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

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DPS Day '25
Department of Physical Sciences, IISER Kolkata

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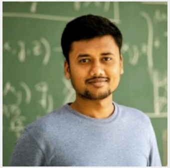
Prof. Siddhartha Lal

Debraj Debata



Siddhartha Patra
(Multiverse Computing)

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Prof. Anamitra Mukherjee
(NISER Bhubaneshwar)

Prof. Arghya Taraphder
(IIT Kharagpur)

Prof. N. S. Vidhyadhiraja
(JNCASR Bangalore)

The Advent of Quantum Materials

- Display exotic properties arising due to strong electronic/spin **interactions**.
- **Examples**: heavy fermion compounds ($CePd_2Si_2$), copper oxides ($La_{2-x}Sr_xCuO_4$), iron pnictides ($BaFe_2(As_{1-x}P_x)_2$), twisted bilayer graphene.

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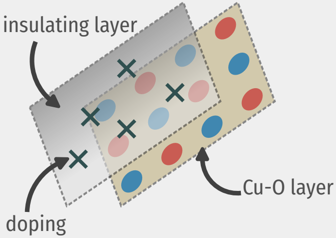

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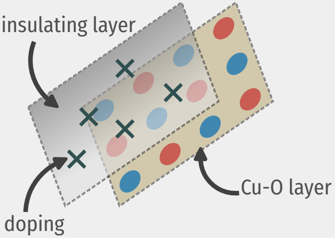

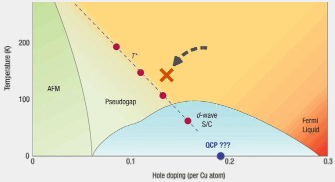

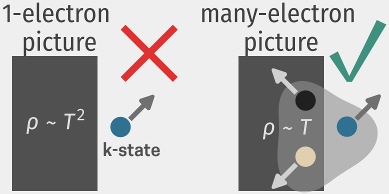

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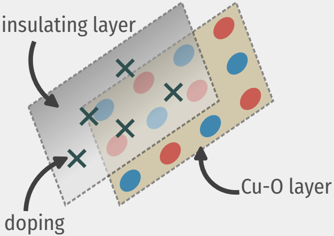

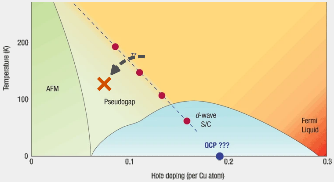

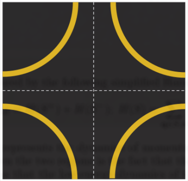

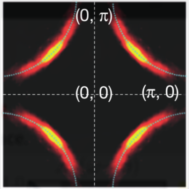

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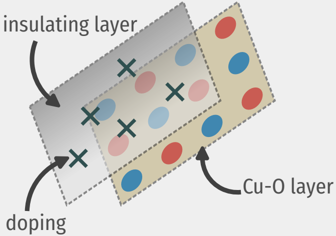
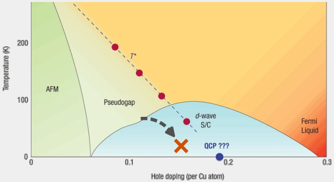
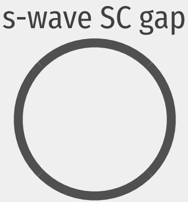
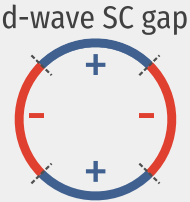
- Superconductivity is **unconventional** (gap vanishes at points on Fermi surface)





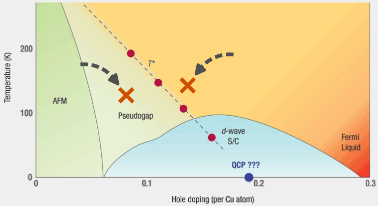




Open Questions

The “normal phases” remain **ill-understood**:

- simple and universal mechanism for strange metals (akin to Fermi liquid theory)
- Microscopic understanding of the pseudogap phase
- How to connect T = 0 results to those at T > 0?



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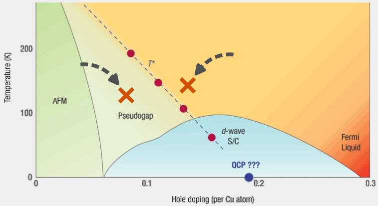
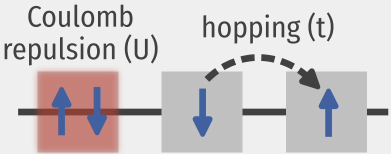


Simplest model for realising these phases
- the 2D **Hubbard model** on square lattice

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



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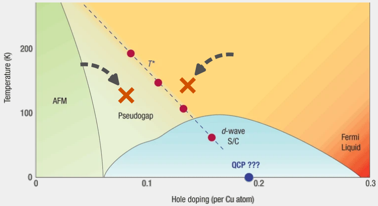

