# Insights on Mott Transition and The Pseudogap Through the Veil of a Quantum Impurity Model

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DPS Day '25
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**Debraj Debata**

**Siddhartha Patra**
(Multiverse Computing)


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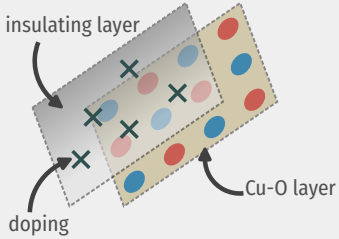
**Prof. Arghya Taraphder**
(IIT Kharagpur)

**Prof. N. S. Vidhyadhiraja**
(JNCASR Bangalore)

# The Advent of Quantum Materials: Cuprate Superconductors

- Cu-O planes separated by insulating layers that can be doped.



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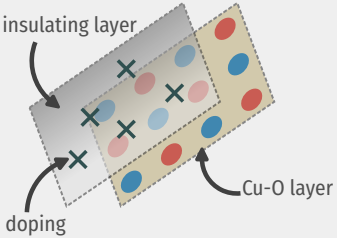


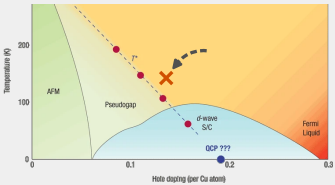


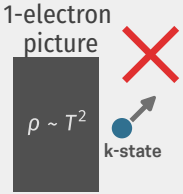


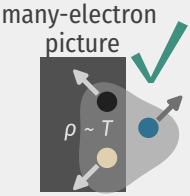

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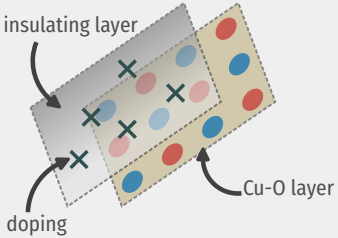


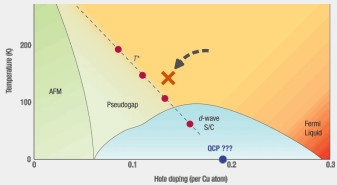


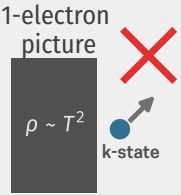


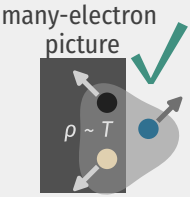

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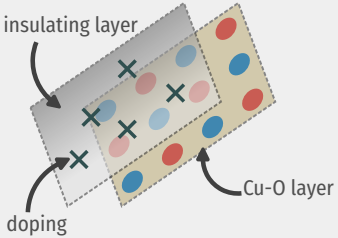


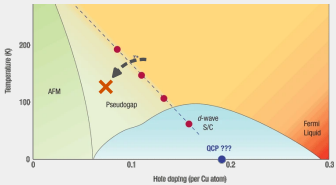


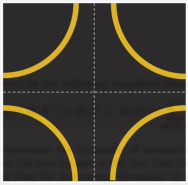

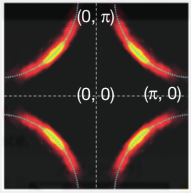

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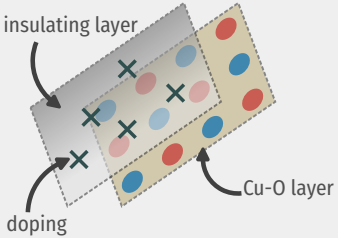
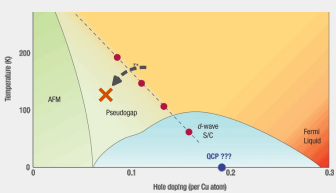
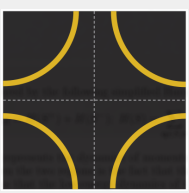
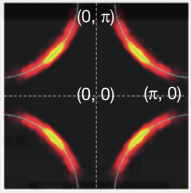
* **Missing:** Microscopic understanding of the pseudogap phase





