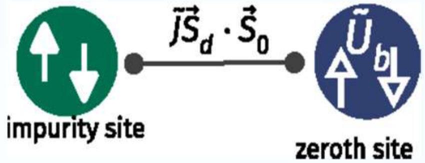

Revisiting the Mott Metal-Insulator transition in DMFT: what lies behind the veil of self-consistency?

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E P Q M

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N. S. Vidhyadhiraja

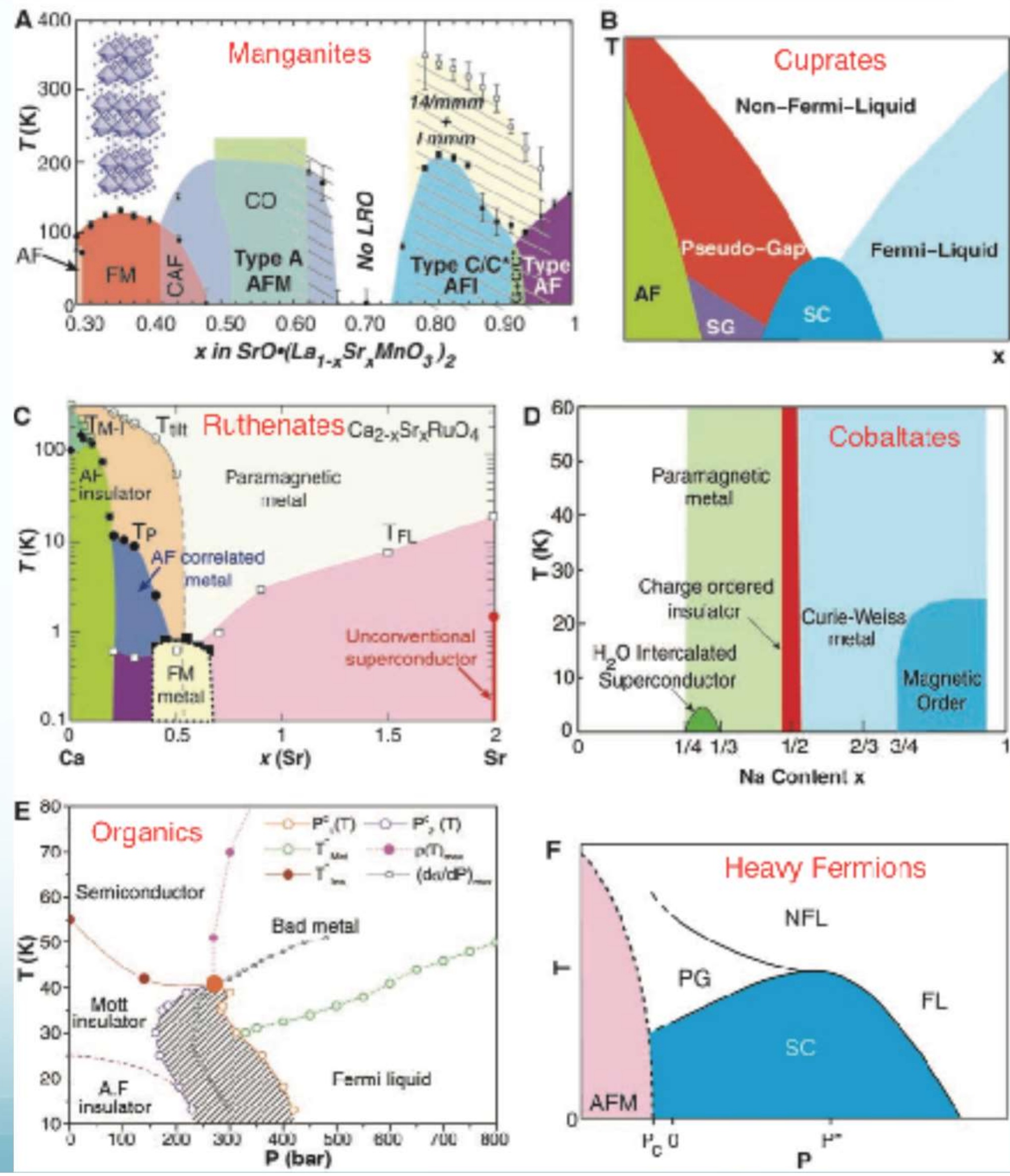
Arghya Taraphder

- also to many colleagues & friends for wonderful discussions,
- the SERB (Govt. of India) for funding through MATRICS & CRG grants; and also to IISER Kolkata

Some big questions

- Complex phase diagrams often observed in strongly correlated electronic materials with a variety of ordered phases. What gives rise to this complexity?

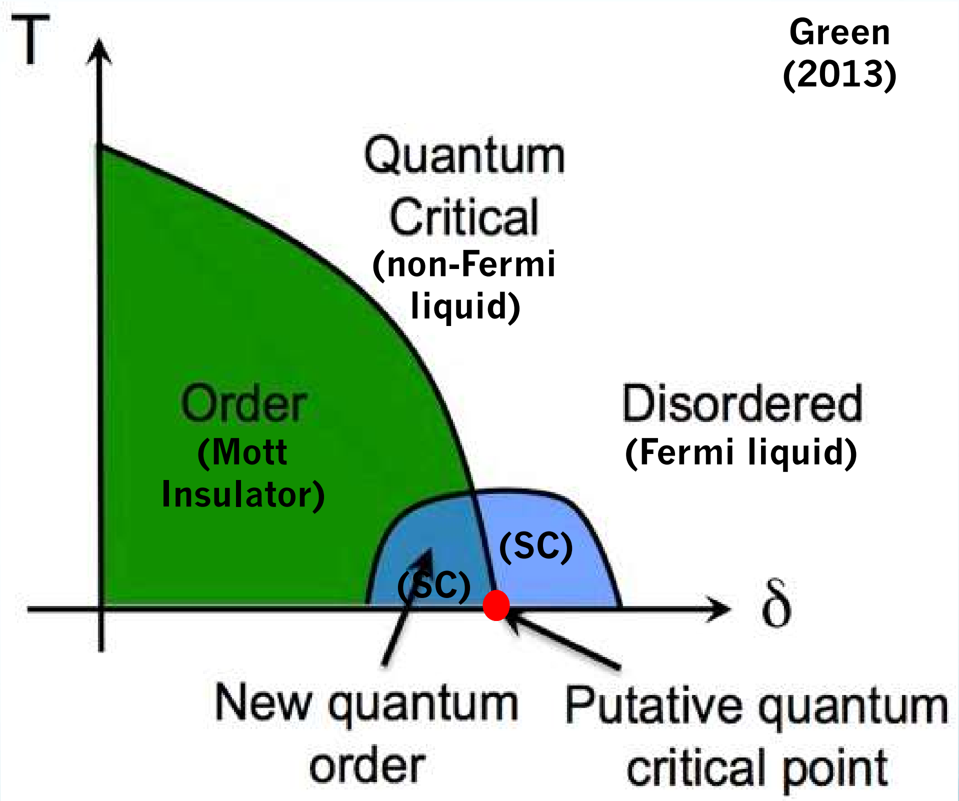
- Can the metal-insulator transition physics of competing tendencies --- electron localisation (due to strong local repulsion) and itineracy (due to hopping) --- be learnt from
  - ➢ simple model Hamiltonians?
  - ➢ a local perspective, i.e., by looking at the same question at a single site (or even a few sites) of the lattice?



Dagotto Science (2005)

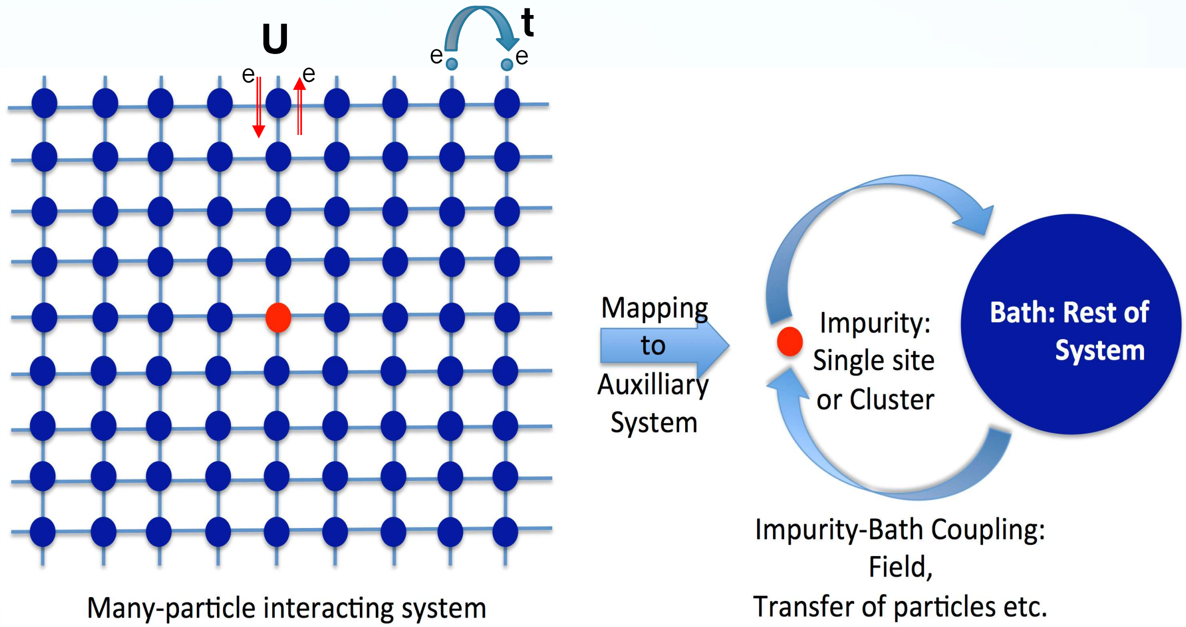
Some big questions

- While we understand the physics of the Fermi liquid metal really well, we encounter strange (or non-Fermi liquids) in many materials.
- Strange metals often found in neighbourhood of quantum critical points, where Fermi liquid is destroyed and an ordered phase emerges. Is this pointing towards some universal?
- Intriguingly, superconducting fluctuations often appear to condense from critical quantum fluctuations of such strange metals. Why?



The Mott Metal-Insulator transition & DMFT

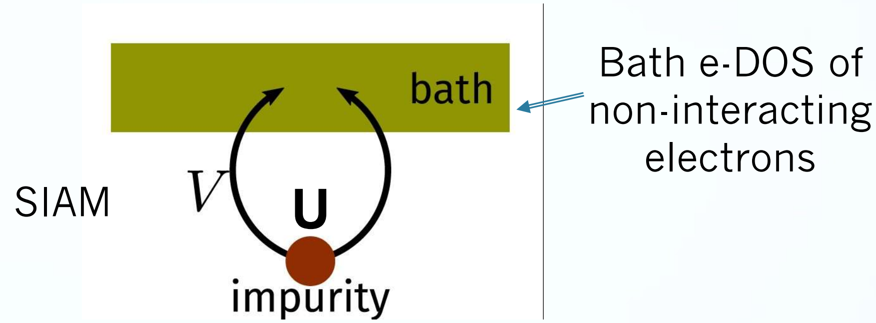
- Mott Metal-Insulator transition involves localisation of itinerant lattice electrons for sufficiently large repulsive interactions
- Easily argued for in the 2D Hubbard model on the square lattice at 1/2–filling : tuning towards U (on-site repulsion) >> D (hopping bandwidth) leads to jamming of electrons
- Dynamical mean-field theory (DMFT) offers a local perspective of the Mott MIT

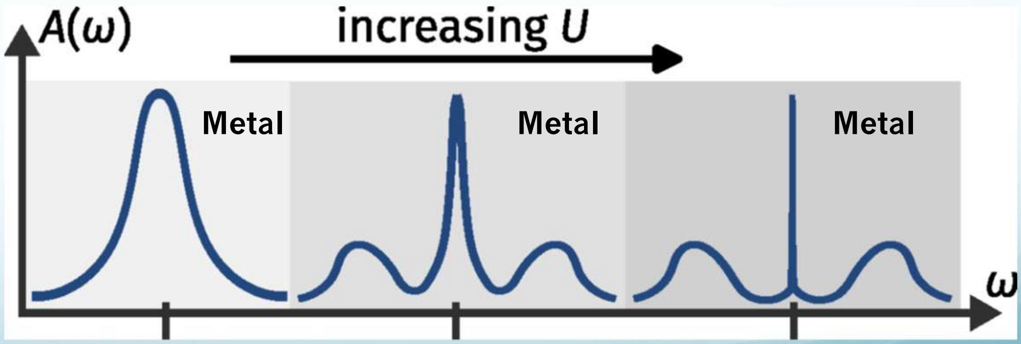


Hubbard Model → DMFT → Single Impurity Anderson Model (SIAM) coupled to a bath of correlated conduction electrons through electronic hybridisation

The Single Impurity Anderson Model (SIAM)

- Standard SIAM involves impurity with on-site Hubbard repulsion, hybridised through electron hopping with conduction bath of non-interacting electrons whose e-DOS is featureless.
- Tuning U to strong coupling shows a dynamical transfer of spectral weight from central peak (Kondo resonance) at small energies to broad features at higher energies (Hubbard sidebands)
- Only Kondo screened impurity phase obtained for any finite U; corresponds to gapless local Fermi liquid
- Local moment (with gapped impurity spectral function) obtained for U= ∞





Impurity Spectral Function

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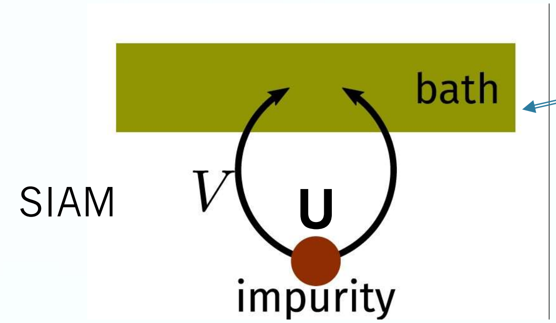
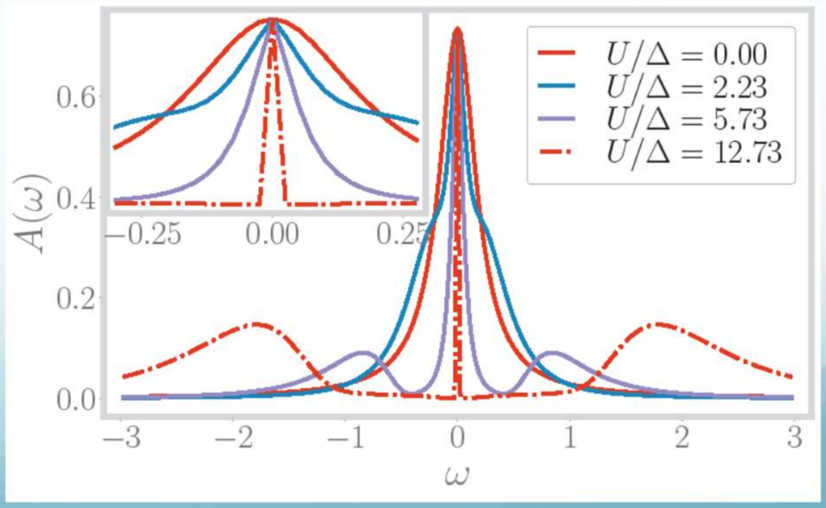


Bath e-DOS of non-interacting electrons



Impurity Spectral Function

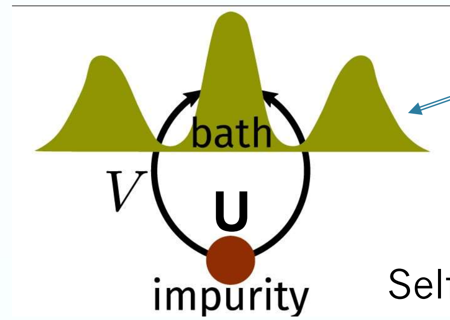
DMFT: Extending the SIAM through self-consistency

