Frustrating the Kondo Effect through Charge Fluctuations: from the Auxiliary Model to the Bulk

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Emergent Phenomena in Quantum Matter
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Outline of the Discussion

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- Some **preliminaries**: Hubbard model, DMFT, and the Anderson impurity model
- What, then, are the **questions**?
- Explaining the Mott MIT: the **extended** Anderson impurity model
- Some more **questions**!
- **Tiling** with the extended Anderson impurity model

The Hubbard model

The Hubbard model: What and Why

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

$U/t = 0 \longrightarrow$ free electron model

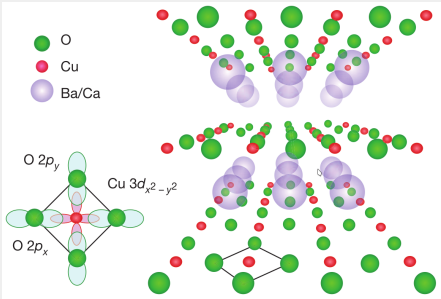
$U/t = \infty \longrightarrow$ array of free spins

Is there a transition at finite U/t?

The Hubbard model: What and Why

Believed to describe the physics of the cuprates

- inert spacer layers render the material quasi-2D
- physics happens in the Cu-O planes
- 3d-electrons from copper hybridise with the oxygen p-orbitals



Might also describe superconducting Nickelate (replace Cu with Ni) and organic charge transfer salts

[0]Keimer et al., Nature (2015); Souza1 and Pouget, JPCM (2013); Qin et al., Annu. Rev. Condens. Matter Phys (2022); Kitatani at al., NPR Quantum Mater (2020)

The Hubbard model in infinite dimensions

$$H_{\text{hub}} = \underbrace{-t \sum_{\langle i,j \rangle} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.} \right)}_{N \times z \text{ terms}} + \underbrace{U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu N}_{N \text{ terms}}$$

In order to retain competition between t and U:

$$t \to t/\sqrt{z}$$

Enormously simplifies calculations: $\Sigma(\vec{k}, \omega) = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} \Sigma(\vec{r}, \omega), \quad \Sigma(\vec{r}, \omega) \sim z^{-r/2}$

$\Sigma(\vec{k}, \omega) = \Sigma_{\text{local}}(\omega)$: **lattice self-energy becomes independent of momentum**

How to calculate this local self-energy? DMFT!

[1]

[1] Miiller-Hartmann, Z. Phys. B-Condensed Matter (1989); Metzner and Vollhardt, PRL (1989); Georges et al, RMP (1996)

Dynamical mean-field theory

How does classical mean-field theory work?

- Replace fluctuations by an **effective mean field** $h(y)$, where y is some order parameter.

$$J \sum_i S_i^z S_{i+1}^z \to h \sum_i S_i^z, h = \beta J m$$

How does classical mean-field theory work?

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- Construct a **self-consistency equation** for the simplified model, typically of the form: $y = f(h)$.

$$m = \tanh(h)$$

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- By starting with some **guess value** h_{guess} for the mean-field, calculate the order parameter y_{guess} corresponding to the guess field.

$$h = 0.01 \implies m = 0.02(say)$$

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- From the consistency equation, the order parameter gives the next value of the field: $h = f^{-1}_{\text{next}}(y_{\text{guess}})$, leading to an **updated mean-field Hamiltonian**.

$$h = 0.01 \implies m = 0.02 \implies h_{\text{next}} = \arctan(0.02)$$

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- **Keep solving** this updated Hamiltonian until the order parameter resulting from subsequent iterations does not change.

$$h = 0.059 \implies h_{\text{next}} = \arctan(0.0591) \implies h_{\text{next}} = \arctan(0.0589)$$

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$$\Sigma(\vec{k}, \omega) \to \Sigma_{\text{loc}}(\omega)$$

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$$G_{\text{loc}} = 1 / \left(\omega - t^2 G_{\text{loc}} - \Sigma_{\text{loc}}\right)$$

The RHS is the impurity Greens function of an
Anderson impurity model with bath described by G_{loc}!

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Create SIAM with Hubbard U and trial G_{loc}
as the bath Greens function. Solve SIAM to obtain Σ_{loc}

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From G_{loc} and Σ_{loc}, calculate the impurity Greens function, using

$$G_{\text{imp}} = 1 / \left(\omega - t^2 G_{\text{loc}} - \Sigma_{\text{loc}}\right)$$

By the self-consistency equation, this is also the bath Greens function for next iteration.

