Mott Criticality as the Confinement Transition of a Pseudogap-Mott Metal

Presentation for Postdoctoral Position at ICTS-TIFR

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A Brief Introduction

University of Calcutta **(B.Sc. Physics)**	IISER Kolkata **(M.S.)**	IISER Kolkata **(Ph.D., Prof. S Lal)**
2018	***2021***	***2026****

Research Interests

- **Mott transition** and criticality, Kondo breakdown in heavy-fermion systems
- Unconventional superconductivity
- emergent non-Fermi liquid phases, **orbital/band-selective** transitions, and Fermi surface topology change
- Various forms of quantum matter

List of Projects

- ✓ **Mott Criticality as the Confinement Transition of a Pseudogap-Mott Metal**. arXiv:2507.17201 (2025)
- Revealing the magnetic dimensional crossover in the Heisenberg ferromagnet CrSiTe3 through picosecond strain pulses. Phys. Rev. B 111, L140414 (2025)
- **Holographic entanglement renormalisation for fermionic quantum matter**. J. Phys. A: Math. Theor. 57 275401 (2024)
- **Kondo frustration via charge fluctuations: a route to Mott localisation**. New J. Phys. 25 113011 (2023)
- Frustration shapes multi-channel Kondo physics: a star graph perspective. J. Phys.: Condens. Matter 35 315601 (2023)
- Unveiling the Kondo cloud: Unitary renormalization-group study of the Kondo model. Phys. Rev. B 105, 085119 (2022)

A Note Of Thanks

Prof. Siddhartha Lal (IISER K)

Prof. N. S. Vidhyadhiraja (JNCASR)

Prof. A. Taraphder (IIT KGP)

Prof. A. Mukherjee (NISER)

Prof. S. R. Hassan (IMSc)

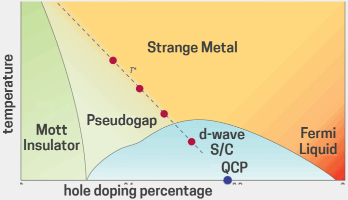
- SERB & IISER Kolkata for funding
- PARAM RUDRA HPC facility for compute time

Mott Criticality as the Confinement Transition of a Pseudogap-Mott Metal

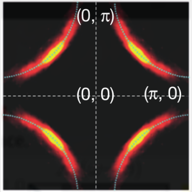
arXiv:2507.17201 (2025). Abhirup Mukherjee, S R. Hassan, A Mukherjee, N S. Vidhyadhiraja, A Taraphder, S Lal

The Challenge: The Pseudogap and Strange Metal

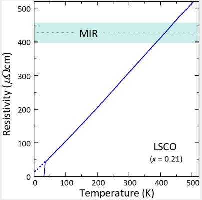
- Nature & origin of pseudogap and strange metal phases of hole-doped Mott insulators
- Difficulty in understanding several puzzling experimental observations.



Schematic **High-Tc SC** Phase Diagram



ARPES plot of **Pseudogap**: gapped and gapless regions coexist



Linear Resistivity in **Strange Metal** crosses MIR bound

Keimer et al. 2015; Proust and Taillefer 2019; Phillips, Hussey, and Abbamonte 2022.

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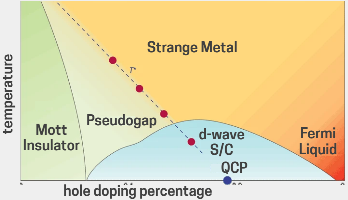

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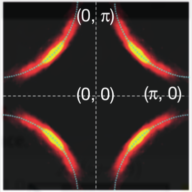

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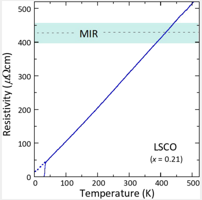
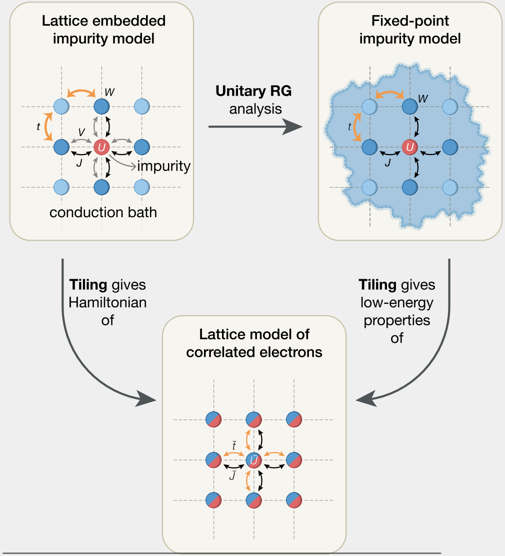


Linear Resistivity in **Strange Metal** crosses MIR bound

- Pseudogap a **precursor** to Mott insulator/ Superconductor? Nature of its excitations?
- Which metal is **parent phase** of Mott insulator, **at 1/2-filling** ?
- Is strange metal a new scale-invariant **long-range entangled** strongly interacting phase?

Keimer et al. 2015; Proust and Taillefer 2019; Phillips, Hussey, and Abbamonte 2022.

Our Approach, In a Nutshell



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

- Lattice symmetry
- Localisation transition

Construct correlated lattice model by applying many-body translation operators ("tiling")

- Restore discrete translation invariance

Analyse impurity mode using **unitary RG** * method.

Tile with **fixed-point impurity model** for low-energy properties of lattice model.

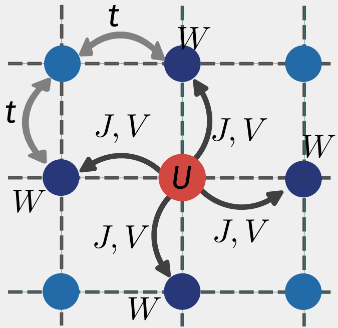
Stoyanova 2006; Mukherjee and Lal 2020a; Mukherjee and Lal 2020b; Mukherjee et al. 2023.