- Gapping the impurity spectral function needs additional physics
- Self-consistency requirement of DMFT leads to conduction bath with non-trivial electronic correlations
- Mott MIT observed through the impurity spectral function:

  Metal – broad Kondo resonance

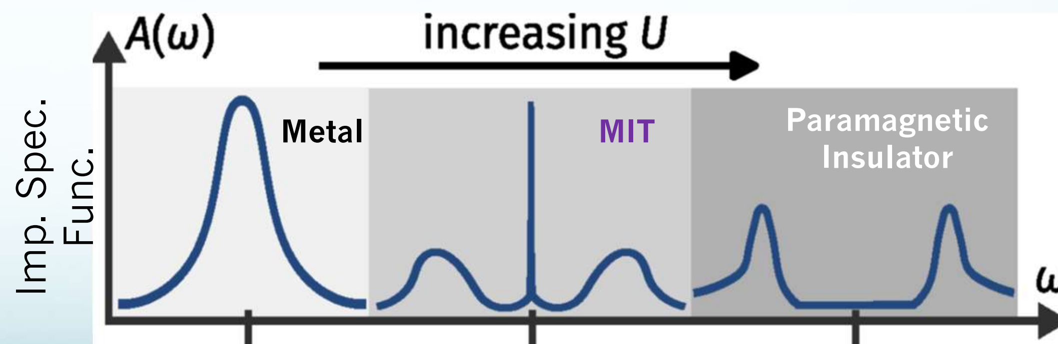
  MIT – sharp central peak lying between Hubbard side bands

  Insulator – Gap separating Hubbard side bands; local moment correspond to frustrated magnetic order



Bath e-DOS of correlated electrons

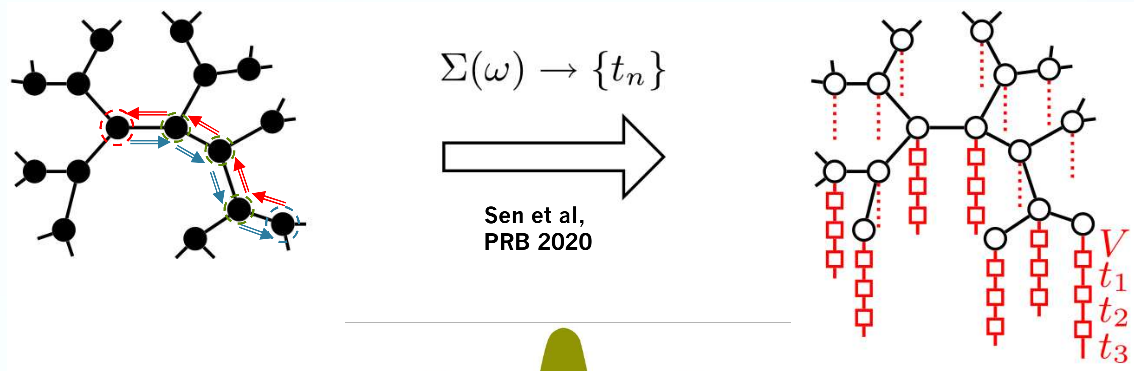
SIAM + Self-Consistency

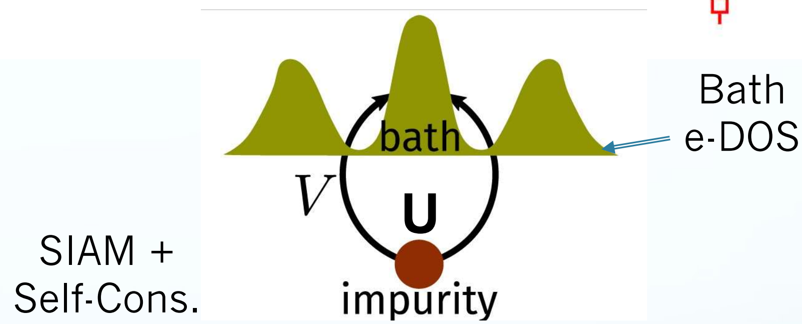


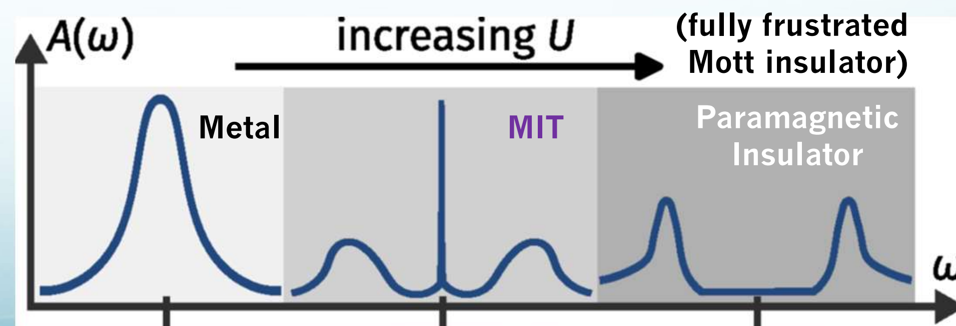
Self-consistency :
Impurity Spec. Func. = local e-DOS of bath

The Mott Metal-Insulator transition & DMFT

- Mott MIT in DMFT is exact for ½-filled Hubbard model on Bethe lattice with ∞ coord. no.
- On this lattice, no non-trivial loops can be formed during round-trip journey of electron from a given site back to itself
- In the limit of ∞ coord. no., all such journeys are rendered independent of & identical to one another: the single-particle self-energy is local (i.e., independent of wavevector k), $\Sigma \equiv \Sigma(\omega)$





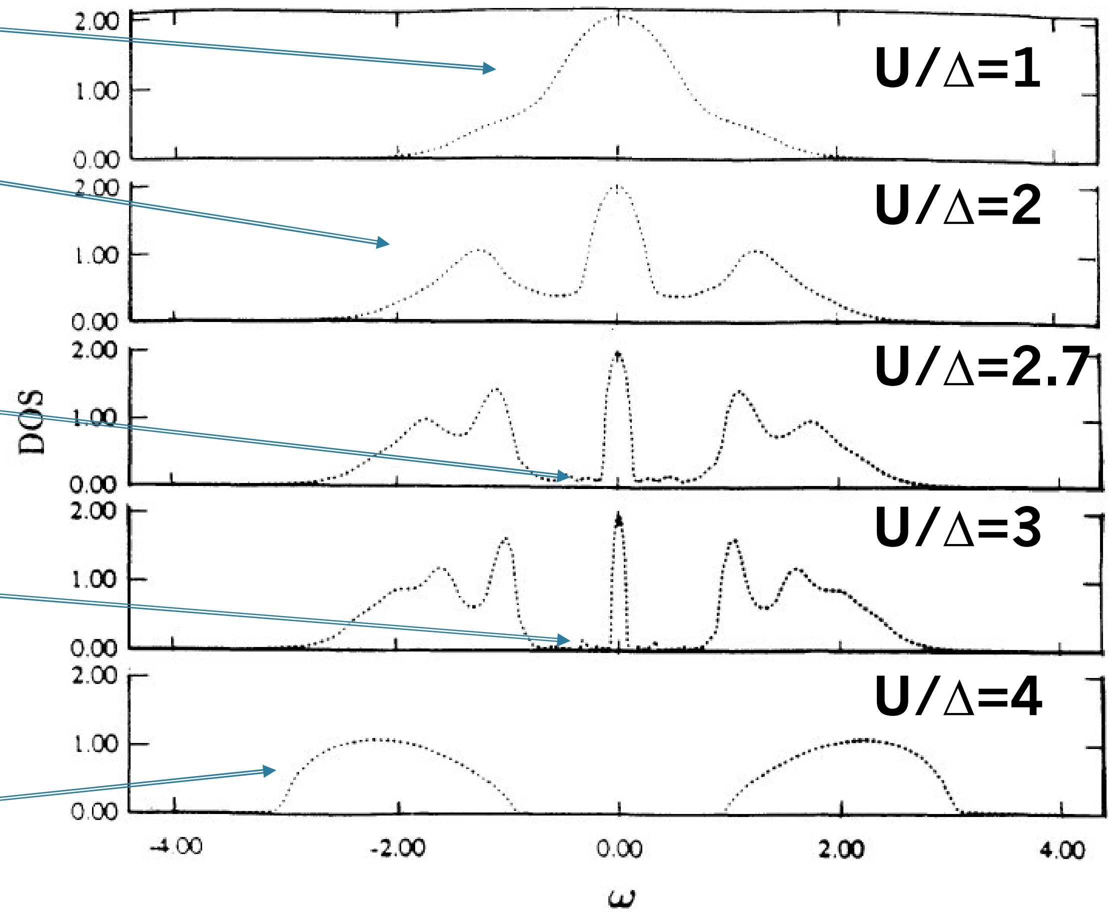


Impurity Spectral Function

DMFT: A local view of the Mott MIT

- Broad Kondo resonance around $\omega = 0$ for small U/Δ : good metal
- Dynamical spectral weight transfer from central peak to (Hubbard) side bands as U/Δ is increased
- Sudden appearance of pre-formed (optical) gap in spectral function at U_{c1} (Mott-Hubbard scenario)
- Pre-formed gap increases, and width of central peak decreases, continuously with tuning U/Δ towards MIT (U_{c2}); signals coexistence of metal & insulator
- Central peak shrinks continuously and disappears at U_{c2} (Brinkman-Rice scenario), and true gap appears smoothly from pre-formed gap: local moment, paramagnetic insulator

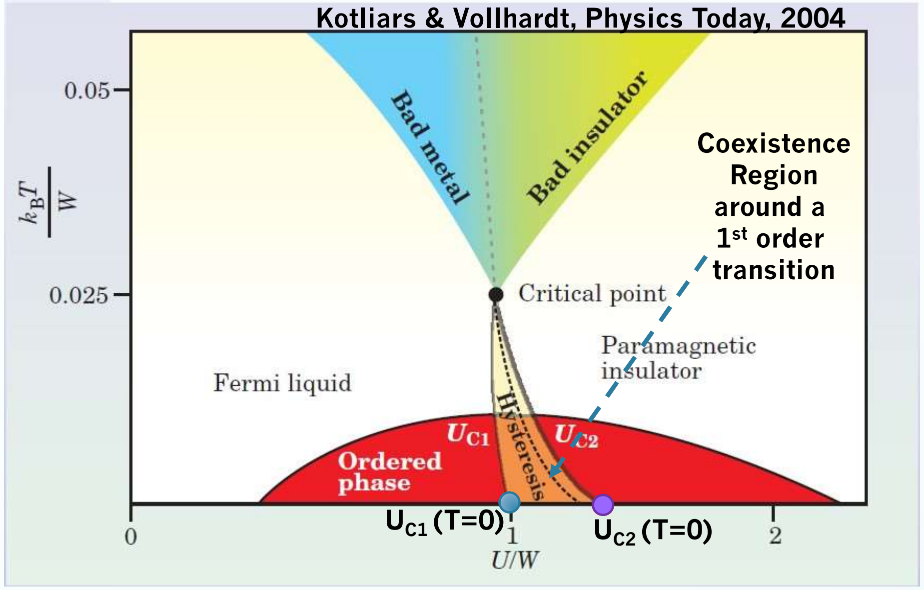
Zhang, Rozenberg & Kotliar, PRL 1993



Impurity Spectral Function

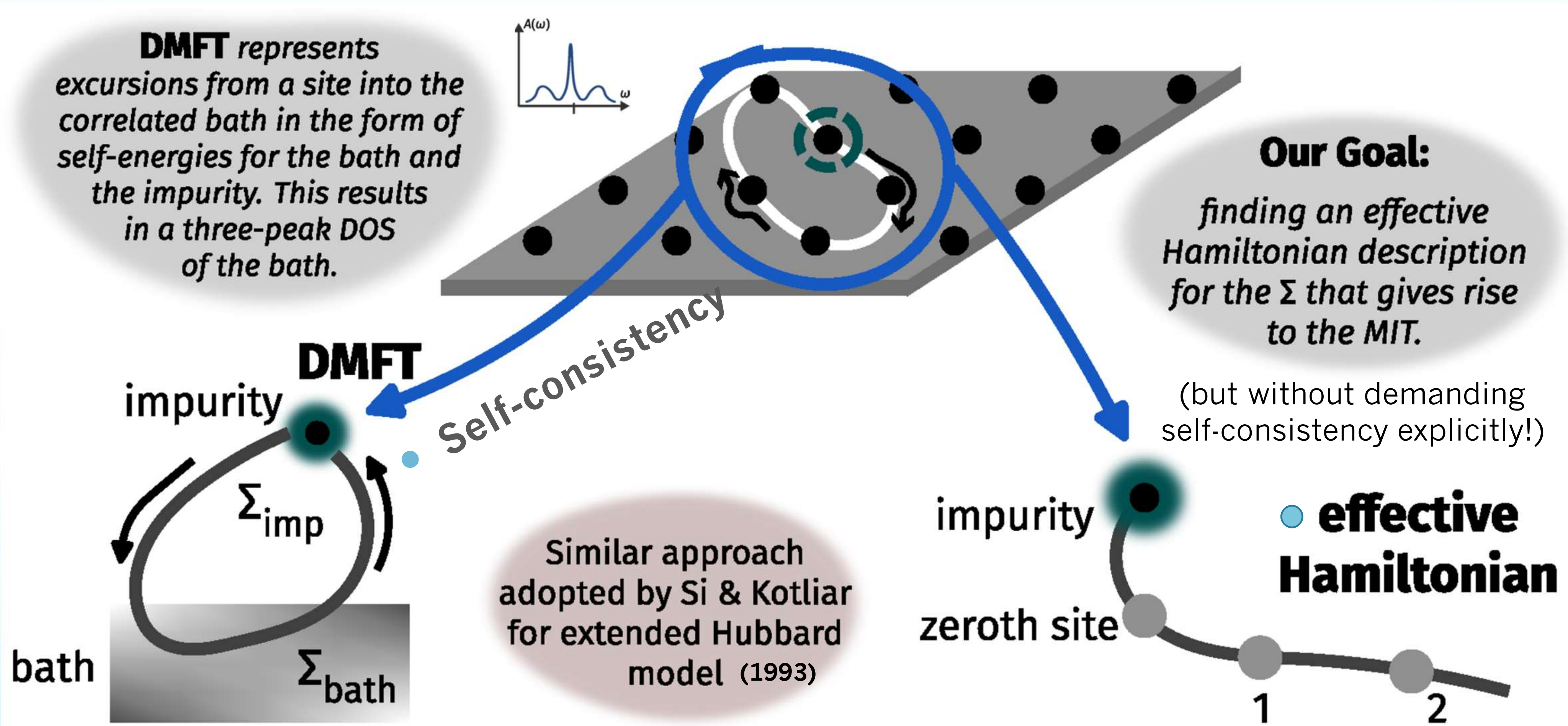
DMFT: A local view of the Mott MIT

- Finite-temperature co-existence region of paramagnetic insulating and metallic phases (light brown region).
- True first order transition at $U_c(T)$ (dashed line). Spinodal lines corresponding to destabilisation of metallic solution ($U_{c2}(T)$) and metastable insulating solution ($U_{c1}(T)$).
- Spinodal lines meet at finite-T critical point, above which there is a crossover between the metal and the insulator.
- Additional physics could lead to a magnetically ordered phase at low-T.

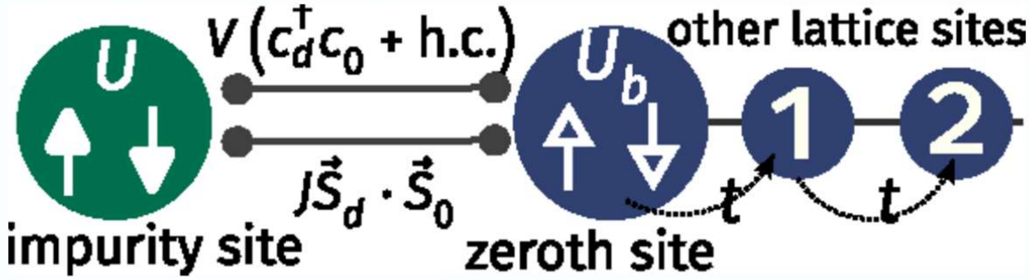


- **Questions:**
  - How does the SIAM change in order to accommodate the MIT, and such a rich phase diagram?
  - What mechanisms drive all this?