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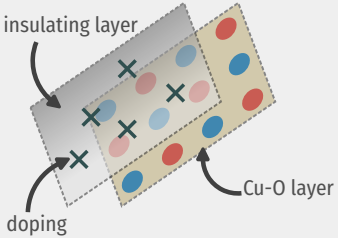
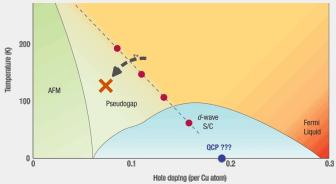
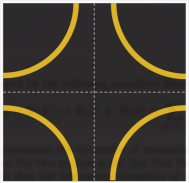
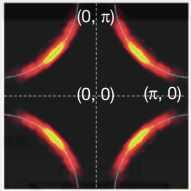


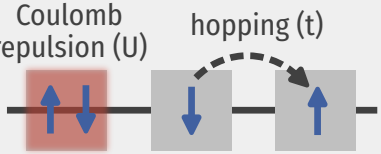






Simplest model for realising these phases
- the 2D **Hubbard model** on square lattice

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

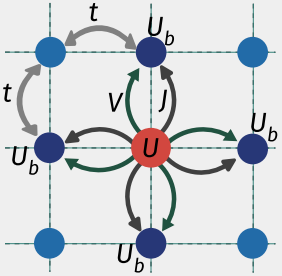



**Too hard to solve**! Alternative approaches needed.

# A Bottom-Up Approach: Starting from an Impurity Model

**What is an Impurity Model?**

- Single **correlated site**, hybridising with conduction **bath**



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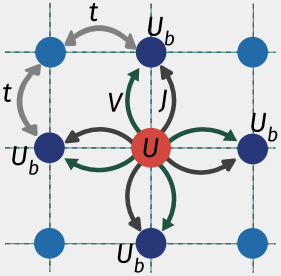
- Impurity-bath hybridisation respects $C_4$ **symmetry** of 2D square lattice (important!)



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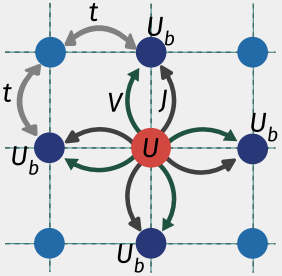

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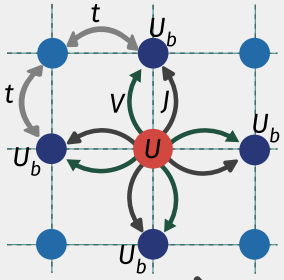
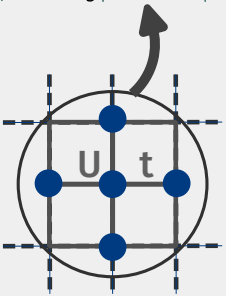



## Mapping to the Lattice Model

- Impurity model describes local environment of each site.



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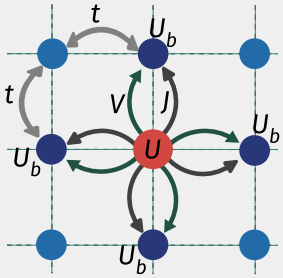
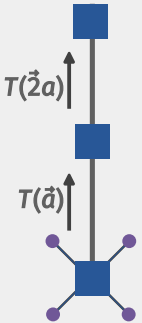
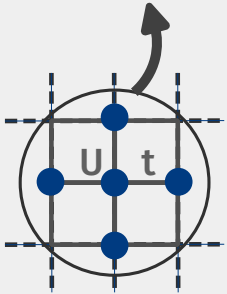



## Mapping to the Lattice Model

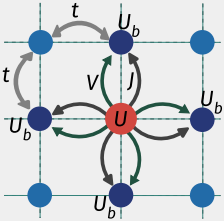
- Impurity model describes local environment of each site.
- **Translation** operator maps impurity model quantities to those on the lattice model