The Core Ingredient: A Lattice-Embedded Impurity Model

Lattice-variant of extended Anderson impurity model

- **Red site**: correlated impurity site (strong local U)
- **Rest of the sites**: conduction bath (hopping t)
- Impurity-bath hybridisation: **Kondo** J, hopping V
- Weak **local interaction** W on N.N bath sites

For $U \gg V$, Mott transition driven by J and W**



**Observed in ∞-dimensional problem: Mukherjee et al., NJP (2023)

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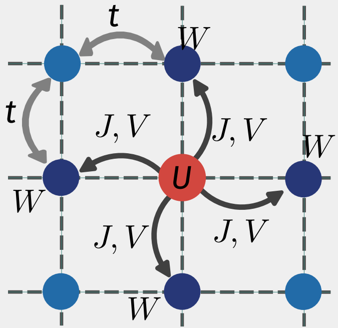


$$H_{\text{aux}} = H_{\text{coup}} + H_{\text{cbath}}$$

$$H_{\text{cbath}} = \sum_{k,\sigma} \epsilon_k n_{k,\sigma} - \frac{W}{2} \sum_{Z} \left(n_{Z\uparrow} - n_{Z\downarrow}\right)^2, \quad Z = \text{N.N}$$

$$H_{\text{coup}} = J \sum_{Z} \mathbf{S}_d \cdot \mathbf{S}_Z, \quad J_{k,k'} = \frac{J}{2}\left[\cos(k_x - k'_x) + \cos(k_y - k'_y)\right]$$

**Observed in ∞-dimensional problem: Mukherjee et al., NJP (2023)

Tiling from Impurity Model to Two Dimensions

"Tiling" allows us to translate physics obtained by from the impurity model into that of the 2D extended Hubbard model

Reconstructed lattice Hamiltonian:

$$-\frac{\tilde{t}}{\sqrt{Z}}\sum_{\langle \mathbf{r}_i,\mathbf{r}_j\rangle;\sigma}\left(c^\dagger_{\mathbf{r}_i,\sigma}c_{\mathbf{r}_j,\sigma}+\text{h.c.}\right)+\frac{\tilde{J}}{Z}\sum_{\langle \mathbf{r}_i,\mathbf{r}_j\rangle}\mathbf{S}_{\mathbf{r}_i}\cdot\mathbf{S}_{\mathbf{r}_j}-\frac{1}{2}\tilde{U}\sum_{\mathbf{r}}\left(\hat{n}_{\mathbf{r},\uparrow}-\hat{n}_{\mathbf{r},\downarrow}\right)^2$$

$$\tilde{t} = 2V/Z$$

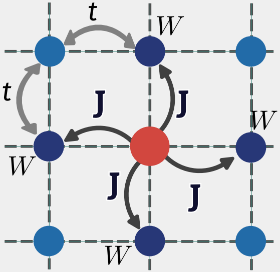
$$\tilde{U} = U + W$$

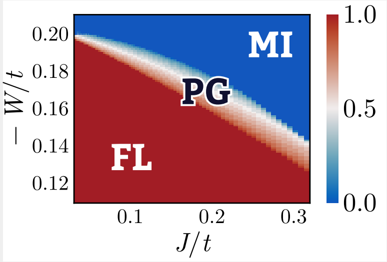
$$\tilde{J} = 2J/Z$$

Unitary RG Phase Diagram and Pseudogapping Transition

Competition between Kondo coupling and local interaction on bath sites:

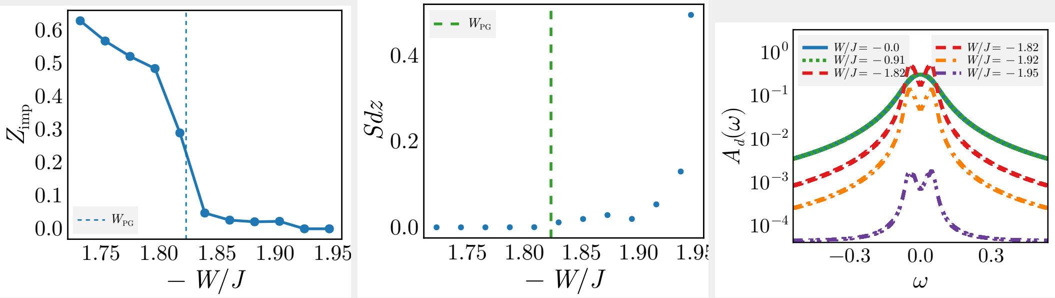
$$\Delta J^{(j)}_{\mathbf{k}_1,\mathbf{k}_2} = -2\sum_{\mathbf{q}} \frac{J^{(j)}_{\mathbf{k}_2,\mathbf{q}} J^{(j)}_{\mathbf{q},\mathbf{k}_1} + 4J^{(j)}_{\mathbf{q},\bar{\mathbf{q}}} W_{\bar{\mathbf{q}},\mathbf{k}_2,\mathbf{k}_1,\mathbf{q}}}{\omega - \frac{1}{2}|\varepsilon_j| + J^{(j)}_{\mathbf{q}}/4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





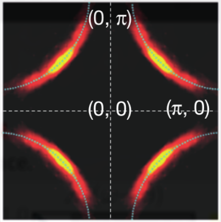
- Competition leads to **Kondo breakdown** for $W < 0$
- Phase diagram shows **pseudogap** phase lying between Fermi liquid (FL) and Mott insulator (MI).
- PG possesses non-Fermi liquid excitations – a ***Mott Metal***

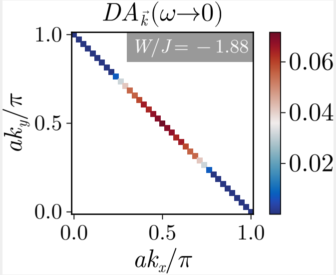
- Strength of Landau quasiparticle excitations of FL (**QP residue** Z) vanishes upon entering PG.
- Impurity magnetisation $\langle S_d^z \rangle$ grows dramatically in PG: **breakdown** of Kondo screening.
- Impurity spectral function shows **pseudogap** at $\omega = 0$!