Mott MIT & DMFT : Our goal



Extending the SIAM (but without demanding self-consistency!)



Wilson chain-like mapping of conduction bath sites; Nozieres local Fermi liquid at site 1 of bath

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

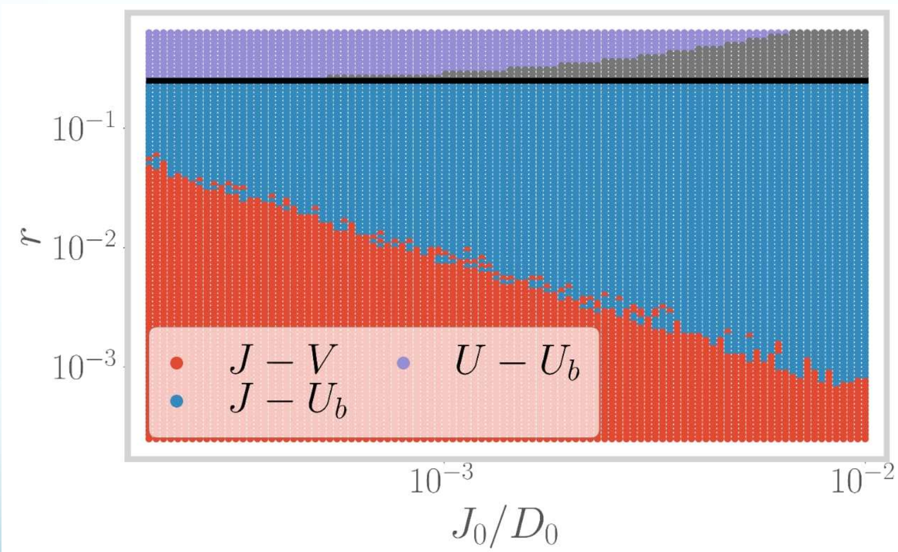
- We extend the particle-hole symmetric SIAM (minimally) to include

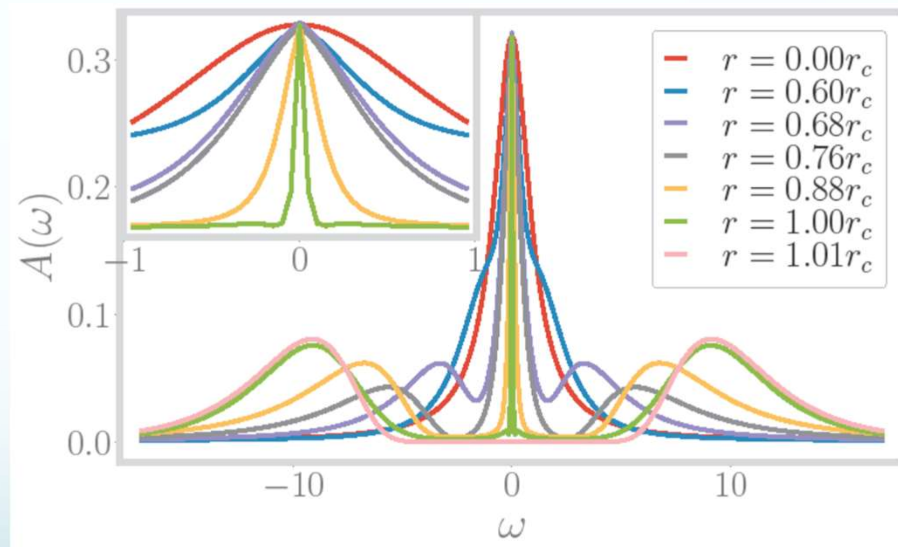
  i. Exchange coupling (J) between impurity and bath zeroth site

  ii. On-site Hubbard interaction (U_b) on bath zeroth site

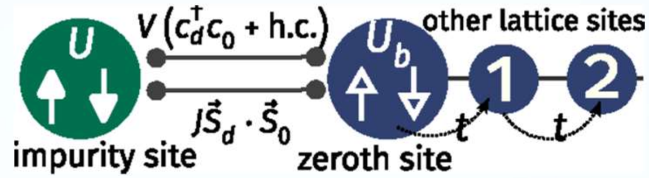
- Analyse this model using Unitary RG method developed recently.

Results from our analysis of the extended SIAM



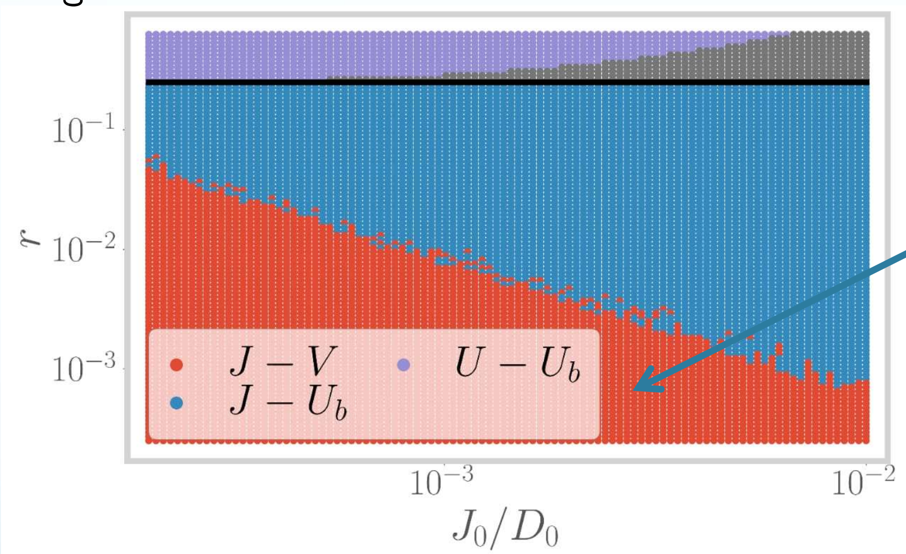


Phases of the extended SIAM



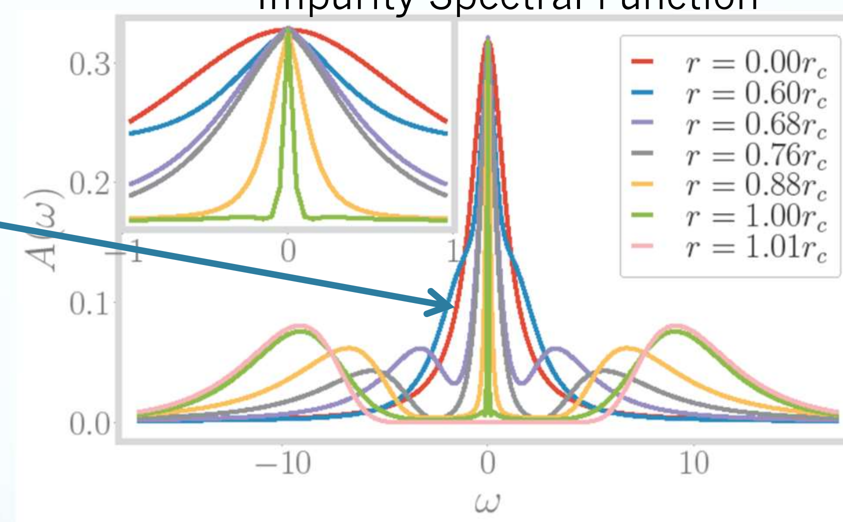
$$r = -\frac{U_b}{J} \quad r_c = \frac{1}{4} \quad U_b = -\frac{U}{10}$$

Phase Diagram



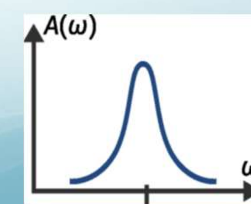
Broad Kondo resonance. Good Fermi liquid metal.

Impurity Spectral Function



: J, V relevant; U irrelevant; U_b negligible. Broad Kondo peak, Weakly correlated local Fermi liquid (red curve)

(Note: Grey region corresponds to a decoupled resonant level impurity model. Disappears from phase diagram upon increasing system size.)



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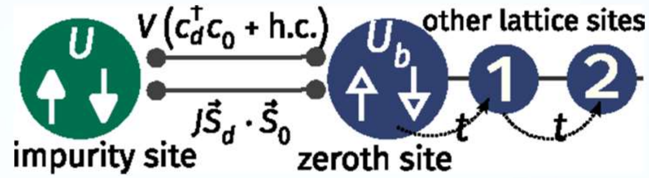

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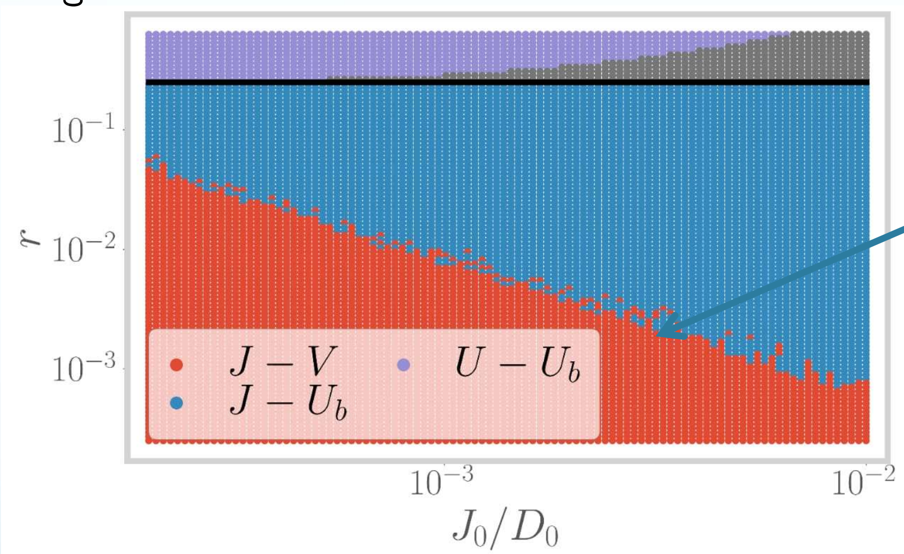
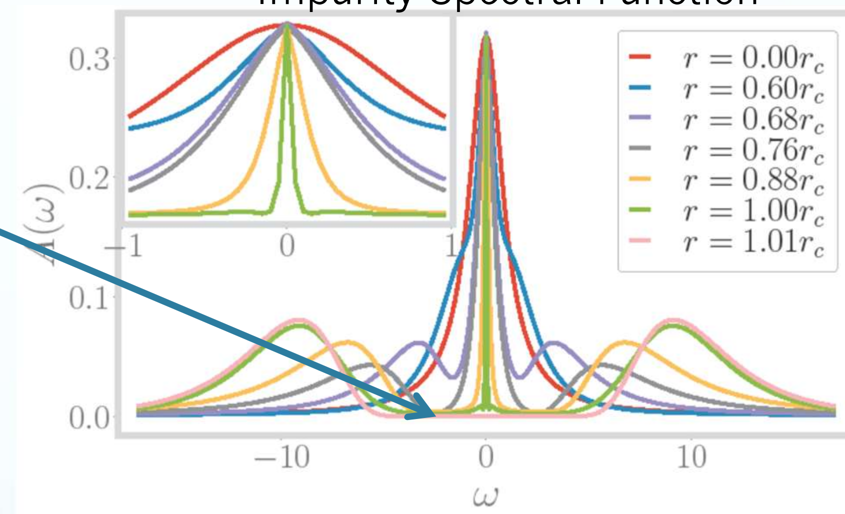
Phase Diagram



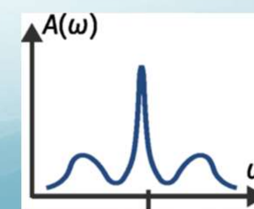
V turns RG irrelevant here. Coincides with well formed dip in Impurity Spectral Function.

Impurity Spectral Function



: J relevant; V, U irrelevant; r < r_c.

3-peak spectral function (sharp Kondo peak + Hubbard side bands), Strongly correlated local Fermi liquid (cyan curve), appearance of pre-formed gap suggests separation of energy scales for opening of gap (Mott-Hubbard transition) and disappearance of Kondo peak (Brinkmann-Rice transition)



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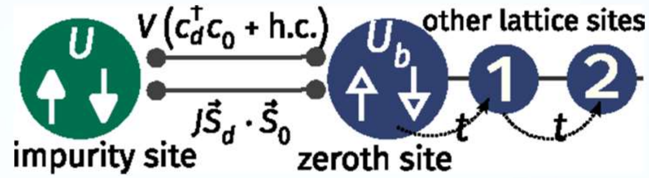
Phases of the extended SIAM



Phase Diagram

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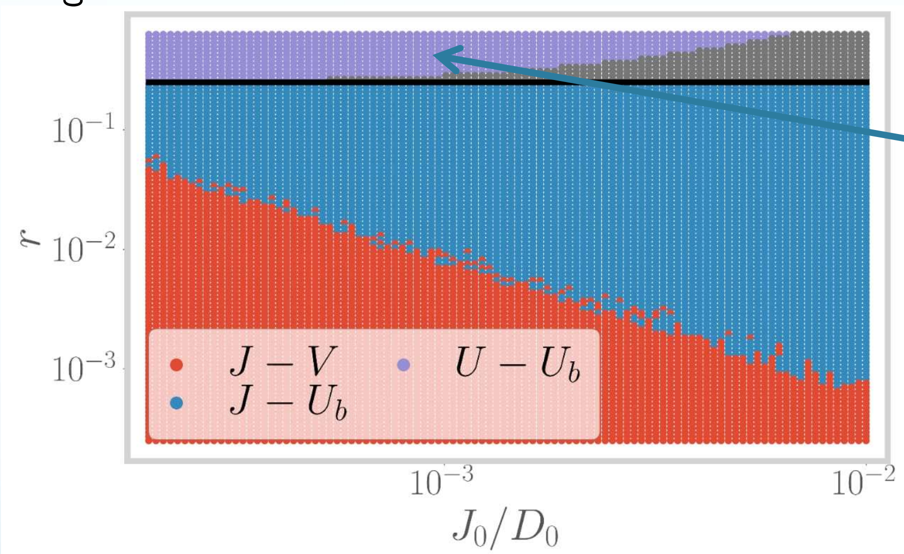
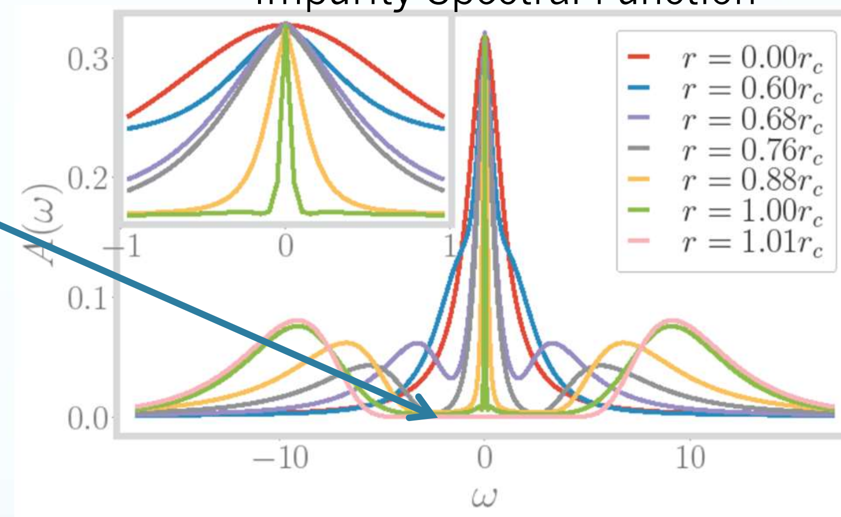


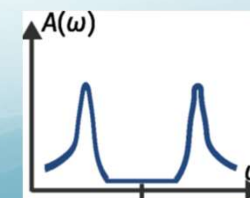
U turns RG relevant here. Gapped DOS of Local Moment. Paramagnetic Insulator.