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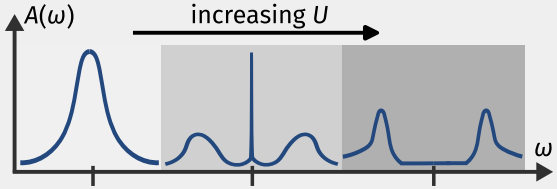
The problem then reduces to finding a SIAM with $G_{\text{imp}} = G_{\text{bath}}$.

This is done iteratively, through a “self-consistency loop”.

DMFT Results on the Bethe lattice in $d = \infty$, at 1/2-filling

Local spectral function **acquires a gap** at a critical value of $\frac{U}{D}(\sim 3)$



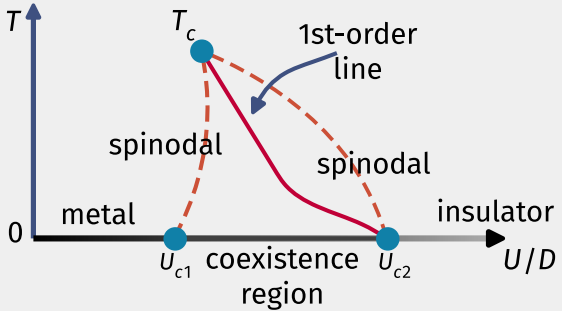
Constitutes a zero temperature **Mott metal-insulator transition**

Good metal with broad peak ⇒ ”Bad” metal with sharp peak ⇒ Mott insulator

DMFT Results on the Bethe lattice in $d = \infty$, at 1/2-filling

Transition is **not bi-continuous**, scales do not vanish simultaneously on both sides

$T = 0$ second order point replaced by a first order line at finite temperatures



Leads to a **metal-insulator coexistence region**, with a finite gap as well as central peak

Physics of the Anderson impurity model

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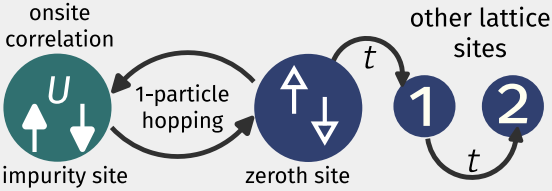
Localised d- or f-electron hybridising with conduction bath

$$H_{\text{SIAM}} = \sum_k \epsilon_k n_{k\sigma} + \epsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k \left[V(k) c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right]$$



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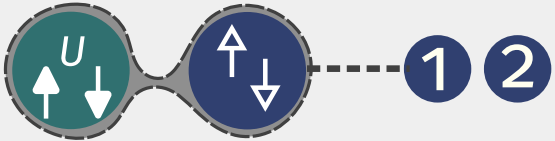
$V/U > 0$

impurity strongly coupled to bath



Gapless excitations are supported; spectral function **has central peak**

Physics of the Anderson impurity model

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$V/U \to 0$

crossover to decoupled local moment

spectral function acquires gap only at $U/V = \infty$

No phase transition as U is tuned!

Physics of the Anderson impurity model

- The standard 1/2–filled SIAM has no local moment phase!
- **Cannot explain** the Mott MIT of DMFT
- Self-consistency must be inserting additional physics.

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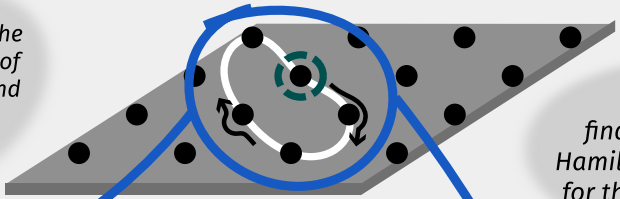
- What is the origin of the **quantum critical fluctuations** observed recently above the finite temperature second-order critical point?
- What is the theory for the infrared gapless excitations **precisely at the MIT**?

DMFT *represents excursions from a site into the correlated bath in the form of self-energies for the bath and the impurity. This results in a three-peak DOS of the bath.*



Our Goal:

finding an effective Hamiltonian description for the Σ that gives rise to the MIT.