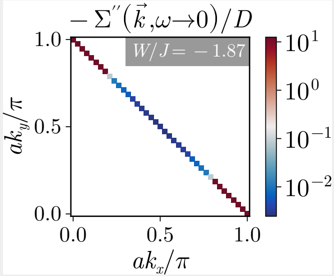


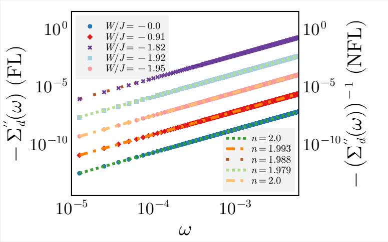
Luttinger Surfaces in the Pseudogap

- PG shows **electronic differentiation** in lattice spectral function: gapped antinodal regions (**Luttinger surfaces**), gapless excitations in nodal regions.
- Electron **scattering rate** shows divergences in gapped antinodal regions, while it is analytic in gapless nodal regions.
- $1/\Sigma'' \sim 1/\Sigma''_0 + \omega^2$. Appearance of power-law exponents such as 2 signals **universality**.





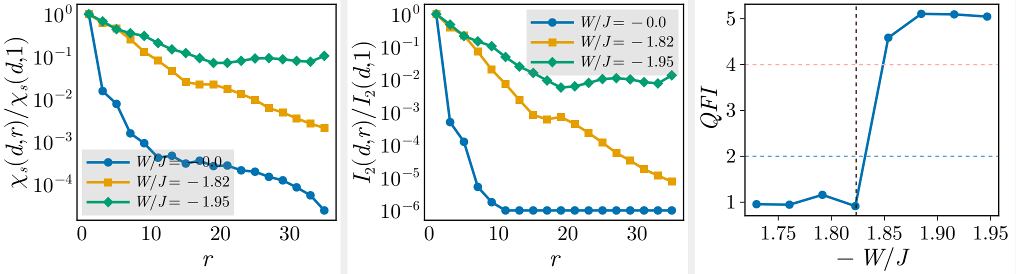




Keimer et al. 2015.

Long-ranged and Multipartite Entanglement in the PG

- real-space correlations $\langle S_d \cdot S_r \rangle$ and entanglement undergo a crossover within the pseudogap from short-ranged to **long-ranged** behaviour
- Quantum Fisher information for $O = \sum_{\text{odd } i} (S_i^+ S_{i+1}^- + \text{h.c.})$ shows a jump in **multipartite entanglement** of 2 in FL to 5 within PG.
- Densely entangled **Quantum Soup** !



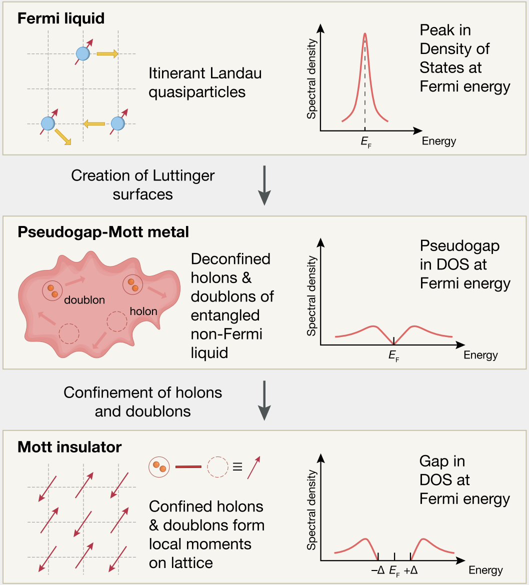
Conclusions: Main Takeaways

Realisation of **Mott's original vision** (1949) with deconfined holes & doubles

- new, (likely) universal phase of **strongly interacting** quantum matter,
- **noisy** , incoherent environment for electron-like excitations,
- a long-ranged and **multipartite** entangled "quantum soup",
- scale invariant at Mott critical point & described by exactly solvable model

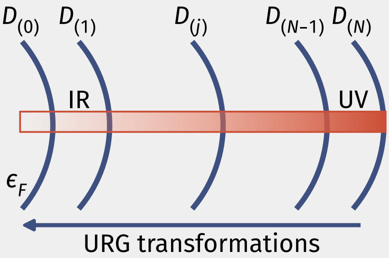
Open Questions:

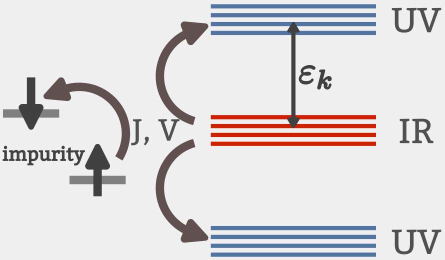
Fate at non-zero temperatures, doping, other geometries?

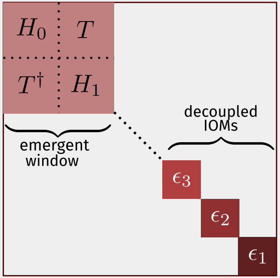


Theoretical Techniques

Unitary Renormalisation Scheme







- Provides access to **low energy fixed-point Hamiltonian**
- RG Proceeds via decoupling of high energy degrees of freedom via many-body **unitary** transformations
- Transformations account for **many-body scattering processes** into various energy sectors
- Also used other RG methods such as **"Poor Man's scaling"**

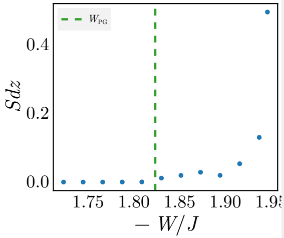
Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

Exact Diagonalisation and Correlation Functions

- Lot of experience working with **fermionic hamiltonians**
- Numerical modelling and exact diagonalisation

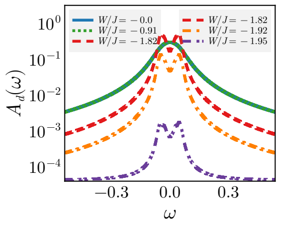
Static correlation functions

- Spin/charge-correlation
- Order parameters



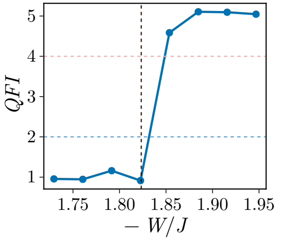
Dynamical responses

- Spectral functions
- Self-energies
- Optical conductivity



Entanglement measures

- Entanglement entropy
- Mutual information
- Quantum Fisher info.