Impurity Spectral Function



(Note: Grey region corresponds to a decoupled resonant level impurity model. Disappears from phase diagram upon increasing system size.)

: J, V irrelevant; U relevant; $r > r_c$. Gapped spec. func., Local Moment (green curve)



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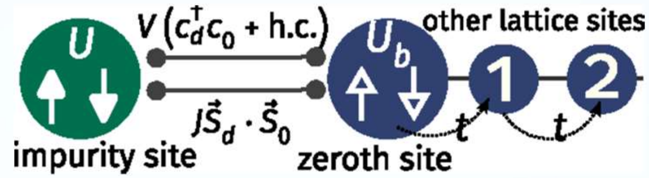

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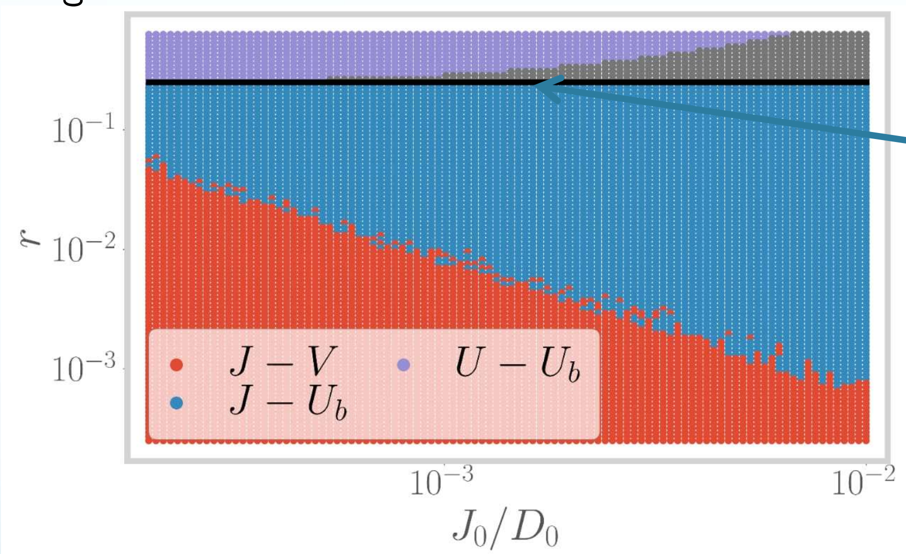
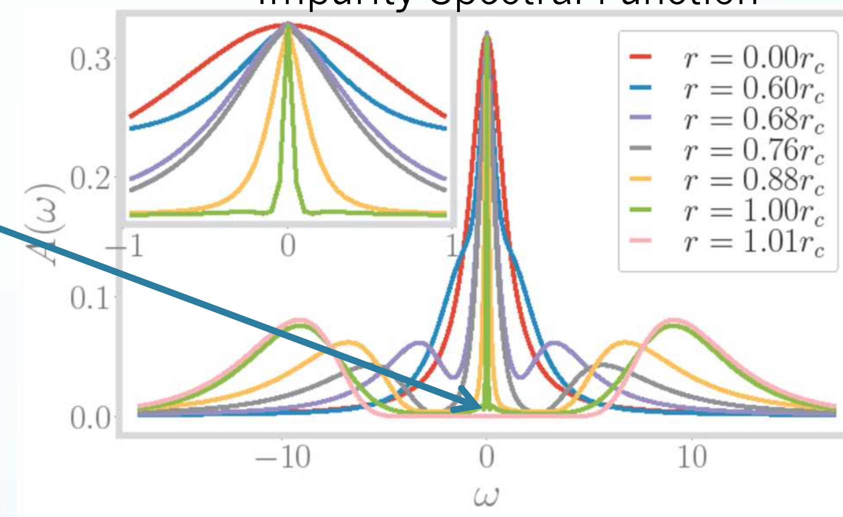
Phase Diagram



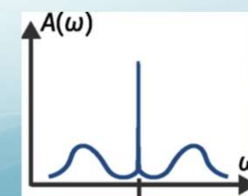
MIT: J turns RG irrelevant here. Sharp Kondo resonance signals breakdown of Fermi liquid metal.

Impurity Spectral Function



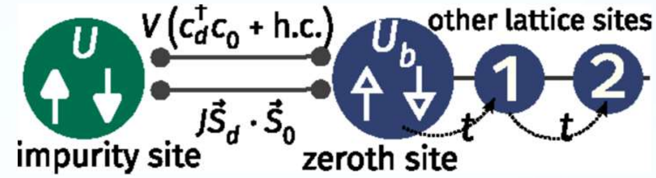
(Note: Grey region corresponds to a decoupled resonant level impurity model. Disappears from phase diagram upon increasing system size.)

— : MIT; $r = r_c$. 3-peak spectral function, sharp central peak corresponds to local non-Fermi liquid (yellow curve)

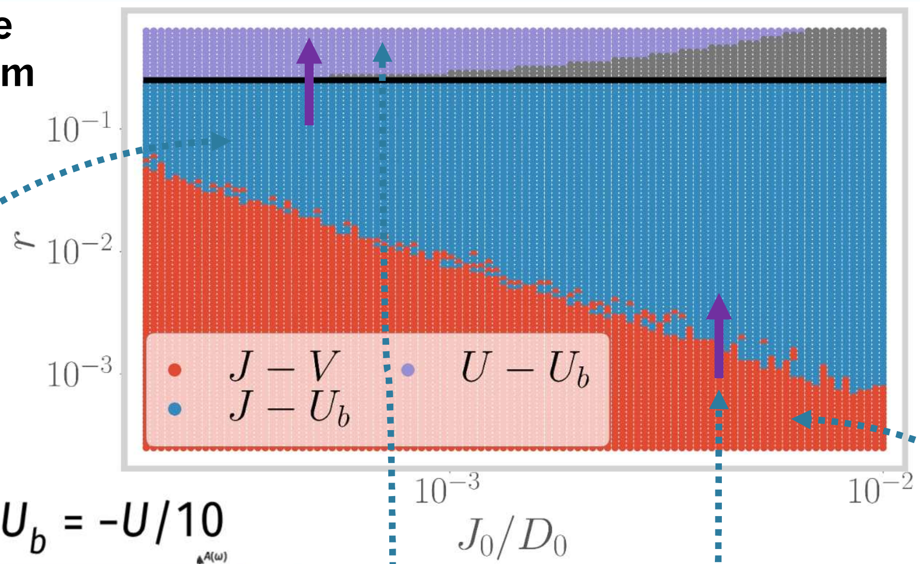


RG flows of the extended SIAM

$$r = -\frac{U_b}{J} \quad r_c = \frac{1}{4} \quad U_b = -\frac{U}{10}$$



Phase Diagram

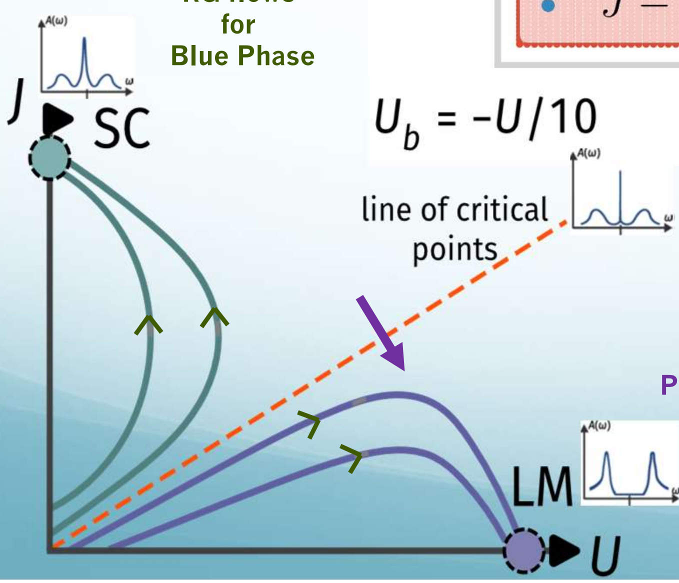


RG Eq. for J :

$$\Delta J \sim J(J + 4U_b)$$

J wants to grow & dominate, but U_b cuts it off at $U_b^* = -J/4$

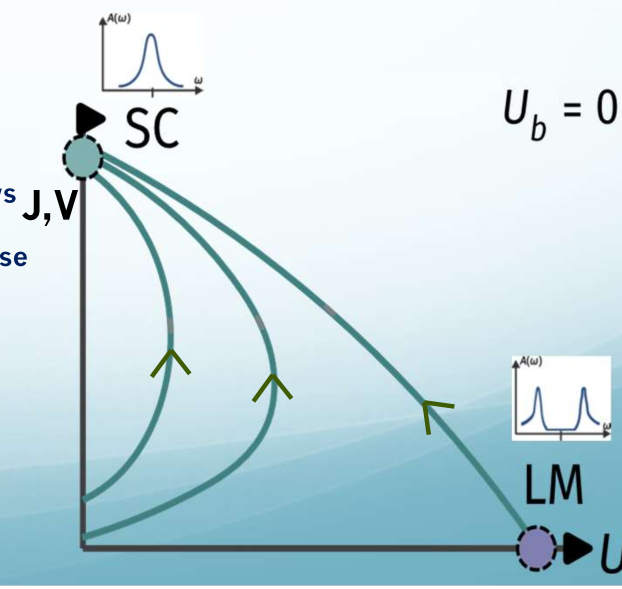
RG flows for Blue Phase



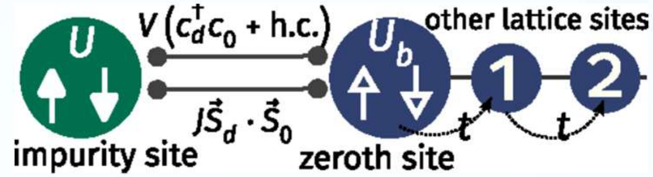
RG flows for Purple Phase

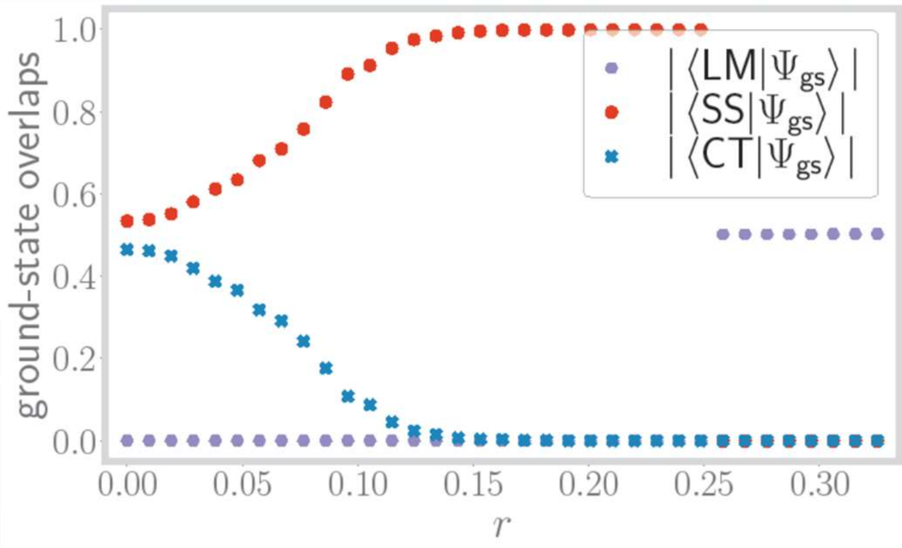
RG Phase diagram for hybridisation (V) is similar to that of J on left, showing transition across red & blue phases.

RG flows for Red Phase



Metallic phase of the extended SIAM: ground state & correlations

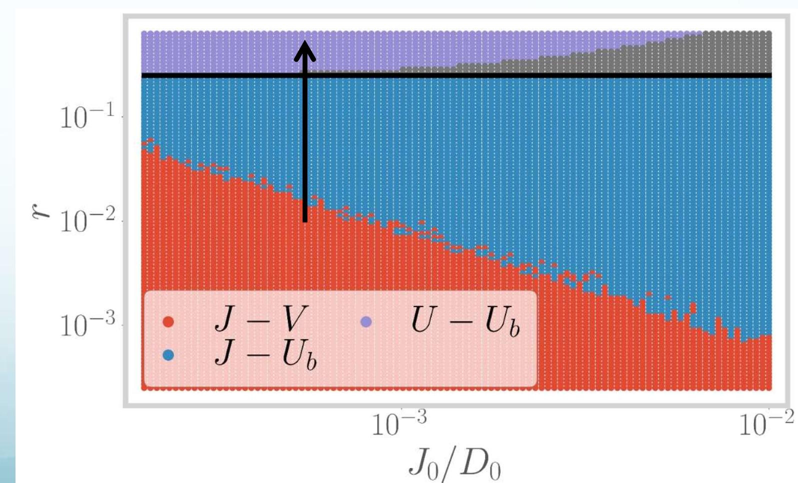




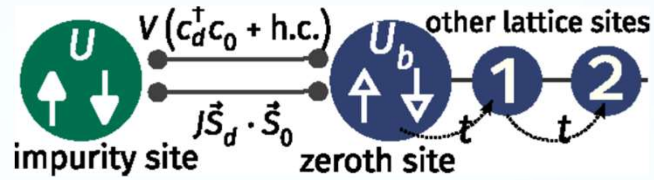
- Overlap of Ground state with spin singlet between impurity and zeroth sites grows upon tuning towards the MIT
- Overlap of Ground state with charge triplet between impurity and zeroth sites decays
- Local Moment appears across the transition

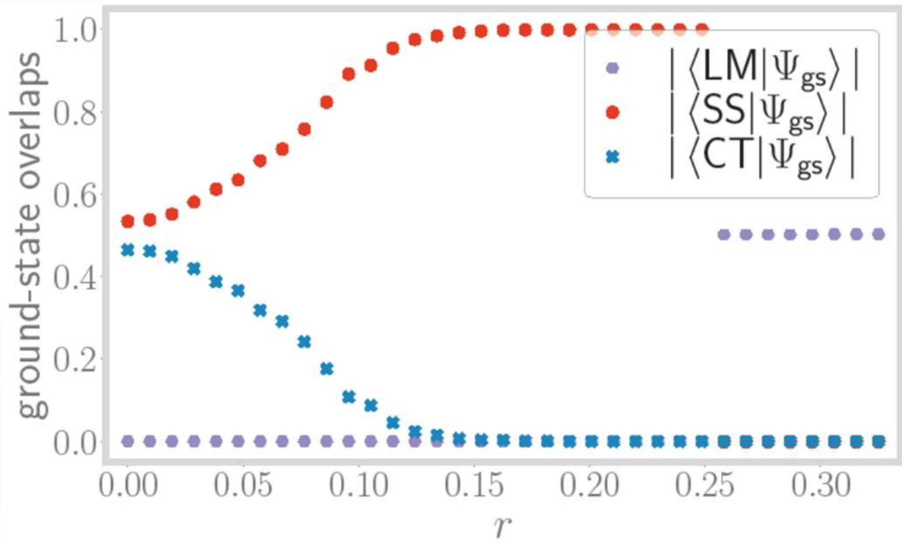
$$|SS\rangle = \frac{1}{\sqrt{2}}(|\uparrow_d \downarrow_0\rangle - |\downarrow_d \uparrow_0\rangle) \qquad |CT\rangle = \frac{1}{\sqrt{2}}(|0_d 2_0\rangle + |2_d 0_0\rangle)$$

$$|LM\rangle = |\uparrow_d O_0\rangle, |\downarrow_d O_0\rangle, |\uparrow_d 2_0\rangle, |\downarrow_d 2_0\rangle$$