# Momentum-space Resolved Impurity Phase Transition

**Raising bath correlation** $W$ tunes the impurity model through three phases



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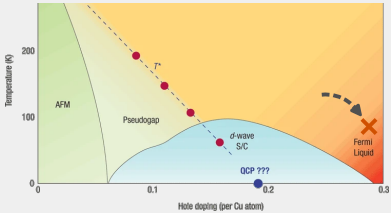
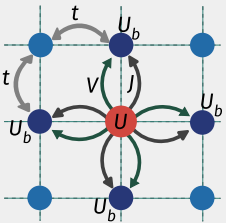
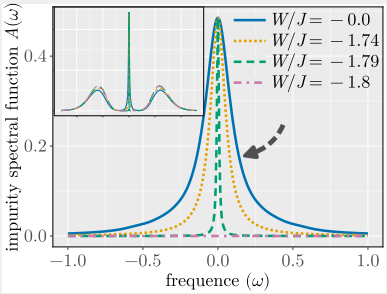
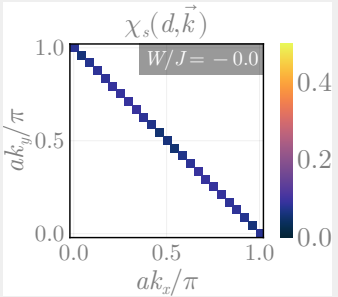
- Impurity **strongly coupled** to Fermi surface



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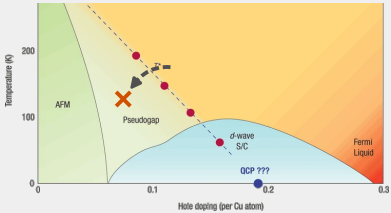
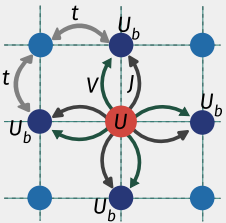
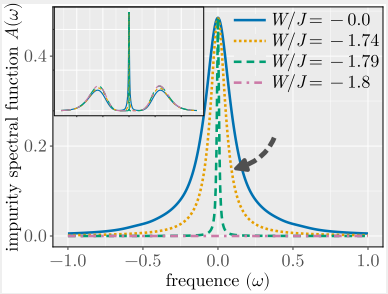
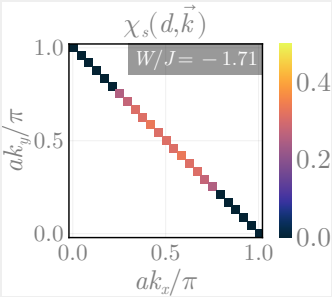
**Raising bath correlation** $W$ tunes the impurity model through three phases

- Impurity **strongly coupled** to Fermi surface
- Impurity coupled **only to parts** of Fermi surface



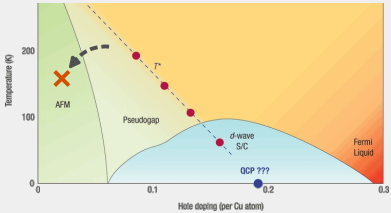



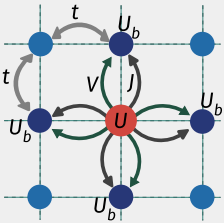



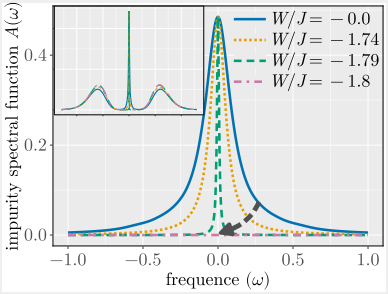
# Momentum-space Resolved Impurity Phase Transition

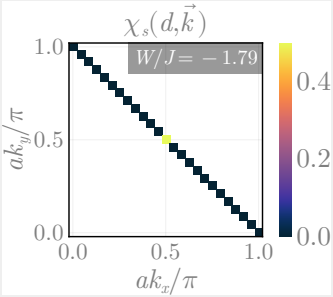
**Raising bath correlation** $W$ tunes the impurity model through three phases