Miscellaneous methods

- Spectral flow insertion techniques
- Effective Hamiltonian computation

Interested in learning **new methods** as well: **DMRG, NRG, DMFT**, etc

Other Projects

Kondo frustration via charge fluctuations: a route to Mott localisation

New J. Phys. 25 113011 (2023). **Abhirup Mukherjee**, N S. Vidhyadhiraja, A Taraphder, S Lal

Precursor to the Mott metal work. Demonstrated how an extended Anderson impurity model captures the $d = \infty$ Mott MIT on the Bethe lattice.

Holographic entanglement renormalisation for fermionic quantum matter

J. Phys. A: Math. Theor. 57 275401 (2024). **Abhirup Mukherjee**, S Patra, S Lal

Demonstration of the holographic principle by showing how entanglement renormalisation in a free fermion system leads to a holographic dimension.

Revealing the magnetic dimensional crossover in the Heisenberg ferromagnet CrSiTe3 through picosecond strain pulses

Phys. Rev. B 111, L140414 (2025). A Kumar N M, S Mukherjee,**Abhirup Mukherjee**, A Punjal, S Purwar, T Setti, S Prabhu S., S Lal, N Kamaraju

Investigated the two-step magnetic dimensional crossover in CrSiTe3. We came up with a simple Ginzburg-Landau model of phonons interacting with the lattice spin fluctuations to explain the softening/gapping of various phonon modes observed from a pump-probe experiment.

Research Interests

- **Studying electronic correlations in MATBG through an exactly solvable model** : The Hatsugai-Kohmoto model is an exactly solvable correlated model displaying non-Fermi liquid and Mott insulating phases. This therefore provides an interesting route to studying the emergence of novel phases in a correlated MATBG system, with **analytical clarity**.

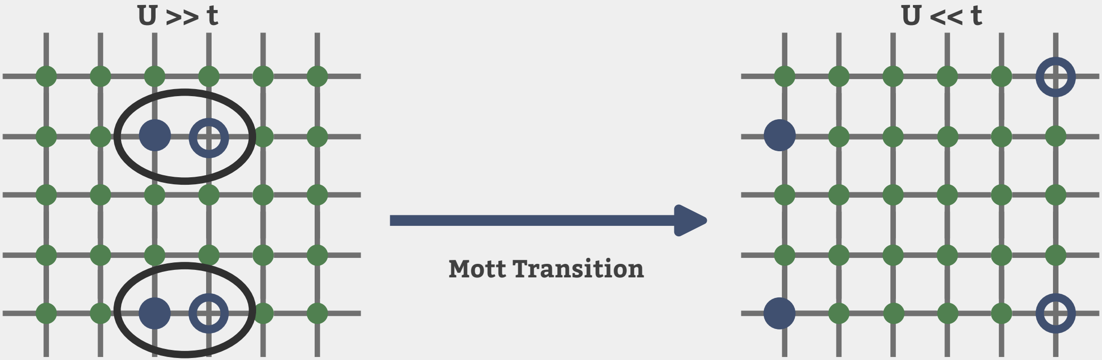
- **Exploring violation of Luttinger's theorem in heavy-fermion systems** : Violation of Luttinger's theorem may result from changes in the anomaly structure of the Fermi surface. One can investigate these claims particularly in the context of heavy-fermion systems to write down **topological order parameters** that track phase transitions in such systems.

- **Studying effect of electronic correlations in MATBG through a bilayer impurity model** : Following Prof. Bernevig's **topological heavy-fermions approach** towards MATBG, it may be fruitful to look at an impurity model analogue of such a THF model by allowing a Kondo impurity to hybridise with a topologically non-trivial conduction bath.

Thank You

Mott MIT as holon-doublon deconfinement

The Mott MIT is essentially a holon-doublon **binding-unbinding** transition



Holons-Doublons tightly bound

Holons-Doublons deconfined

- Delocalised **gas of holons & doublons** form metal: Fermi liquid?
- Nature and mechanism of transition?

Mott 1949.

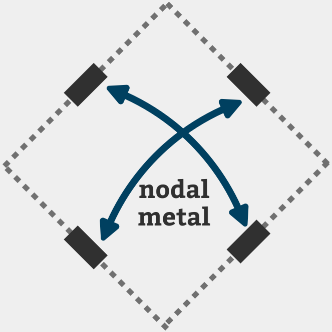
Singular Nodal Metal at Critical Point

- Mott critical point has **nodal non-Fermi liquids** . Theory can be obtained in the form of exactly solvable **Hatsugai-Kohmoto model** !

$$H_{\text{eff}} = \sum_{\mathbf{q},\sigma} \epsilon_{\mathbf{q}} r_{\mathbf{q},\sigma} + U \sum_{\mathbf{q},\sigma} r_{\mathbf{q}\sigma} r_{\mathbf{q}\bar{\sigma}}$$

$r_{\mathbf{q}\sigma}$: nested combination across FS

- Nodal metal is singular, i.e., has a Mott pole in self-energy at Fermi energy, but is still gapless. Gapless excitations are **holons & doublons** .