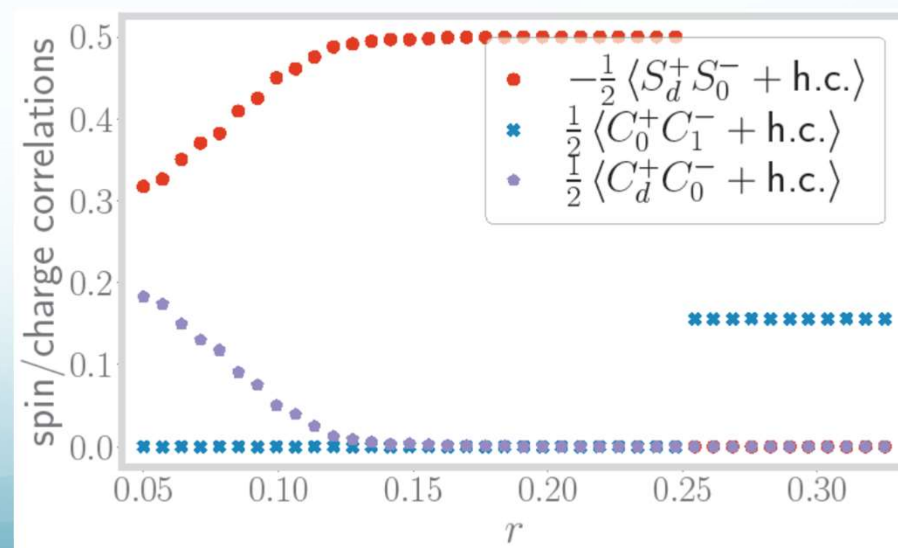
Metallic phase of the extended SIAM: ground state & correlations





- Overlap of Ground state with spin singlet between impurity and zeroth sites grows upon tuning towards the MIT
- Overlap of Ground state with charge triplet between impurity and zeroth sites decays
- Local Moment appears across the transition

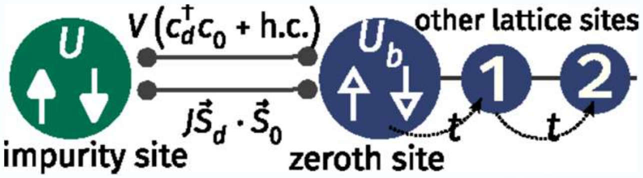
- Spin-flip fluctuations between impurity and zeroth sites grows upon tuning towards the MIT; sudden fall at MIT
- Holon-doublon fluctuations between impurity and zeroth sites decays

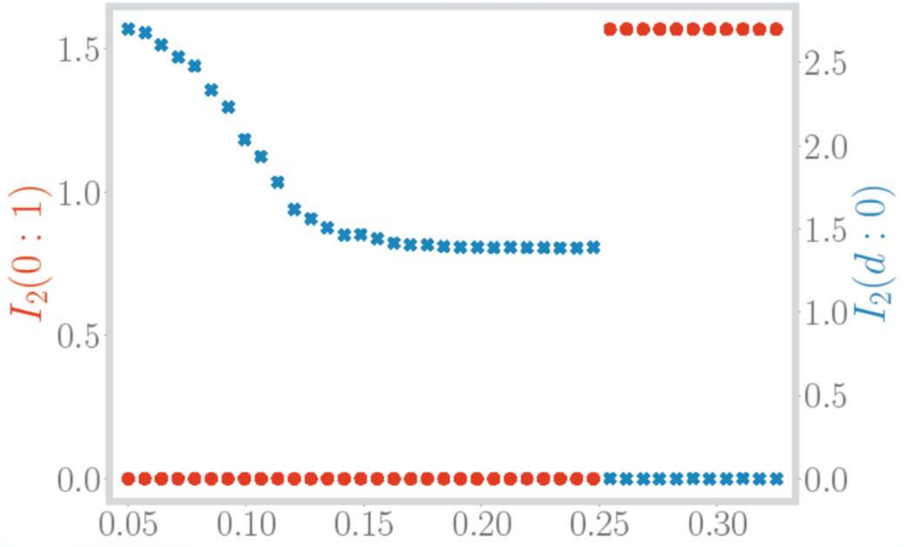


$|SS\rangle = \frac{1}{\sqrt{2}}(|\uparrow_d \downarrow_0\rangle - |\downarrow_d \uparrow_0\rangle)$ $\quad |CT\rangle = \frac{1}{\sqrt{2}}(|0_d 2_0\rangle + |2_d 0_0\rangle)$

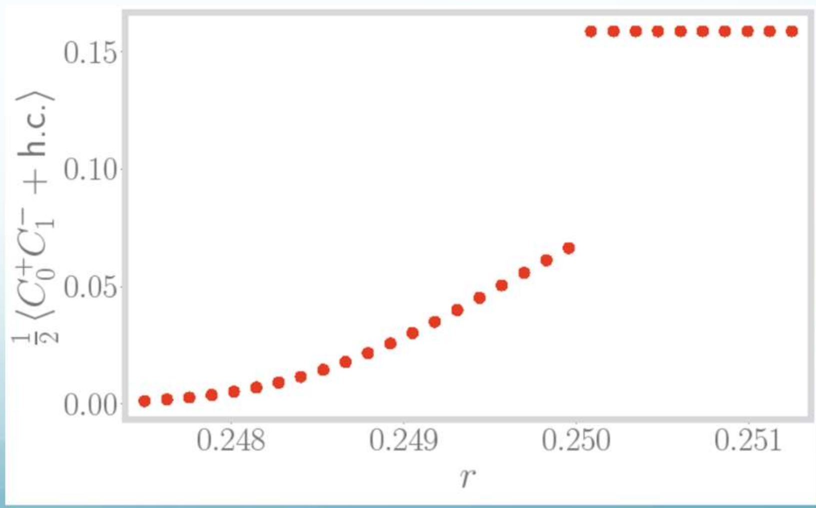
$|LM\rangle = |\uparrow_d O_0\rangle, |\downarrow_d O_0\rangle, |\uparrow_d 2_0\rangle, |\downarrow_d 2_0\rangle$

Metallic phase of the extended SIAM: ground state & correlations



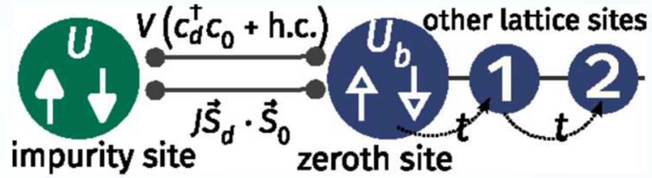


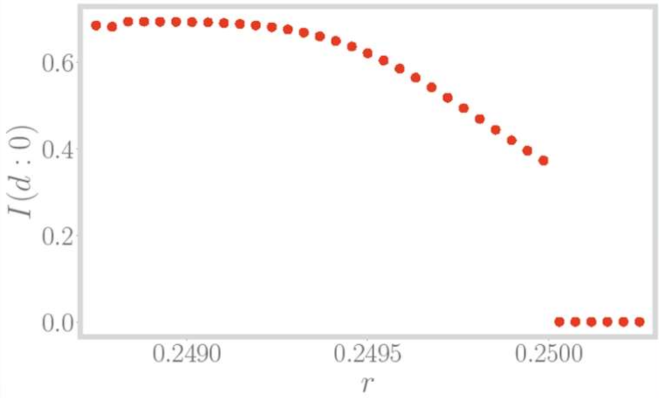
- Mutual Information between impurity and zeroth sites decreases steadily upon tuning towards the MIT, then falls to zero
- Mutual information between zeroth and first sites of bath zero in metal, jumps across MIT



- Holon-doublon fluctuations between zeroth and first sites of bath grows sharply in metallic phase very near MIT
- Coincides with sharp fall in spin-flip fluctuations responsible for Kondo screening
- Holon-doublon (pairing) fluctuations destabilise the Kondo cloud, lead to MIT

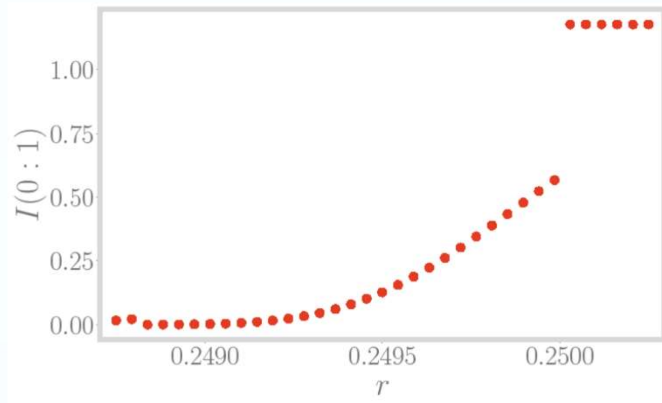
Metallic phase of the extended SIAM: bi- and tri-partite entanglement



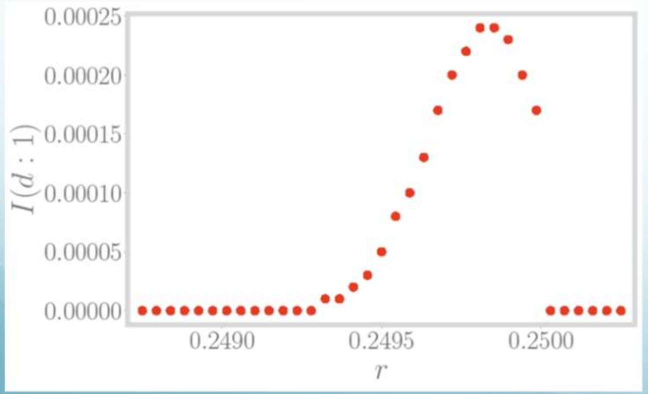


Decreasing entanglement between impurity and bath zeroth sites

Increasing entanglement between bath zeroth & first sites.

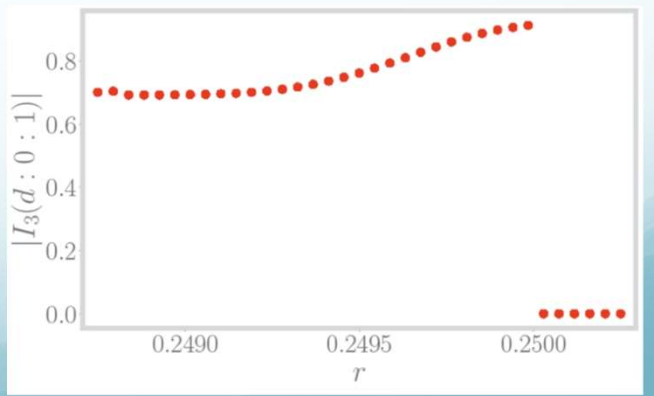


Weakening & Destruction of Kondo screening cloud

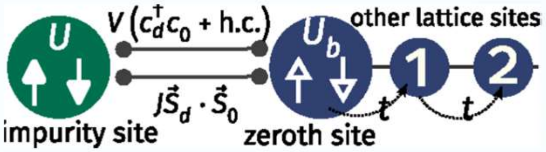


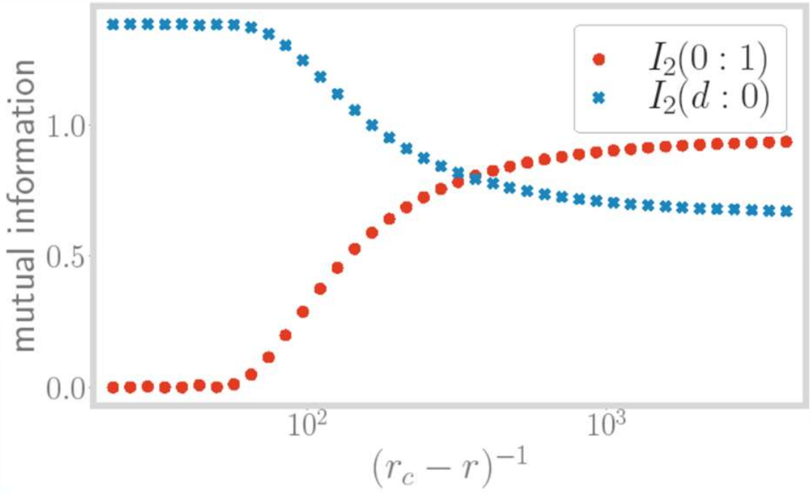
Non-monotonic variation of entanglement between impurity and bath first site

Increasing tripartite entanglement between impurity, bath zeroth & first site



Metallic phase of the extended SIAM: bi- and tri-partite entanglement





- Decreasing entanglement between impurity and bath zeroth sites
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Weakening & Destruction of Kondo screening cloud

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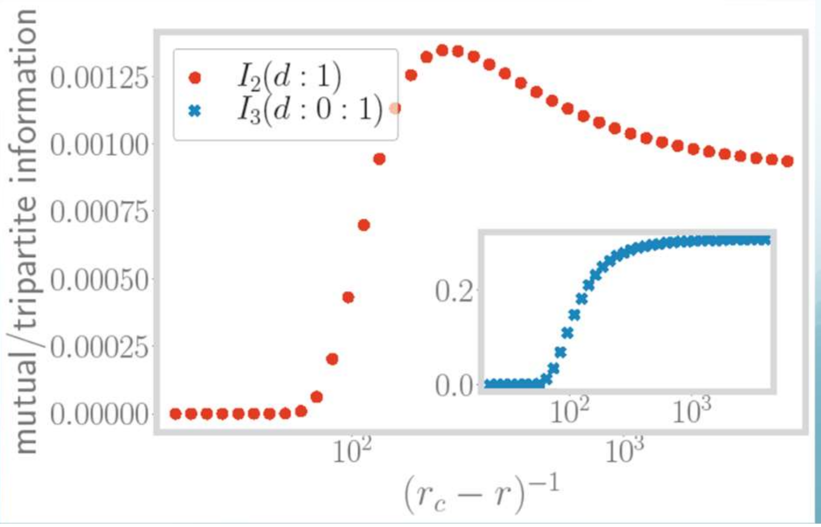
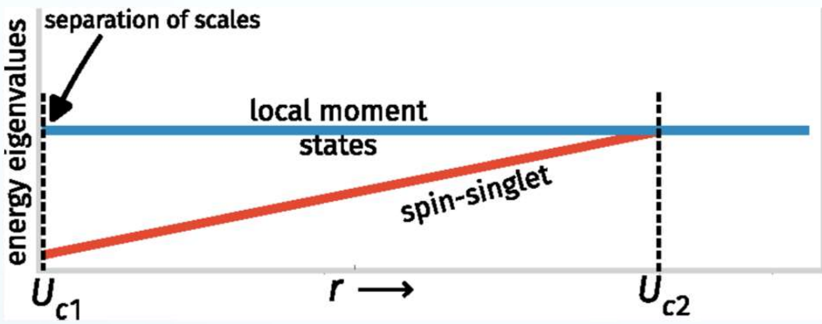
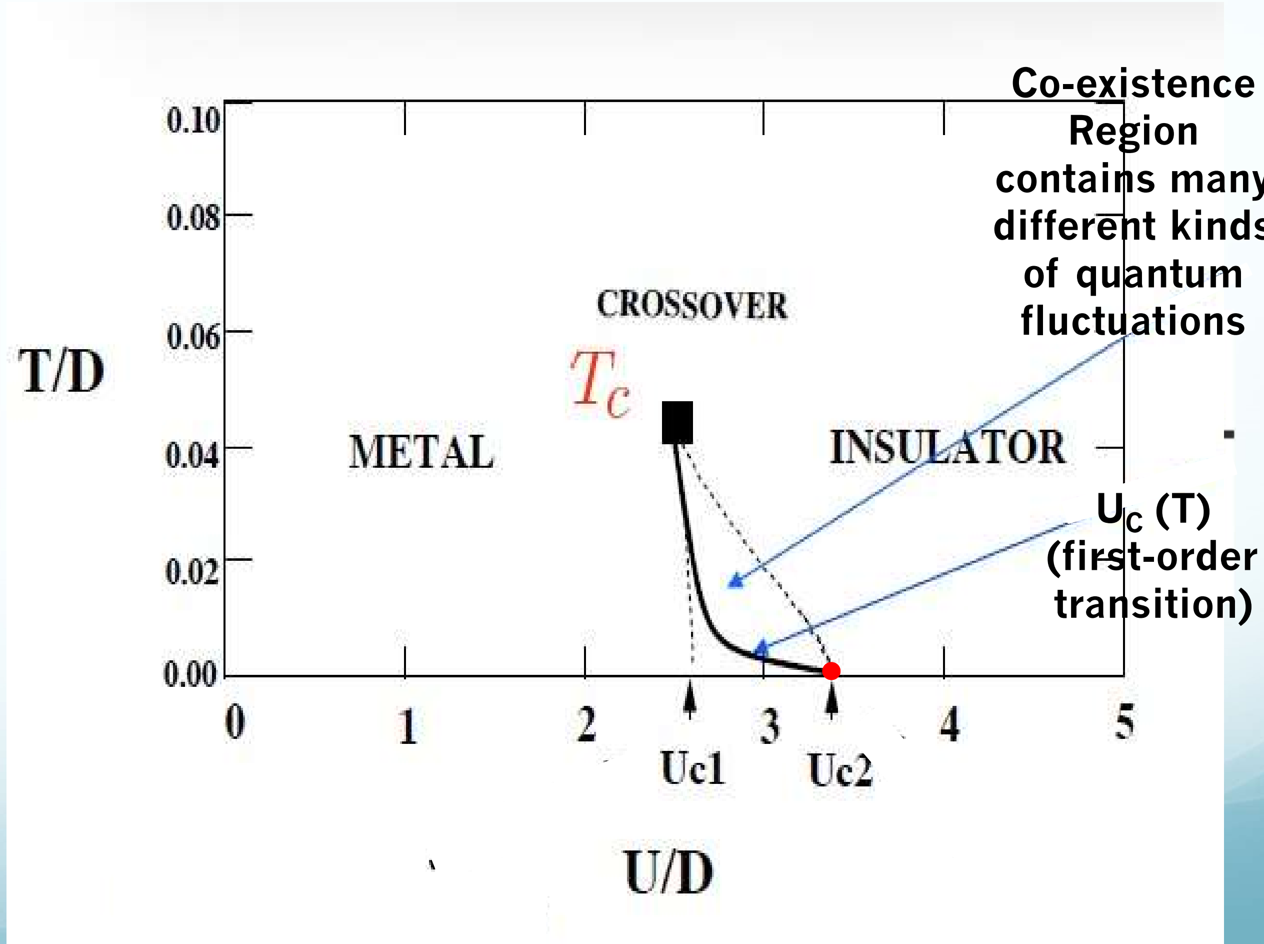