DMFT

impurity

Σ_{imp}

bath

Σ_{bath}

Similar approach adopted by Si & Kotliar for extended Hubbard model

impurity

zeroth site

1

2

effective Hamiltonian

Extending the Anderson impurity model

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Add some **additional terms** in the Hamiltonian

- an explicit Kondo term
- a local correlation on bath site connected to the impurity

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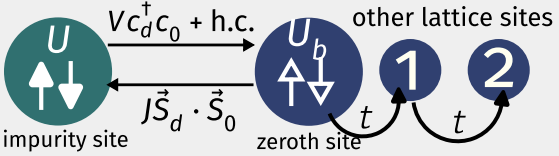
$$H = H_{\mathrm{KE}} + V \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{0\sigma} + \mathrm{h.c.} \right) + \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + \underbrace{J \vec{S}_d \cdot \vec{S}_0 + \frac{1}{2} U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow} \right)^2}$$

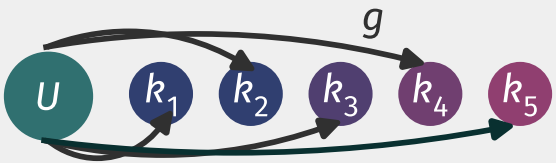


Renormalisation of Couplings

Renormalisation of couplings

Check how the Hamiltonian looks like at **low energies**!

1. Separate the Hamiltonian into a tower of energy scales



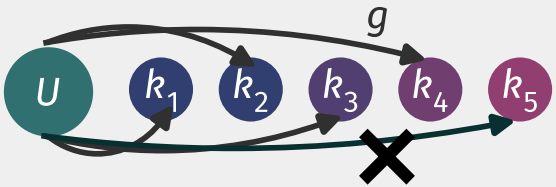
Kinetic energy of non-interacting problem provides an obvious scheme.

$$\epsilon_0 > \epsilon_1 > \ldots > \epsilon_N$$

Renormalisation of couplings

Check how the Hamiltonian looks like at **low energies**!

2. Integrate out the high energy degrees of freedom



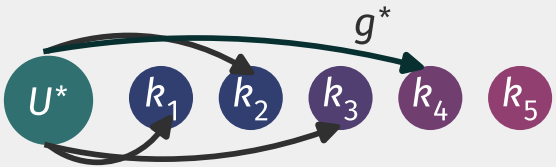
Involves removing number fluctuations in these states:

$$c^{\dagger}_{\mathrm{UV}}, c_{\mathrm{UV}} \rightarrow n_{\mathrm{UV}}$$

Renormalisation of couplings

Check how the Hamiltonian looks like at **low energies**!

3. Obtain renormalisation of remaining degrees of freedom



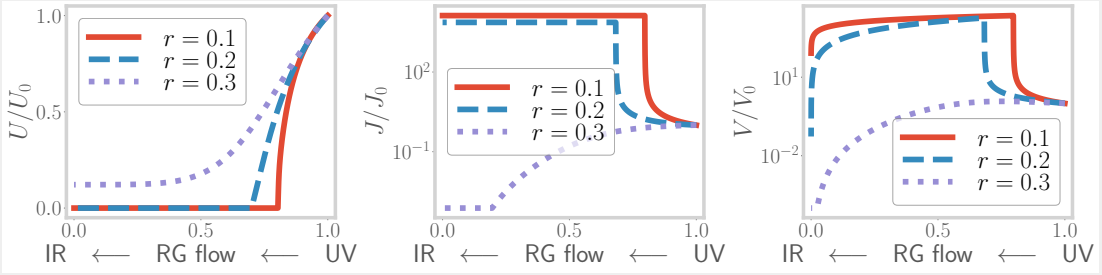
Virtual number fluctuations are taken into account:

$$g^2 c^\dagger_{\mathrm{UV}} c^\dagger_{\mathrm{IR},1} G_{\mathrm{UV}} c_{\mathrm{IR},2} c_{\mathrm{UV}} \sim g^* c^\dagger_{\mathrm{IR},1} c_{\mathrm{IR},2}$$

Renormalisation of couplings

$$\Delta J(D) = \frac{1}{\omega - D/2 + J/4}\rho(D)J\left(J + 4U_b\right)$$

Similar equations for V and U; U_b **is marginal**



A closer look at the RG equation for J

In terms of dimensionless couplings $g = \rho\left(J + 2U_b\right)$ and $\gamma = -2\rho U_b$:

$$\Delta g \sim g^2 - \gamma^2$$

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U_b acts in two ways:

- The first term represents an **effective Kondo** RG flow with reduced strength g
- The second term is a **new term that competes** with the effective Kondo effect

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U_b acts in two ways:

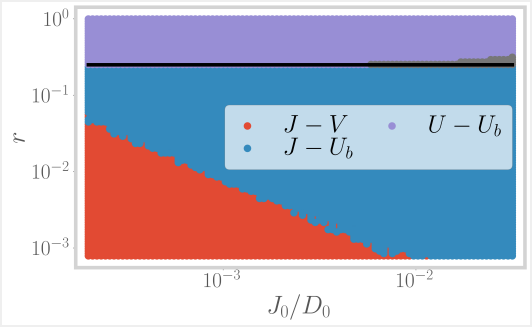
- The first term represents an **effective Kondo** RG flow with reduced strength g
- The second term is a **new term that competes** with the effective Kondo effect