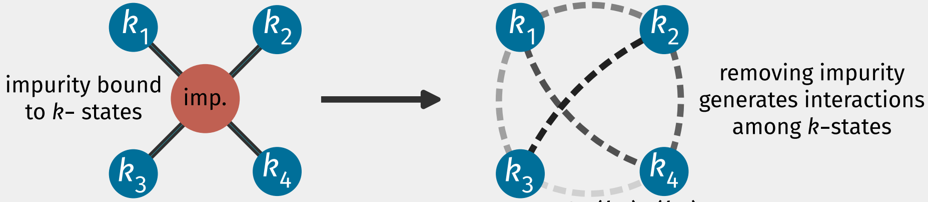
The single-channel Kondo problem: Anatomy of the Kondo cloud

Anirban Mukherjee et al., Phys. Rev. B 105, 085119

Effective Hamiltonian for the Kondo cloud

We first applied the **unitary RG** to obtain a low energy fixed point theory.

To obtain a theory for the Kondo cloud, we **trace out impurity** from fixed point Hamiltonian.



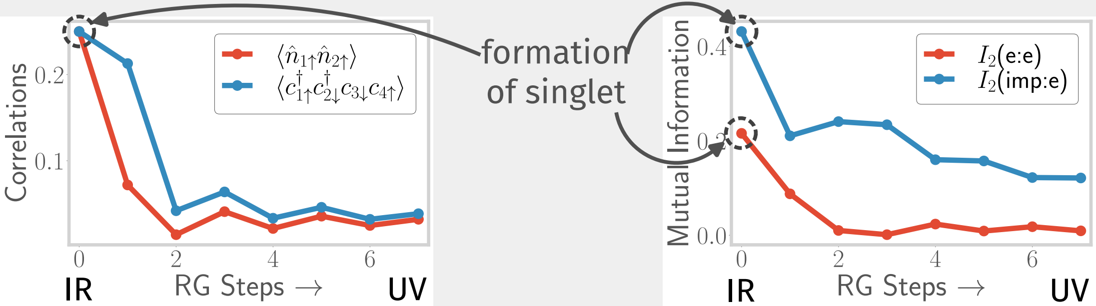
$$KE + J^*\vec{S}_d \cdot \sum_{kk'} \vec{s}_{kk'} \longrightarrow KE + \sum_{k_1,k_2} \frac{2\varepsilon(k_1)\varepsilon(k_2)}{J^*}\hat{n}_{k_1}\hat{n}_{k_2} + \sum_{\{k_i\}} V_{1234}\, c^\dagger_{k_4\uparrow} c^\dagger_{k_3\downarrow} c_{k_2\downarrow} c_{k_1\uparrow}$$

- all-to-all interactions between momentum states, **large entanglement**
- 2-particle interaction terms **not** present in Fermi liquid, are **responsible for screening**

Mukherjee et al. 2022; Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

Quantifying entanglement within the Kondo cloud

In order to demonstrate formation of Kondo cloud, we study the **variation of entanglement** and correlations under RG transformations.



- Both entanglement and k-space correlations **increase** as RG proceeds from UV to IR.
- This shows the formation of the **Kondo singlet** and the growth of two-particle correlations in the **Kondo cloud**.

Mukherjee et al. 2022.

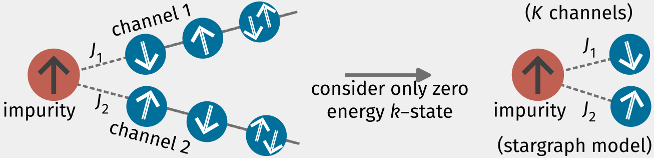
Distorting the Kondo singlet: The multi-channel Kondo Problem

Siddhartha Patra et al., 2023 J. Phys.: Condens. *Matter* 35 315601

What is the multichannel Kondo problem?

Single impurity interacting with **multiple channels** in the bath

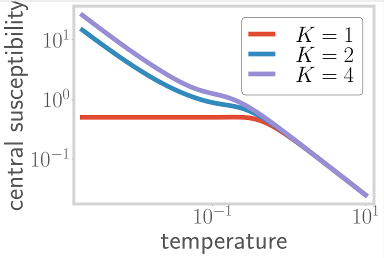
$$H_{\text{Kondo}} = KE_{\text{bath}} + \sum_l J_l \vec{S}_{\text{imp}} \cdot \vec{s}^{(l)}$$



Known to display divergent $T = 0$ impurity susceptibility (incomplete screening), and orthogonality catastrophe, **non-Fermi liquid** excitations.

Zero bandwidth limit is (analytically) solvable: $\{|S^z_{\text{tot}}\rangle\}$

- Ground state degeneracy for $K > 1$ explains **orthogonality catastrophe**
- $S^z_{\text{tot}} \neq 0$ in ground states shows incomplete screening
- Excitations shows **non-Fermi liquid** physics in the form of inter-channel scattering.



Nozières, Ph. and Blandin, A. 1980; Affleck and Ludwig 1993; Emery and Kivelson 1992; Andrei and Destri 1984.

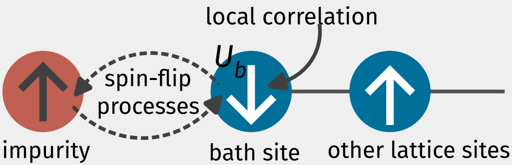
How to destroy the Kondo cloud: Effect of local interactions in the bath

Abhirup Mukherjee et al 2023., New J. Phys. 25 113011

What is the new physics ingredient?