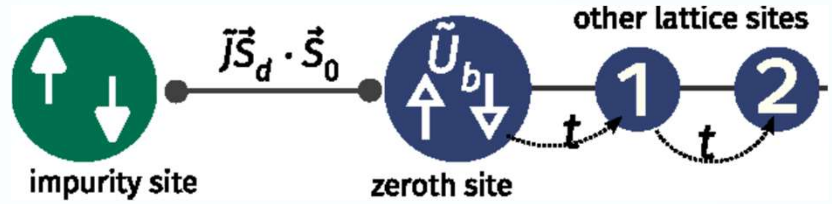
A closer look at the transition





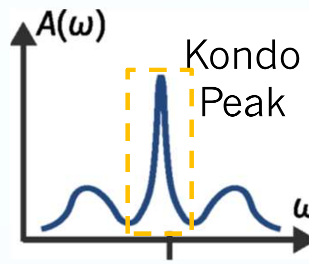
Minimal effective theory for MIT

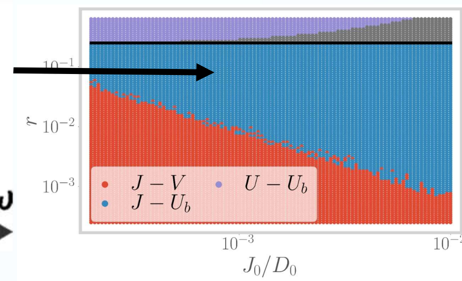
- Minimal effective theory for Kondo regime of effective SIAM is J-U_b model

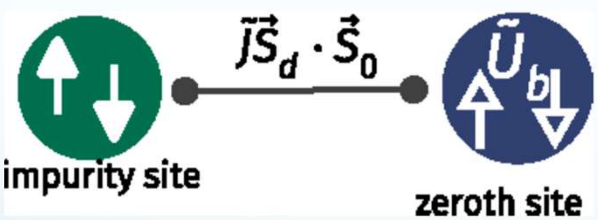


Eff. Ham^n $$H_{\rm eff} = J\vec{S}_d \cdot \vec{S}_0 - U_b\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2 + H_{\rm K.E.}$$

RG eq. $$\Delta J \sim J\left(J + 4U_b\right)$$

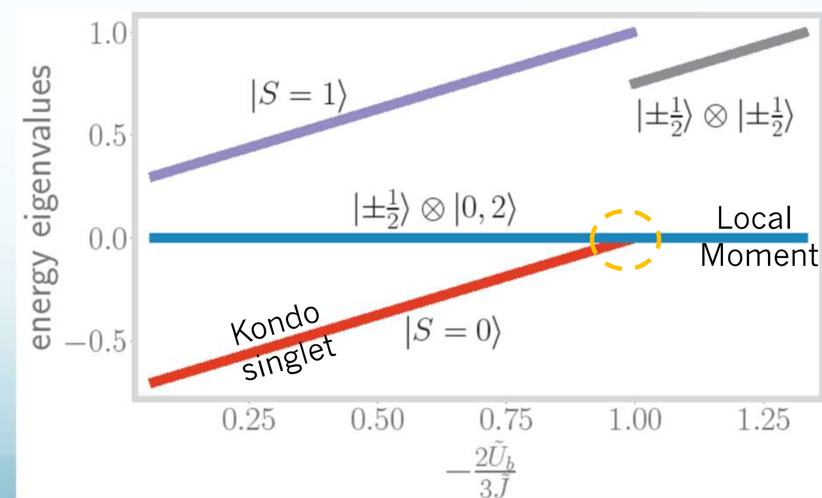






(Neglect excursion into rest of bath)

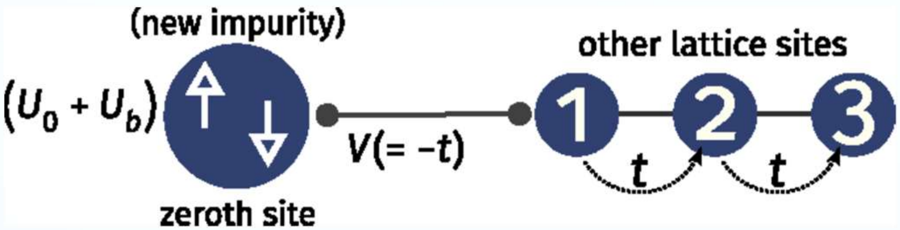
- 2-site J-U_b model obtained by taking zero bandwidth shows level crossing between unique Kondo singlet and doubly-degenerate local moment states

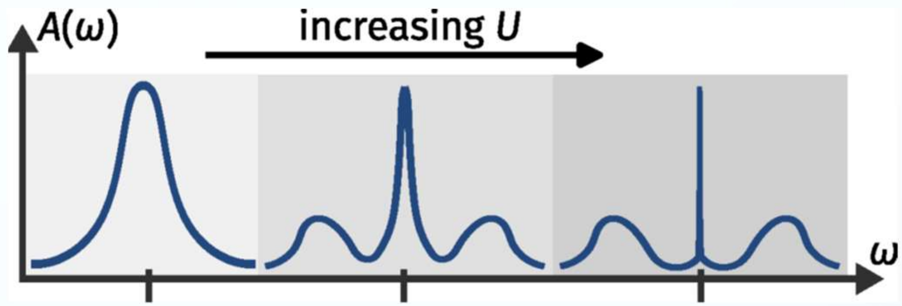


Self-consistency within the extended SIAM

(Moeller et al., PRL 1995)

- Self-consistency in DMFT: identical e-DOS at impurity and bath zeroth sites
- In the extended SIAM, we obtain the effective e-DOS on the bath zeroth site by integrating out the impurity site altogether.





- This generates additional repulsive interaction on the bath zeroth site, effective SIAM: $U_0 = J^*/4 - U_b >> 0$
- Spectral function of the bath zeroth site (the new "impurity") is that of the standard SIAM

- **Equivalence of spectral functions on impurity & bath zeroth sites achieved in metallic phase of extended SIAM.**

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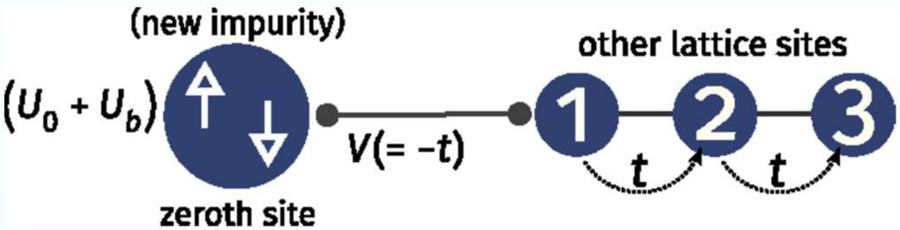

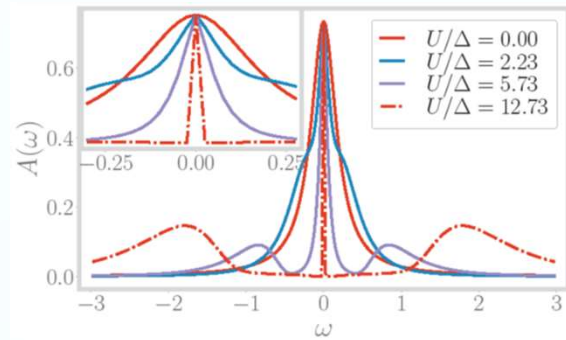

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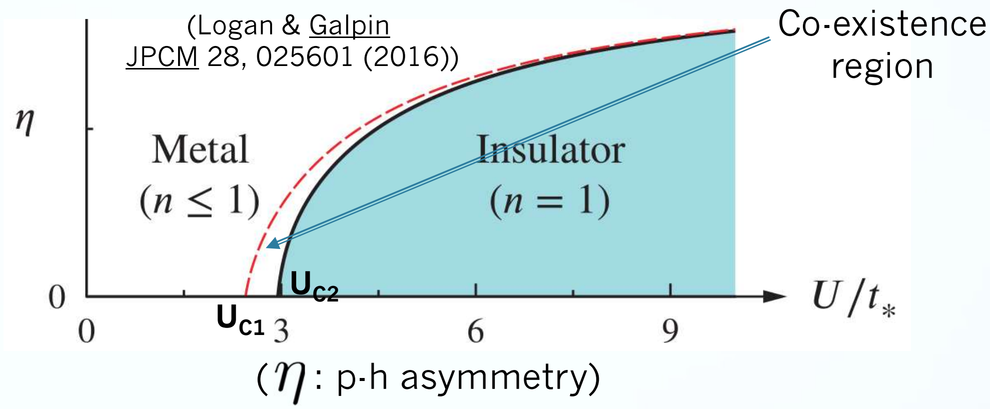
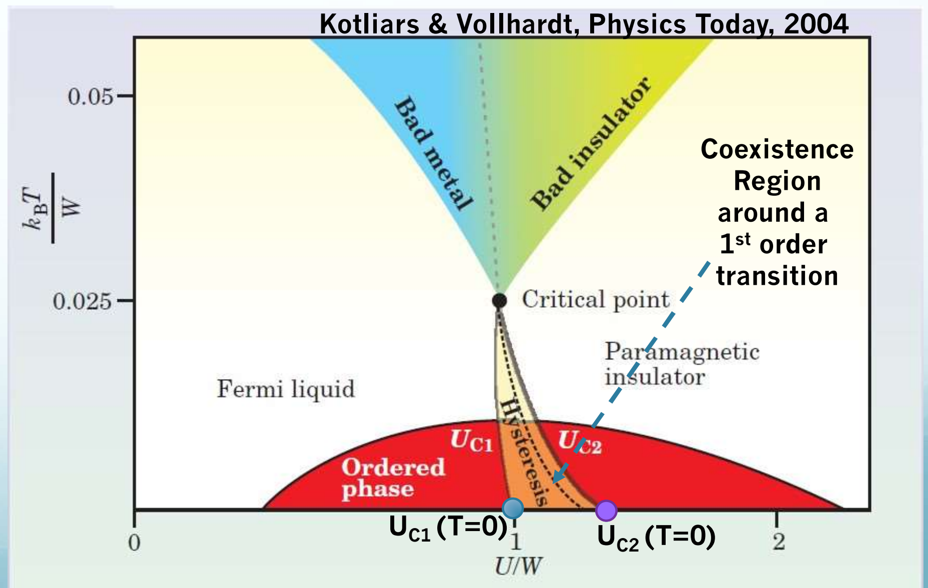
Co-existence of metal and insulating phases within the extended SIAM

- DMFT obtains a co-existence of metallic and insulating phases at T>0 in regime $U_{C1} < U < U_{C2}$
- Metallic solution is true ground state for all $U \le U_{C2}$ at T=0. MIT at $U = U_{C2}$.
- MIT: continuous sharpening of Kondo peak, Kondo scale $T_K \to 0$, Landau QP residue $Z \to 0$
- Gap appears discontinuously at $U = U_{C2}$.
- Insulating solution adiabatically continued upon lowering U from above U_{C2} till $U = U_{C1}$.





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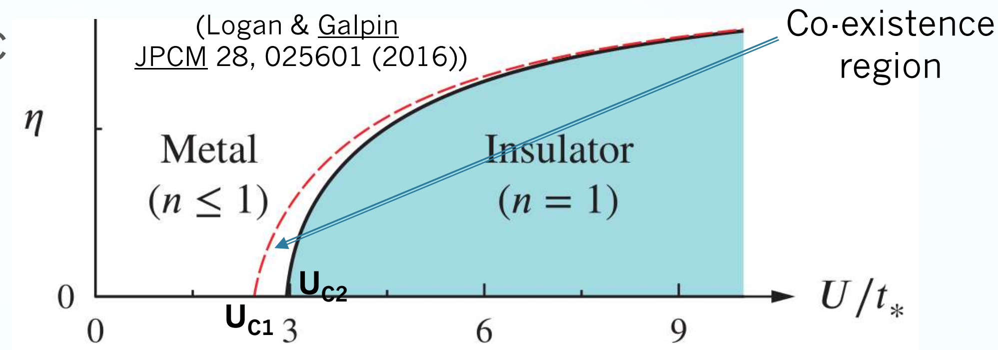
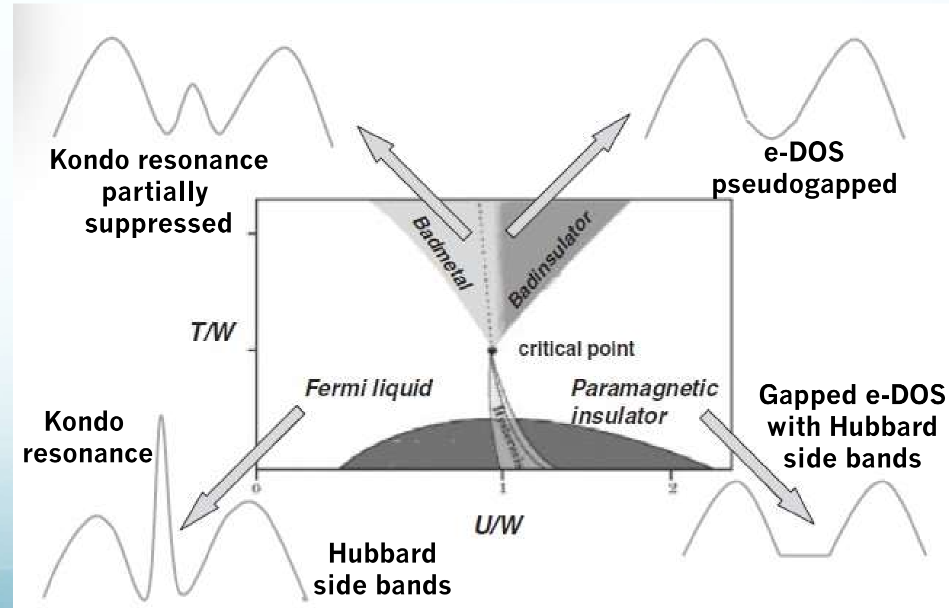
- Gap appears discontinuously at U = U_{C2} .
- Insulating solution adiabatically continued upon lowering U from above U_{C2}(T) till U = U_{C1}(T).