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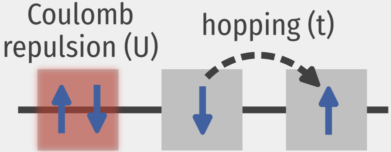
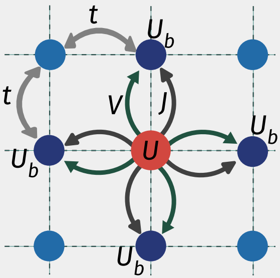


Existing methods suffer from a variety of problems:

- Quantum Monte Carlo suffers from fermion **sign problem** at low temperatures
- Dynamical mean-field theory: low lack of ***k*-space resolution** & large computation cost
- DMRG only works in **quasi-1D** systems

A Bottom-Up Approach: Starting from an Impurity Model



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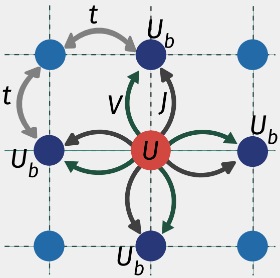

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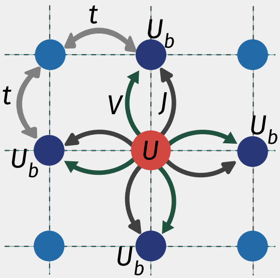

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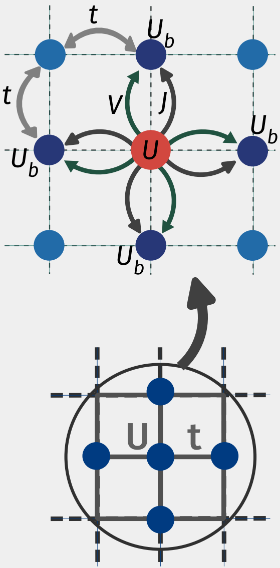

Mapping to the Lattice Model

- Impurity model describes local environment of each site.

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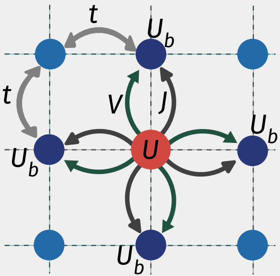

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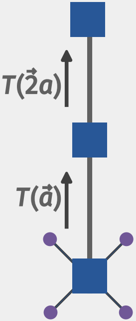
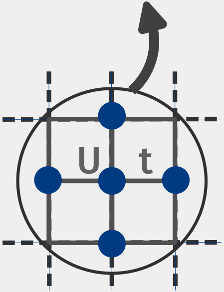


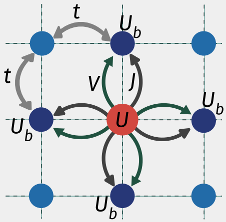


Mapping to the Lattice Model

- 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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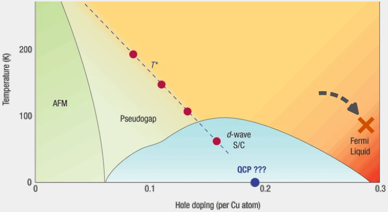
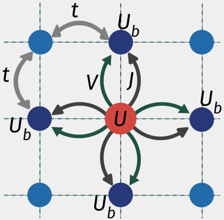
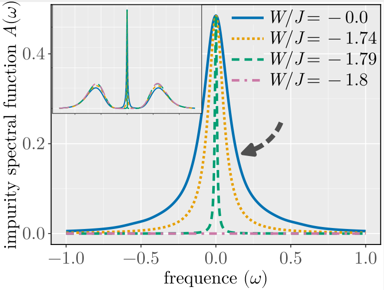
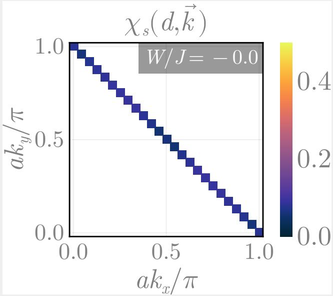
- Impurity **strongly coupled** to Fermi surface









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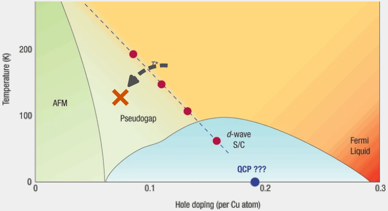
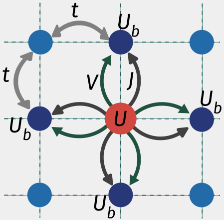
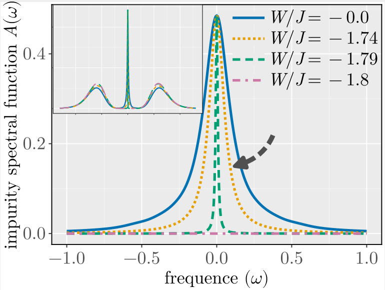
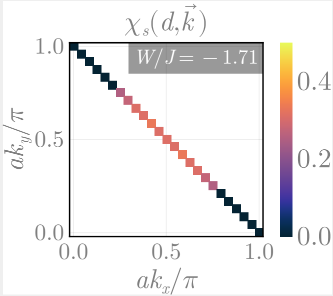
- Impurity **strongly coupled** to Fermi surface
- Impurity coupled **only to parts** of Fermi surface