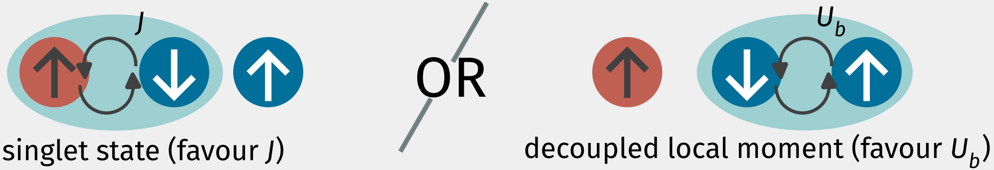
Add **local correlation** on bath (zeroth) site coupled to impurity

$$KE_{\text{bath}} + J\vec{S}_{\text{imp}} \cdot \vec{S}_{\text{bath}} - U_b \left(\vec{S}_{\text{bath}}\right)^2$$



URG equations show that an **attractive** U_b frustrates the zeroth site.

$$\Delta J \sim J^2 + 4U_b J \implies \textbf{phase transition} \text{ at } J = -4U_b$$



Such a model sheds light on the Mott MIT in ∞-dimensions (as seen from DMFT).

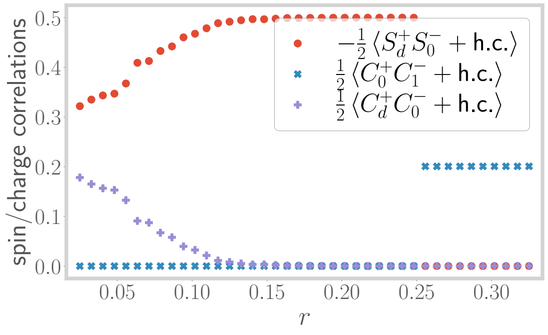
Georges et al. 1996.

Nature of the transition

Across the transition,

- impurity correlations vanish
- bath correlations become non-zero

Shows that **pairing correlations** in the bath are responsible for the transition.



The state **precisely at the transition** is special:

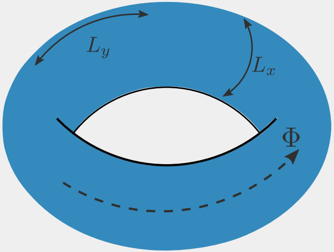
- non-Fermi liquid excitations
- **fractional** impurity magnetisation and occupancy

Holography of entanglement in 2D free fermions

Abhirup Mukherjee, Siddhartha Patra, Siddhartha Lal

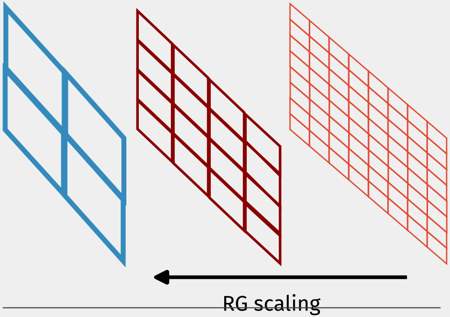
J. Phys. A: Math. Theor. 57 275401 (2023)

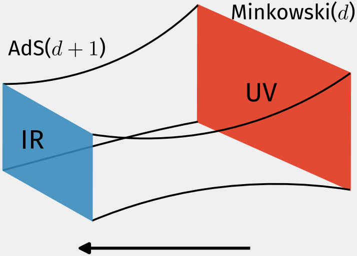
Some broad questions



We consider 2D electrons placed on a torus in a flux Φ.

- Is the entanglement content of this system **holographic**?
- Is there any **topological** notion within the entanglement measures?



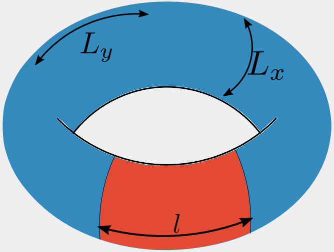


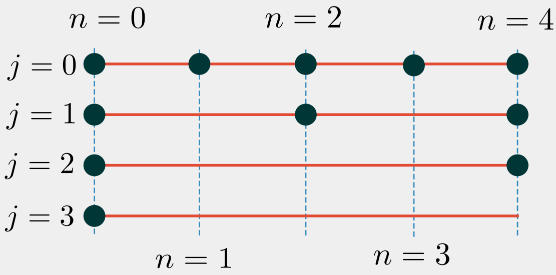
Arias, Blanco, and Casini 2015; Zaanen et al. 2015.

Results

- Choose subsystem in real space (red region)
- Apply **coarse-graining transformations** in k-space

Evolution of subspace entanglement shows interesting properties.



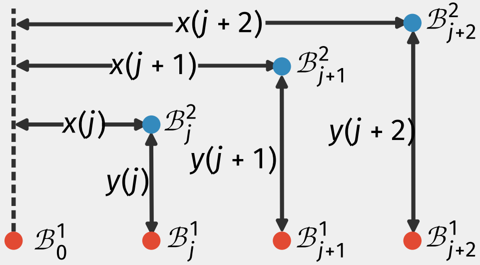


Results

Use mutual information I_2 to define **distance**.

- Larger $I_2 \implies$ smaller distance
- Allows notion of **curvature** as well.

Coarse-graining transformations lead to **emergent** spatial dimension



Van Raamsdonk 2010.

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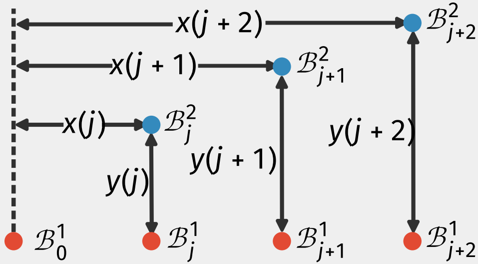


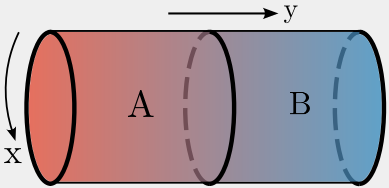
Other consequences:

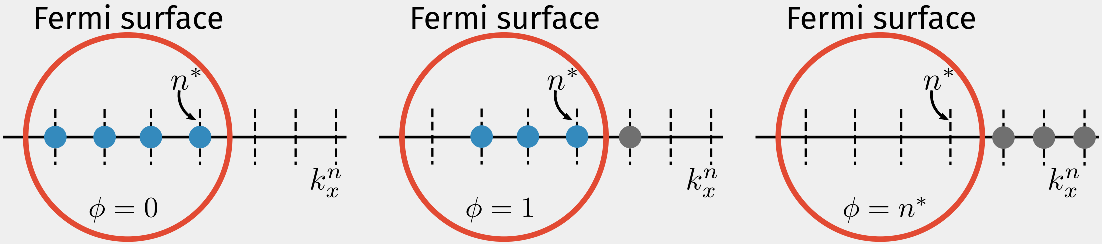
- **hierarchy** of entanglement exists along the RG
- hierarchy also present in **multipartite entanglement**

Van Raamsdonk 2010.