(η: p-h asymmetry)



Kotliars & Vollhardt, Physics Today, 2004

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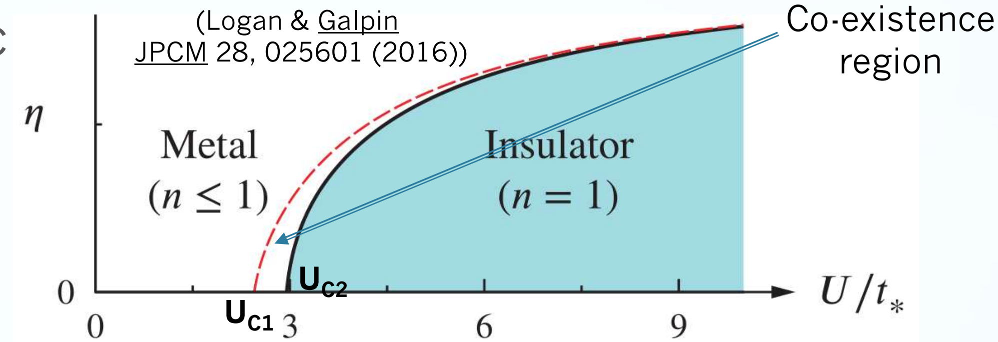

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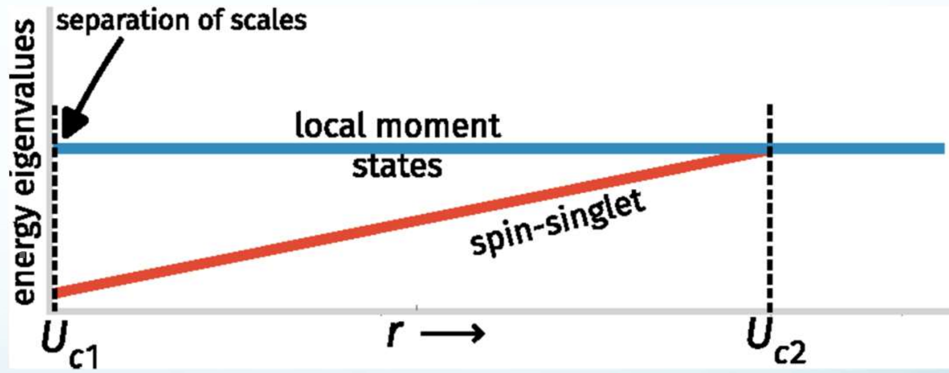

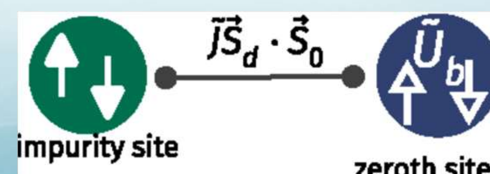

(Neglect excursion into rest of bath)

Co-existence of metal and insulating phases within the extended SIAM

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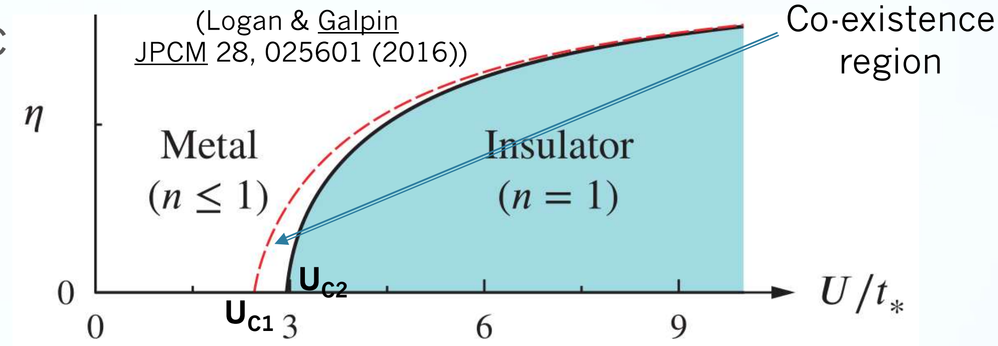

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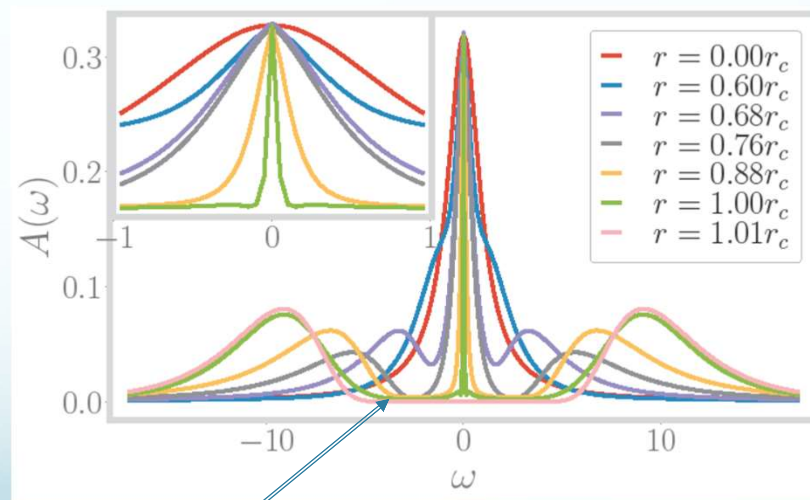
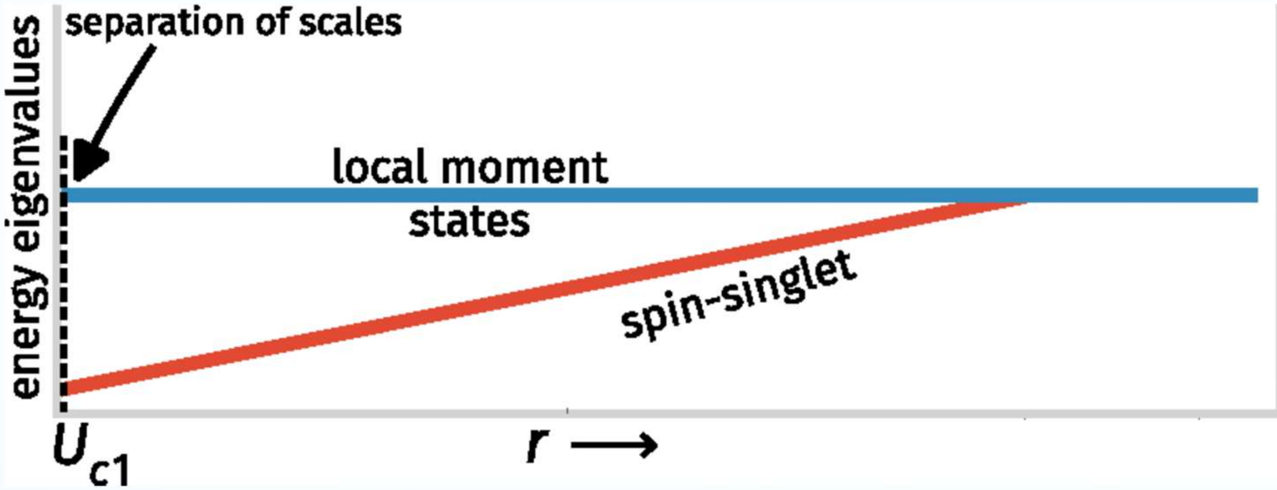
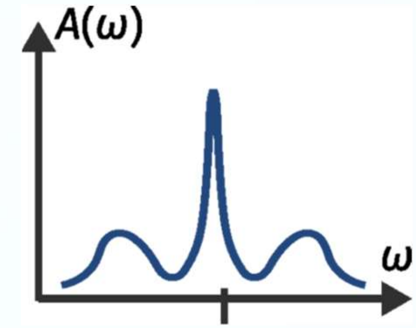
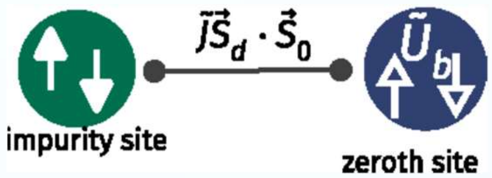


Sign of pre-formed/optical gap within metallic phase

Origin of Co-existence within extended SIAM: physics at U_{c1}

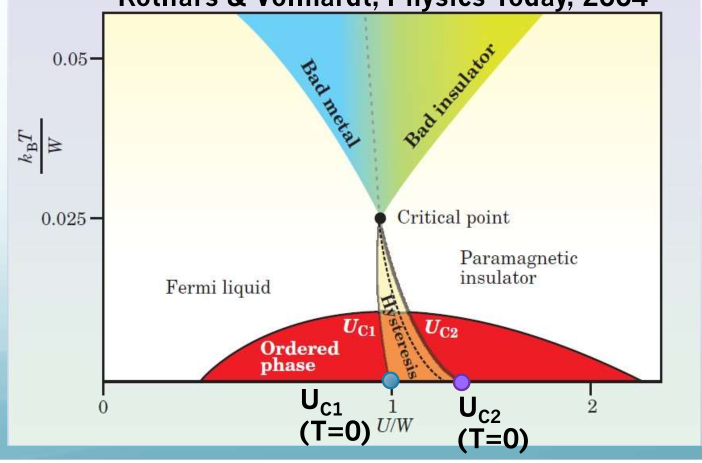




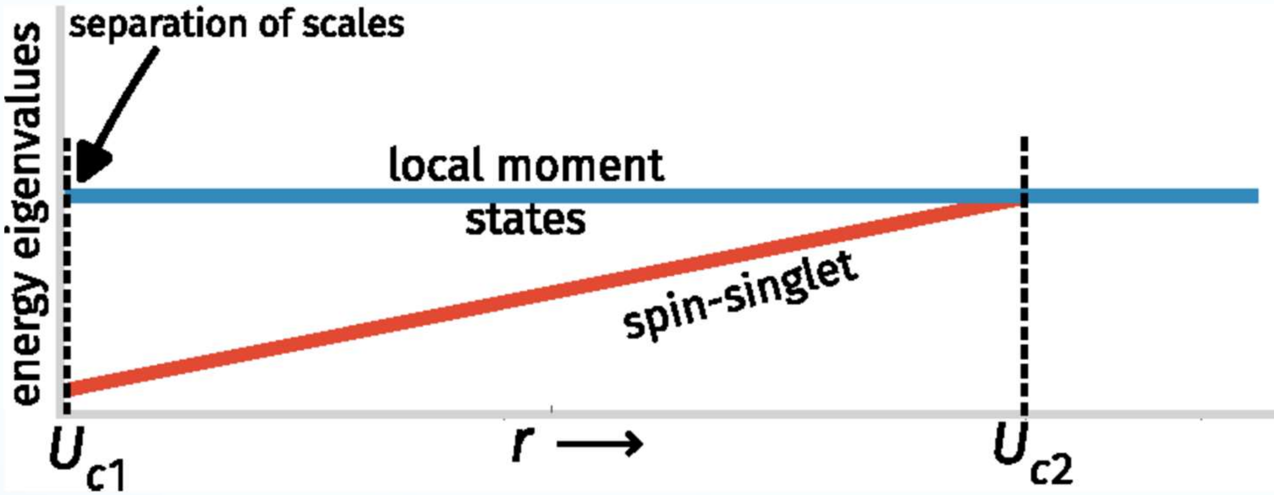


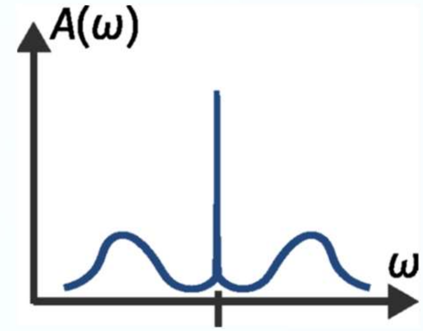
- U_{C1} is when the side peaks get separated from the sharp central Kondo resonance, i.e., appearance of near-zeroes in the impurity spectral function as RG irrelevant single-particle hybridization (V) vanishes
- Singlet ground state stabilized; local Fermi liquid with (local) Landau qp excitations

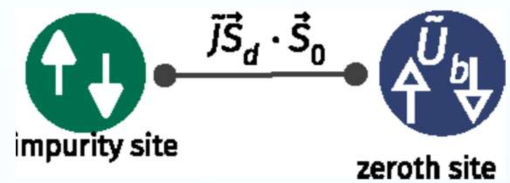
Kotliars & Vollhardt, Physics Today, 2004



Origin of Co-existence within extended SIAM: physics at U_{c2}

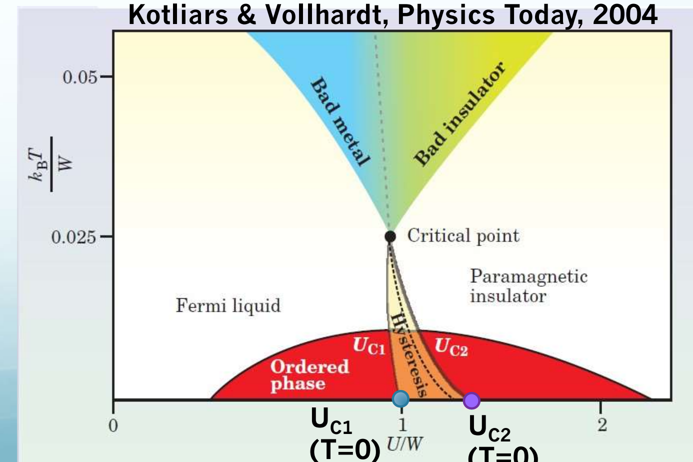




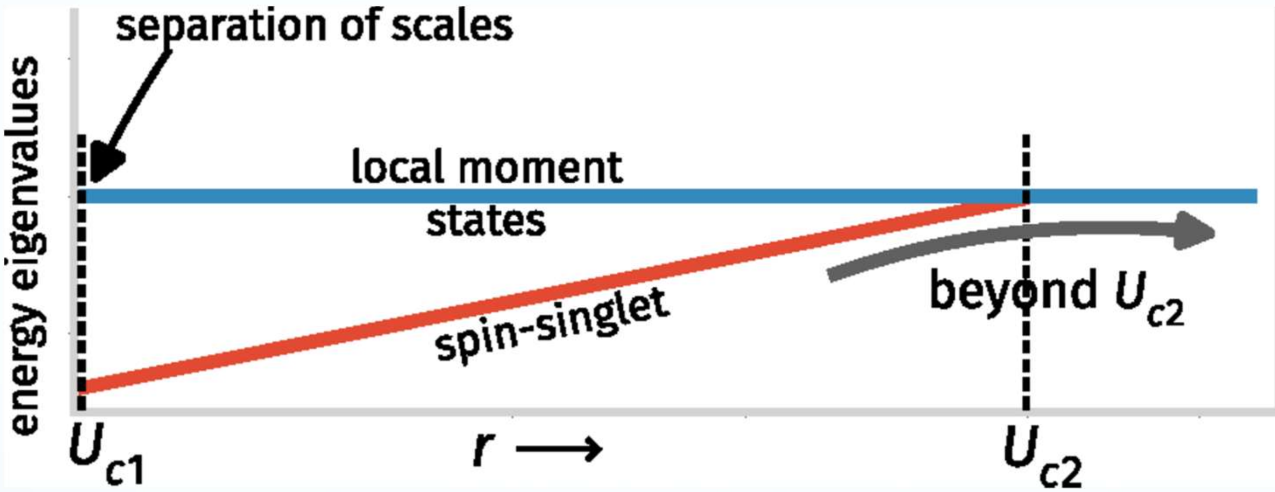


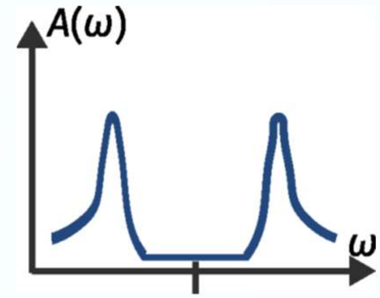
- U_{C2} is when the singlet ground state and the degenerate local moment excited states cross (MIT) ; Kondo peak extremely sharp; Kondo coupling J turns RG marginal
- Flattening of the near-zero regions of the impurity spectral function show pre-formed gap in the metallic phase