- Impurity **strongly coupled** to Fermi surface
- Impurity coupled **only to parts** of Fermi surface
- Impurity **decoupled** from the Fermi surface



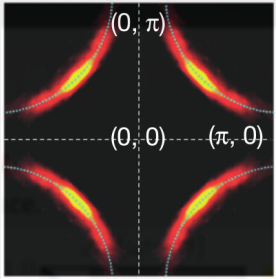



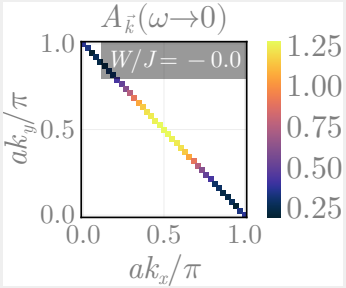



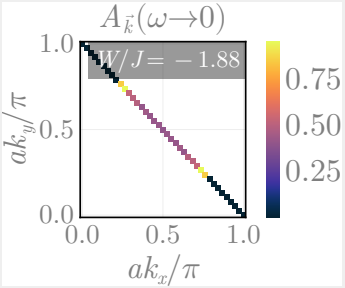



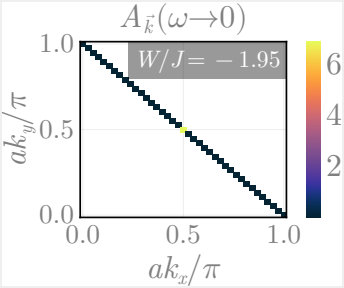
# Pseudogapping Transition on the Lattice Model

- Map Greens functions from impurity model to **lattice model**.
- Momentum-space DOS reveals **partially gapped** Fermi surface.



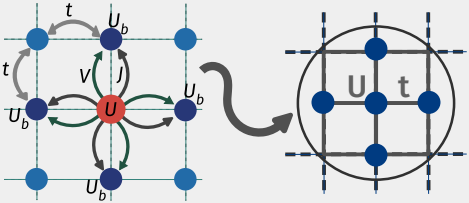



# Main takeaways

**Simplifies** the study of lattice models through appropriate **impurity models**.



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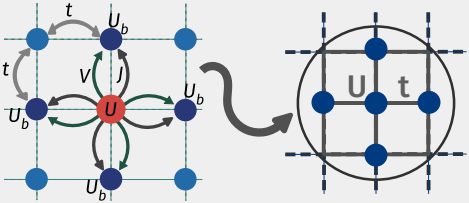
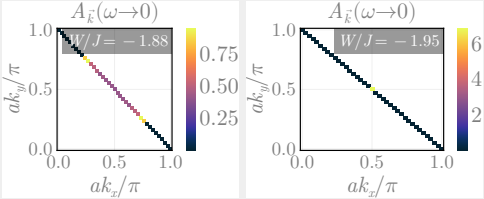
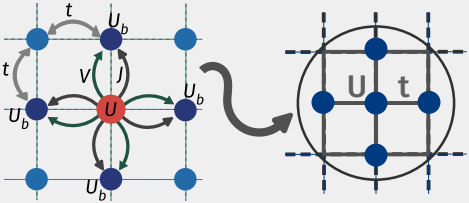



Our impurity model realises a **pseudo-gapping transition** in a correlated model.

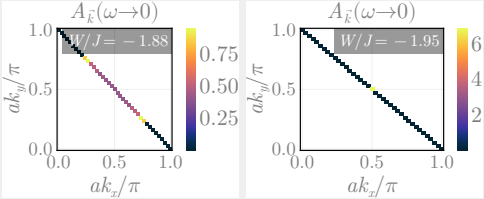


# Main takeaways

**Simplifies** the study of lattice models through appropriate **impurity models**.




Our impurity model realises a **pseudo-gapping transition** in a correlated model.




## Generalisations and Extensions

- Tune impurity filling - simulate **doping**!
- Multiple impurities - symmetry-broken or **spin liquid** phases