Results

- By tuning flux, we relate Luttinger's volume to functions of entanglement
- Entanglement spectral flow is also related to Chern numbers in presence of magnetic field





Oshikawa 2000; Seki and Yunoki 2017; Alexandradinata, Hughes, and Bernevig 2011.

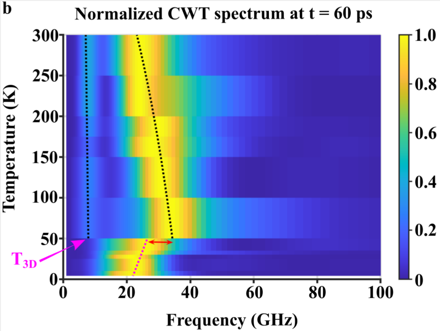
Revealing the magnetic dimensional crossover in the Heisenberg ferromagnet $CrSiTe_3$ through picosecond strain pulses

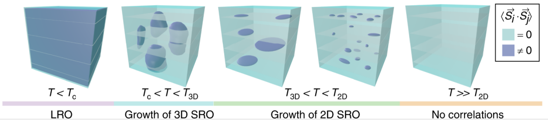
A Kumar N M, S Mukherjee,Abhirup Mukherjee, A Punjal, S Purwar, T Setti, S Prabhu S., S Lal, N Kamaraju

Phys. Rev. B 111, L140414 (2025)

GL Theory for Spin-Phonon Interaction

Prof. Kamaraju's group investigated the **magnetic dimensional crossover** (paramagnet → 2D short-range order → 3D long-range order) in $CrSiTe_3$ using **pump-probe** spectroscopy.





Ron et al. 2019; N M et al. 2025.

- The acoustic strain pulses show a red-shift (**softening**) of the high-frequency phonons and a **gapping** out of the low-frequency phonon modes.
- We came up with a **Ginzburg-Landau model** of phonons interacting with lattice spin fluctuations to explain these features.

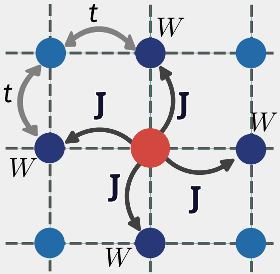
$$L = \sum_j [\dot{Q}_j^2 - (\lambda - M^2\chi)(Q_{j+1} - Q_j)^2 - M^2\xi Q_j^2]$$

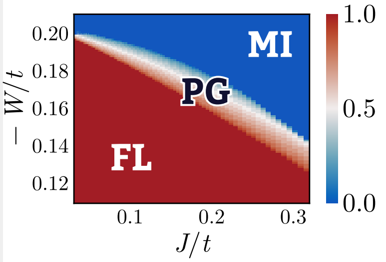
- Renormalisation of **phonon dispersion and spring constant** due to interactions explains the softening and gapping.

Unitary RG Phase Diagram and Pseudogapping Transition

Competition between Kondo coupling and local interaction on bath sites:

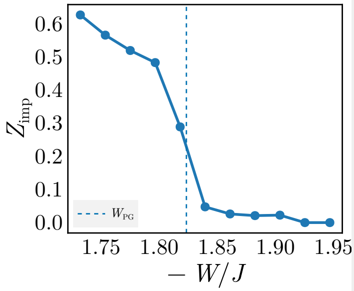
$$\Delta J^{(j)}_{\mathbf{k}_1,\mathbf{k}_2} = -2\sum_{\mathbf{q}} \frac{J^{(j)}_{\mathbf{k}_2,\mathbf{q}} J^{(j)}_{\mathbf{q},\mathbf{k}_1} + 4 J^{(j)}_{\mathbf{q},\bar{\mathbf{q}}} W_{\bar{\mathbf{q}},\mathbf{k}_2,\mathbf{k}_1,\mathbf{q}}}{\omega - \frac{1}{2}|\varepsilon_j| + J^{(j)}_{\mathbf{q}}/4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

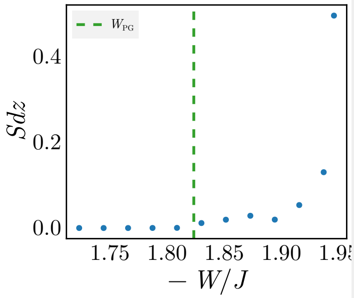


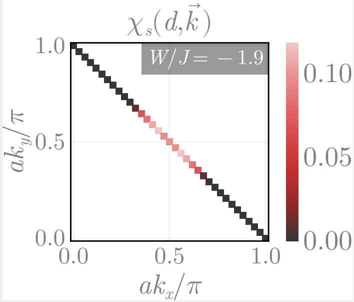


- Competition leads to **Kondo breakdown** for $W < 0$
- Phase diagram shows **pseudogap** phase lying between Fermi liquid (FL) and Mott insulator (MI).
- PG possesses non-Fermi liquid excitations – a **Mott Metal**

- Strength of Landau quasiparticle excitations of FL (**QP residue** Z) vanishes upon entering PG.
- Impurity magnetisation $\langle S_d^z \rangle$ grows dramatically in PG: **breakdown** of Kondo screening.
- Impurity-bath spin correlations vanish around antinode: signature of **pseudogap**

