kondo** description - each pair of opposite quadrants forms a channel



NON-FERMI LIQUID NATURE OF THE PSEUDOGAP

2CK guaranteed by **symmetry** of Kondo coupling:

$$|J(k_1, k_2)| = |J(k_1 + \vec{\pi}, k_2)|$$

2CK \rightarrow **non-Fermi liquid** excitations!



Coleman, Ioffe, and Tsvelik 1995; Schofield 1997; Varma, Nussinov, and Van Saarloos 2002; Patra et al. 2023.

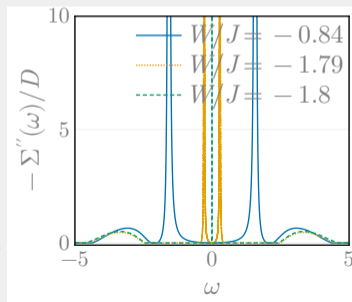
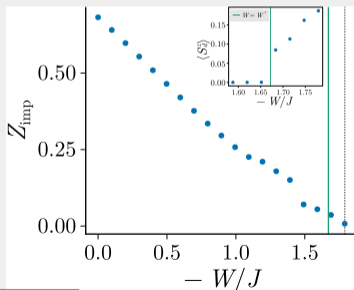
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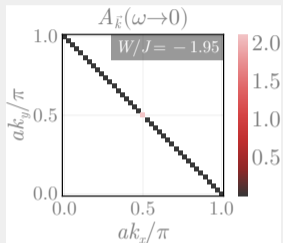
- **Marginal FL** behaviour: $\Sigma' \sim \omega \ln \omega$
- quasiparticle residue, $Z \sim 1 / \ln \omega$ (vanishes logarithmically)
- Partially **unscreened** moment



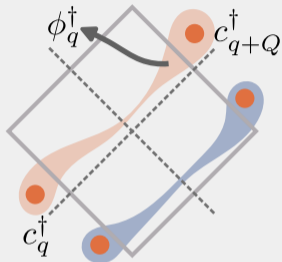
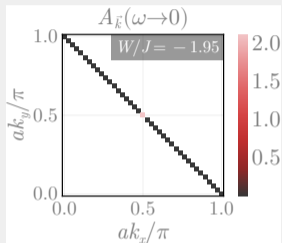
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Close to transition, screening concentrated in **nodal regions**



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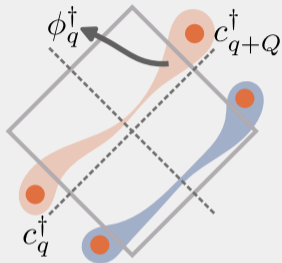
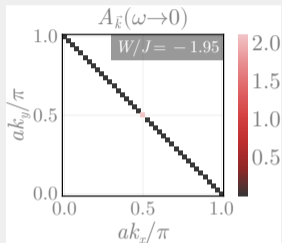
Low-energy excitations:

- Integrate out impurity spin-flips (J^2/W)
- SW transformation \rightarrow effective Hamiltonian

Emergent modes:

$$\phi_{\mathbf{q},\sigma} = \frac{1}{\sqrt{2}} (c_{\mathbf{N}_1+\mathbf{q},\sigma} - c_{\mathbf{N}_1+\mathbf{Q}_1-\mathbf{q},\sigma}), \quad r = \phi^\dagger \phi$$

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$$\Delta \tilde{H} = \underbrace{\sum_{\mathbf{q},\sigma} \frac{|\varepsilon_{\mathbf{N}_1+\mathbf{q}}| \varepsilon_{\mathbf{N}_1+\mathbf{q}}}{-W} r_{\mathbf{q},\sigma}}_{\text{dispersion}} + \sum_{\mathbf{q}_1, \mathbf{q}_2, \sigma} \frac{J^{*2}}{-4W} \left[\underbrace{r_{\mathbf{q}_1\sigma} (1 - r_{\mathbf{q}_2\bar{\sigma}})}_{\text{density interaction}} - (1 - \delta_{\mathbf{q}_1, \mathbf{q}_2}) \underbrace{\phi_{\mathbf{q}_1, \bar{\sigma}}^\dagger \phi_{\mathbf{q}_1, \sigma}^\dagger \phi_{\mathbf{q}_2, \sigma} \phi_{\mathbf{q}_2, \bar{\sigma}}}_{\text{fwd/tang. pair transfer}} \right]$$

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- Nodal metal is described by a **Hatsugai-Kohmoto model**.
- Non-Fermi liquid excitations.

$$\Sigma \sim \frac{u^2}{\omega}, Z \sim \omega^2$$

Σ pole continues into **Mott insulator**.

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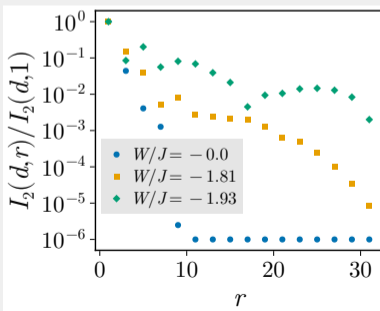
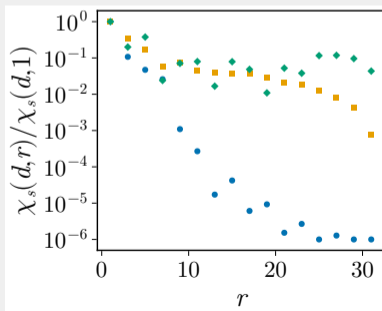
For $q_1 \neq q_2$, we find **charge fluctuations**:

$$\phi_{\mathbf{q}_1,\bar{\sigma}}^\dagger \phi_{\mathbf{q}_1,\sigma}^\dagger \phi_{\mathbf{q}_2,\sigma} \phi_{\mathbf{q}_2,\bar{\sigma}}$$

Might become dominant upon **doping**!

NON-LOCAL NATURE OF THE PSEUDOGAP

- real-space correlations and entanglement undergo a crossover within the pseudogap from short-ranged to **long-ranged** behaviour
- This is further evidence of the **breakdown of local Kondo screening**, and resulting Landau quasiparticle excitations
- the Mott transition observed by us for the Hubbard-Heisenberg model on the square lattice lies well beyond the paradigm of **local quantum criticality**



CONCLUSIONS

- On a 2D square lattice, a Fermi liquid must morph into a **non-Fermi liquid pseudogap phase** in order to give rise to a Mott insulator
- k -space differentiated **Kondo breakdown** lies at the heart of this physics
- the pseudogap features increasingly **non-local correlations** as the system is driven towards the transition

Future Directions

- Heavy fermions?
- Doping the pseudogap phase?
- Other impurity model geometries - spin liquids?

BACKUP SLIDES

TILED ENTANGLEMENT

Concentration of S_{EE} and I_2 within the nodal region