Momentum-space Resolved Impurity Phase Transition

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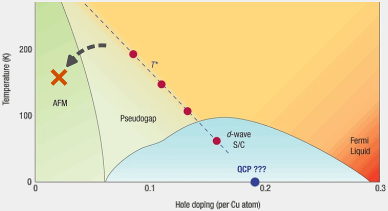
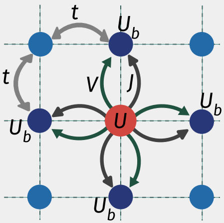
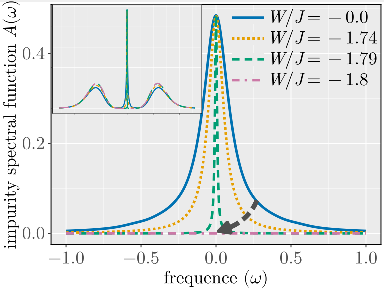
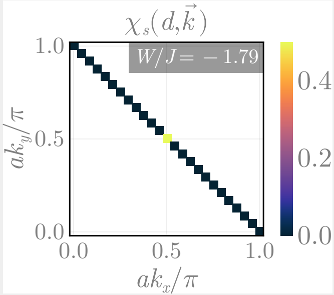
- Impurity **strongly coupled** to Fermi surface
- Impurity coupled **only to parts** of Fermi surface
- Impurity **decoupled** from the Fermi surface



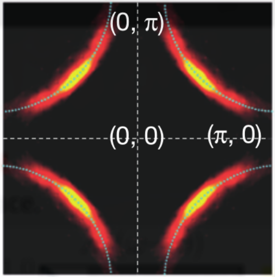


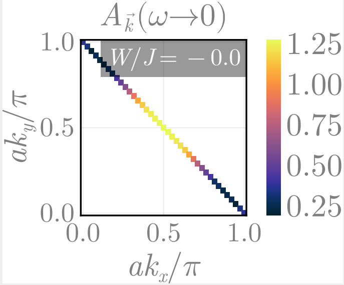


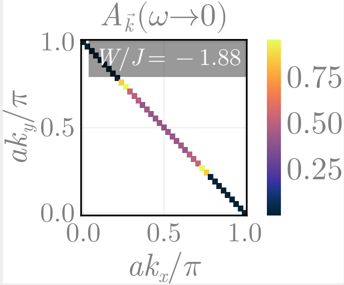


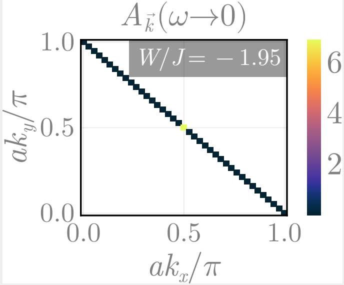
Pseudogapping Transition on the Lattice Model

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



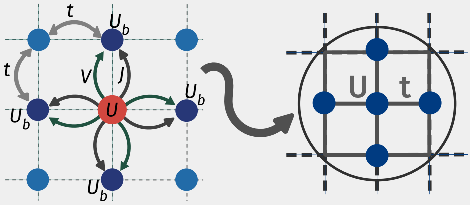






Main takeaways

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



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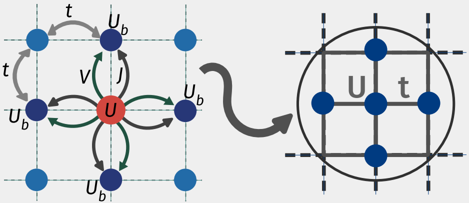

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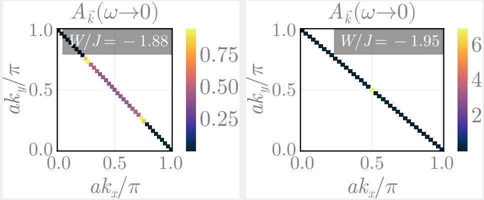

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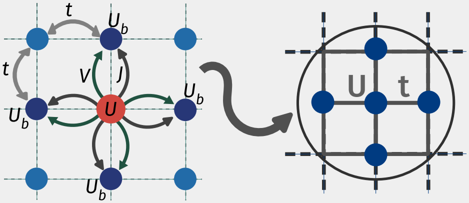

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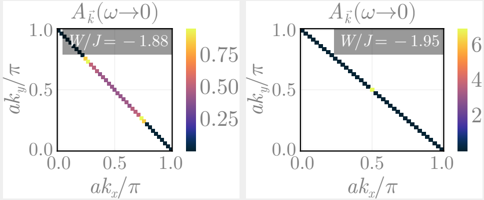

Generalisations and Extensions

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