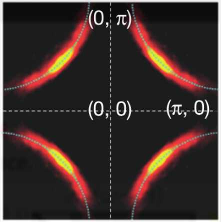


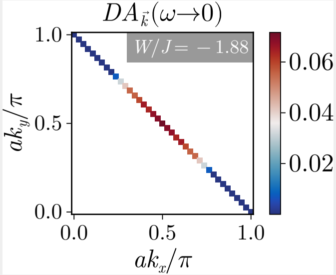


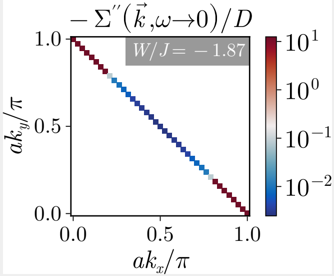


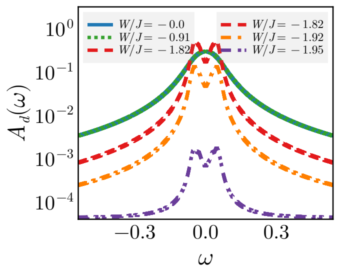
Luttinger Surfaces in the Pseudogap

- PG shows **electronic differentiation** in lattice spectral function: gapped antinodal regions (**Luttinger surfaces**), gapless excitations in nodal regions.
- Electron **scattering rate** shows divergences in gapped antinodal regions, while it is analytic in gapless nodal regions.
- Impurity spectral function shows **pseudogap** of Fermi arcs!





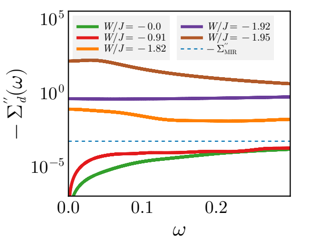


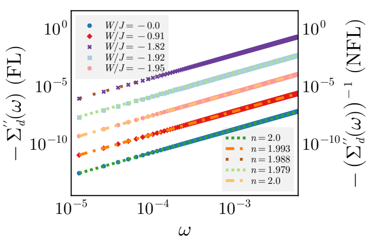


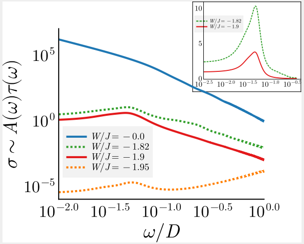
Keimer et al. 2015.

Universal Scaling of Spectral Features

- Electron Scattering Rate of NFLs cross **Mott-Ioffe-Regel (MIR) bound** (no electron-like excitations!), while FLs are within it.
- $1/\Sigma'' \sim 1/\Sigma''_0 + \omega^2$. Appearance of power-law exponents such as 2 signals **universality** .
- Optical Conductivity $\sigma \sim A(\omega)\tau(\omega)$ shows a **shifted “Drude” peak**







Tiling Details: Greens Function

$$G(k,\sigma;\omega) = \sum_{v,n} C_{v,k} \left[\frac{\langle \psi_{\mathrm{gs}}(r_d)|T_{v,\sigma}|\psi_n(r_d)\rangle \langle \psi_n(r_d)|T^{\dagger}_{v,\sigma}|\psi_{\mathrm{gs}}(r_d)\rangle}{\omega - (E_n - E_0 + \epsilon_v)} \right. \\ \left. + \frac{\langle \psi_{\mathrm{gs}}(r_d)|T^{\dagger}_{v,\sigma}|\psi_n(r_d)\rangle \langle \psi_n(r_d)|T_{v,\sigma}|\psi_{\mathrm{gs}}(r_d)\rangle}{\omega + (E_n - E_0 - \epsilon_v)} \right] . \tag{1}$$

$$G_{\mathrm{loc}}(\omega) = G(d\sigma;\omega - \epsilon_{\mathrm{loc}}) + \sum_{v} C_v \left[G(T_{v,\sigma}, d\sigma; \omega - \epsilon_v) + \sum_{\mathbf{k}} G(T_{v,\sigma}, T_{k,\sigma}; \omega - \epsilon_v) \right] \\ + \sum_{k} G(d\sigma, T_{k,\sigma}; \omega) , \tag{2}$$

Tiling Details: Static Correlation

$$
\begin{aligned}
&\sum_{r_d} \langle \Psi_{\mathrm{gs}} | c_{r_d+r,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \Psi_{\mathrm{gs}} \rangle \\
&= \sum_{n} F_n^*(r) \langle \psi_{\mathrm{gs}}(r_d) | c_{r_d,\sigma}(t) | \psi_n(r_d) \rangle \langle \psi_n(r_d) | c^{\dagger}_{r_d,\sigma} | \psi_{\mathrm{gs}}(r_d) \rangle \\
&+ \sum_{k,n} F'_n(k) F_n^*(r) \langle \psi_{\mathrm{gs}}(r_d) | T_{k,\sigma}(t) | \psi_n(r_d) \rangle \langle \psi_n(r_d) | c^{\dagger}_{r_d,\sigma} | \psi_{\mathrm{gs}}(r_d) \rangle \\
&+ \sum_{k,n} F'_n(k)^* F_n^*(r) \langle \psi_{\mathrm{gs}}(r_d) | c_{r_d,\sigma}(t) | \psi_n(r_d) \rangle \langle \psi_n(r_d) | T^{\dagger}_{k,\sigma} | \psi_{\mathrm{gs}}(r_d) \rangle \\
&+ \sum_{k_1,k_2} F'_n(k_1) F'_n(k_2)^* F_n^*(r) \langle \psi_{\mathrm{gs}}(r_d) | T_{k_1,\sigma}(t) | \psi_n(r_d) \rangle \langle \psi_n(r_d) | T^{\dagger}_{k_2,\sigma} | \psi_{\mathrm{gs}}(r_d) \rangle \ ,
\end{aligned} \tag{3}
$$