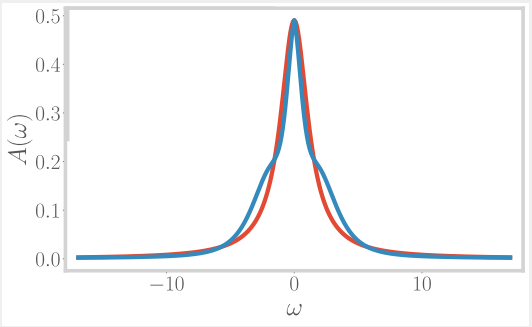
Kondo effect is **destroyed** when the terms become of equal strength:

$$g = \gamma \implies r = -U_b/J = 0.25$$

$T = 0$ Phase Diagram

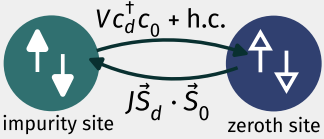
Phase diagram



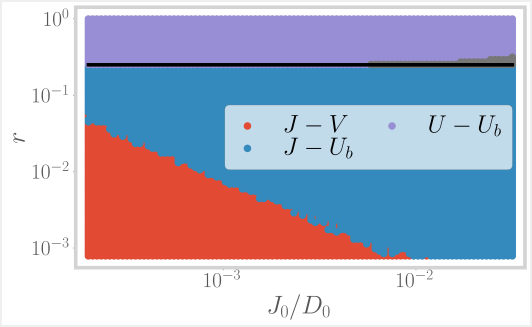


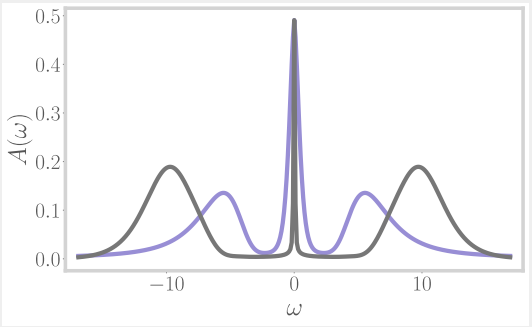
Red phase: weakly correlated metal

- V, J are relevant; broad spectral function
- Effective Hamiltonian: $H^*_{\text{KE}} + V^*\left(c^\dagger_{d\sigma}c_{0\sigma} + \text{h.c.}\right) + J^*\vec{S}_d \cdot \vec{S}_0$
- Ground state has both spin and charge content;



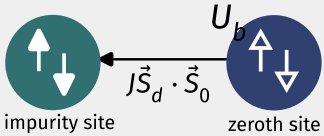
Phase diagram





Blue phase: strongly correlated metal

- J relevant, V irrelevant; sharp spectral function
- Effective Hamiltonian: $H^*_{\mathrm{KE}} + J^* \vec{S}_d \cdot \vec{S}_0 + \frac{U_b}{2}\left(n_{0\uparrow} - n_{0\downarrow}\right)^2$
- Ground state has only spin - Kondo singlet;



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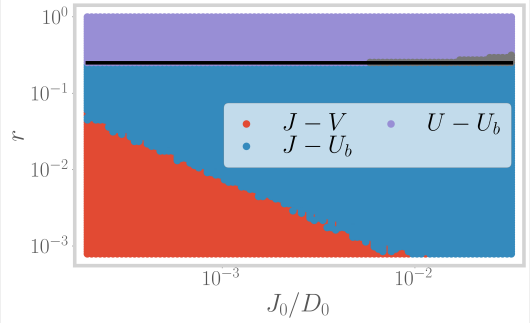

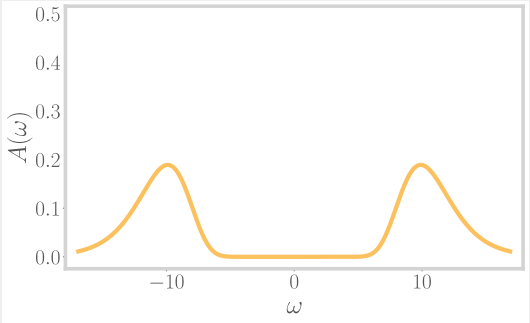

Violet phase: local moment

- V, J are irrelevant; gapped spectral function
- Effective Hamiltonian: $H^*_{\mathrm{KE}} + \frac{U^*}{2}\left(n_{0\uparrow} - n_{0\downarrow}\right)^2$
- Ground state reduces to a decoupled moment;

References I