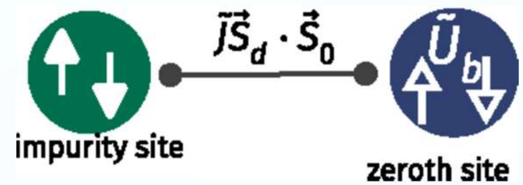
Kotliars & Vollhardt, Physics Today, 2004



Crossing the MIT: emergence of local moment ground states

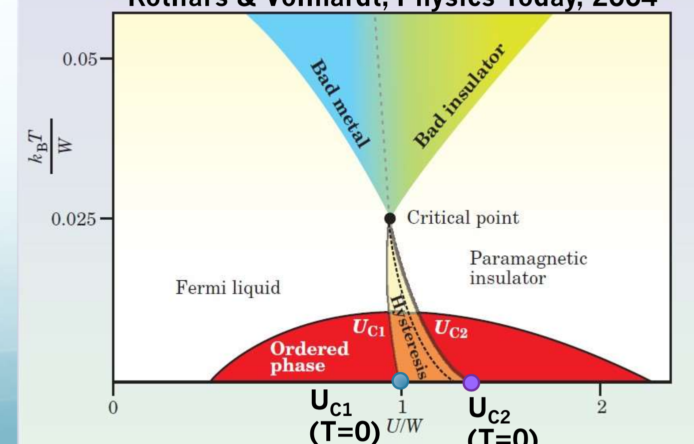






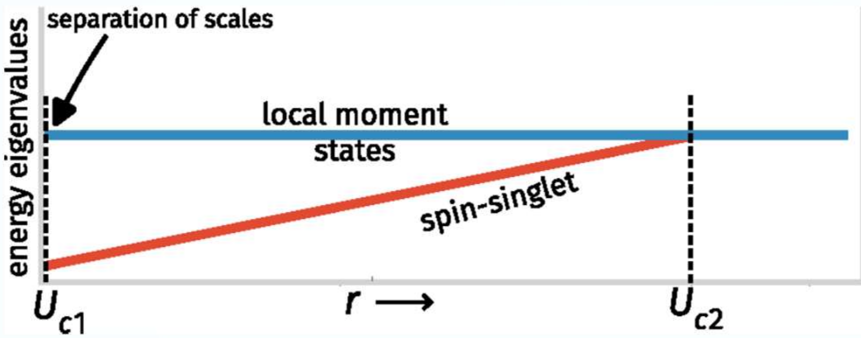
- $U > U_{C2}$: Kondo peak disappears suddenly; J turns RG irrelevant
- Sudden/ discontinuous appearance of spectral gap; local moment (paramagnetic) insulating phase; U turns RG relevant

Kotliars & Vollhardt, Physics Today, 2004

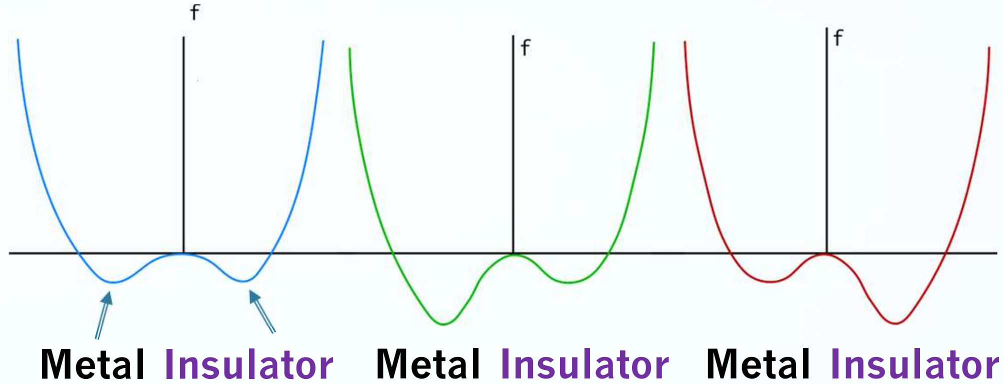


Why Co-existence of metal and insulating phases at T > 0 ?

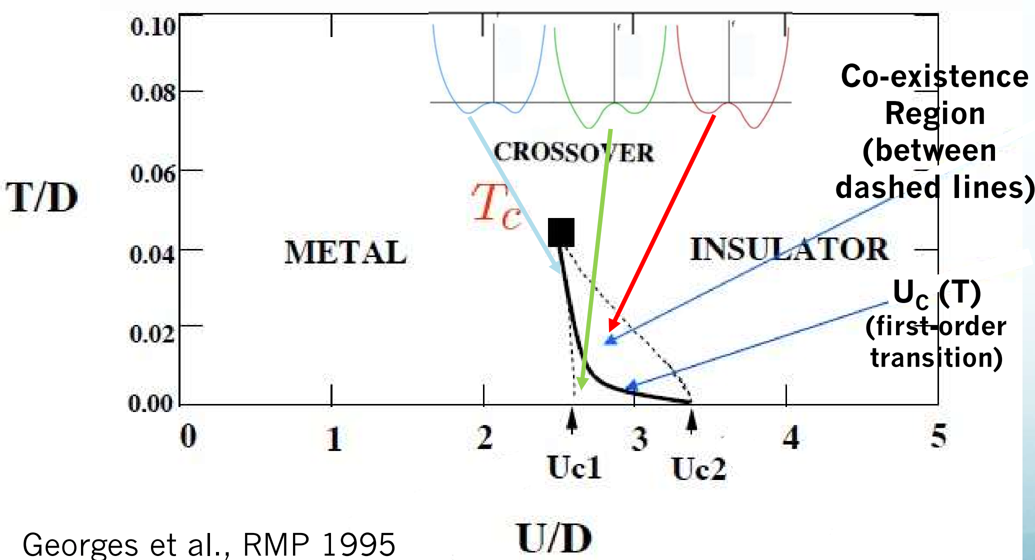
Quantum (T = 0) Energy Spectrum



Thermal Free Energy for T > 0



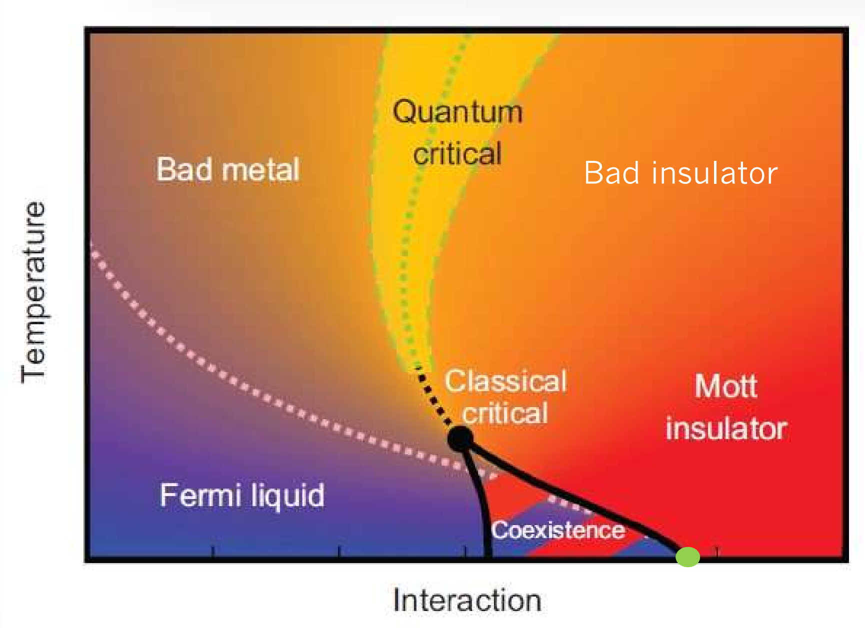
$U(T) = U_c(T)$	$U_{c1}(T) < U < U_c(T)$	$U_c(T) < U < U_{c2}(T)$
$F_{metal} = F_{insulator}$	$F_{metal} < F_{insulator}$	$F_{metal} > F_{insulator}$



Georges et al., RMP 1995

- **Free energy of Metallic State** $F_{metal} = E_{metal} - T\,S_{metal}$
- **Free energy of Insulating State** $F_{ins} = E_{ins} - T\,S_{ins}$
  $S_{ins} > 0$: degeneracy of local moment excited states
- $U_C(T=0) = U_{C2}(T=0)$: Only transition at T=0
- $U_{C1}(T_C) = U_{C2}(T_C)$: Finite-T critical point

A special finite temperature Critical Point



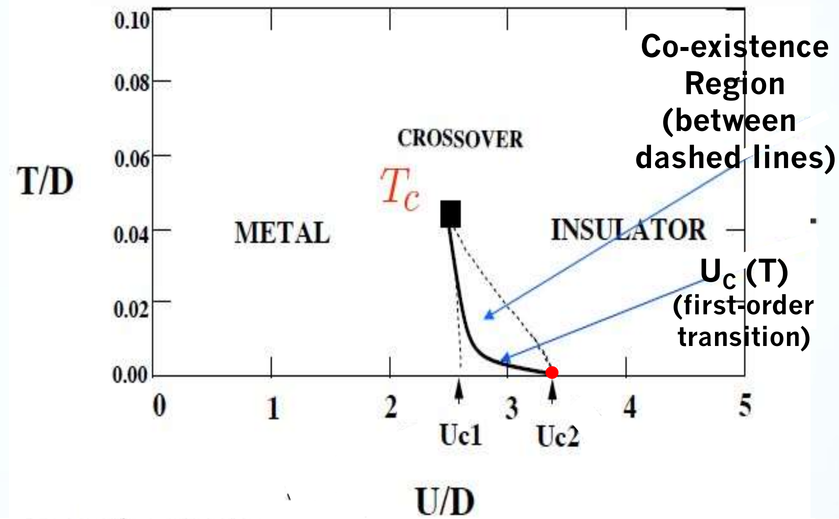
- Why are critical quantum fluctuations observed in the conical finite-T region above the (finite-T) critical point via CT-QMC simulations of the DMFT transition ? (Terletska et al, PRL 2011; Vucicevic et al, PRB 2013)
- Is there a quantum phase transition (QPT) at T=0 hidden beneath the co-existence region?

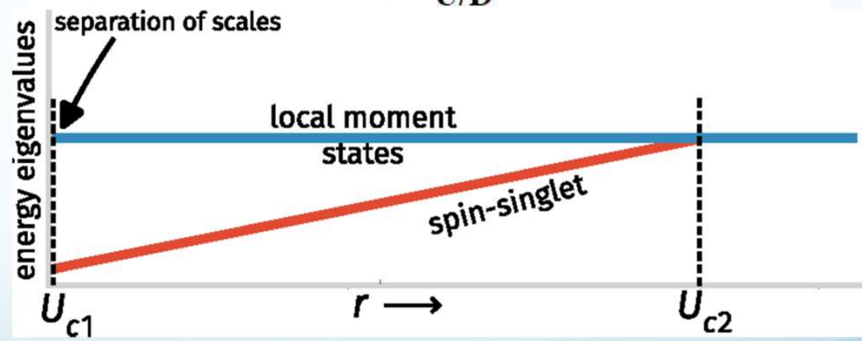
QCP at U_{c2}: MIT as breakdown of local Fermi liquid metallic phase

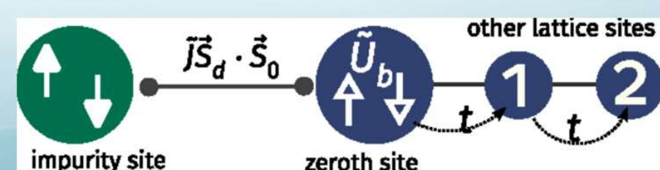
- The J-U_b obtains a local Fermi liquid for U < U_{C2} , with
  - qp residue $Z \propto T_K$ and
  - qp lifetime $\tau \sim \left(\frac{\omega}{T_K}\right)^{-2}$
- Breakdown of the local FL at MIT (U=U_{c2})

$$T_K \;,\; \tau \rightarrow 0 \text{ as } r \rightarrow 1/4$$
$$T_K \sim (1 - \frac{4U_b}{J})^{\alpha}, \alpha > 0$$

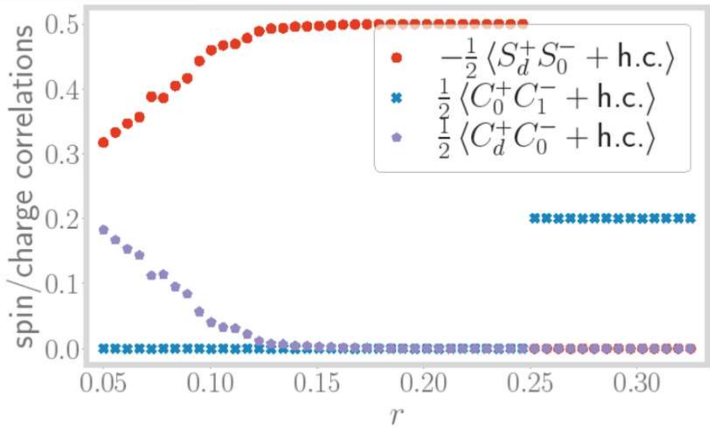
- **QCP** : Degeneracy of singlet and local moment states leads to new scattering processes for electron tunnelling onto zeroth site from first site. Involves coherent holon-doublon transfer between 0 and 1 sites: **non-Fermi Liquid behaviour at MIT**!



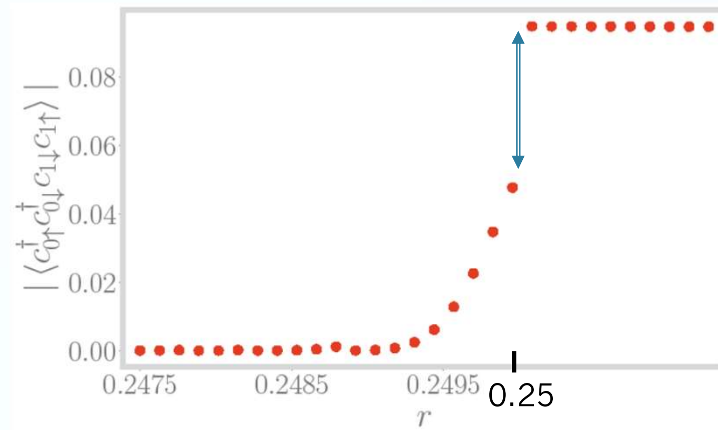


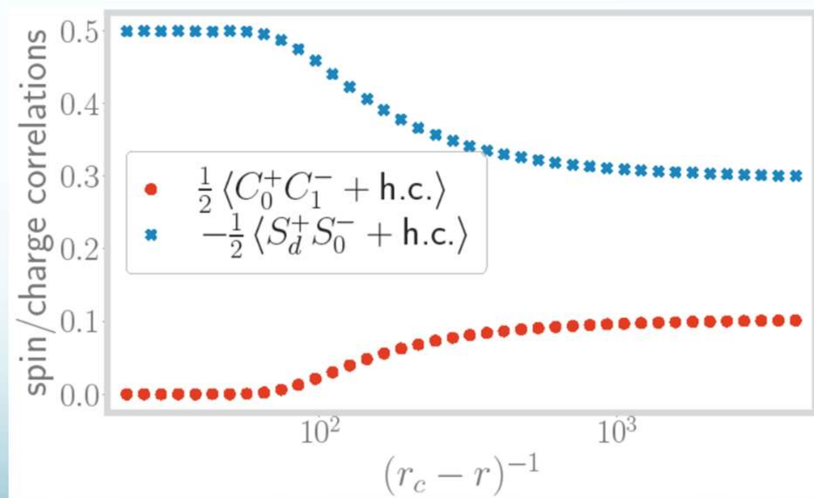


QCP at U_{c2}: MIT as breakdown of local Fermi liquid metallic phase

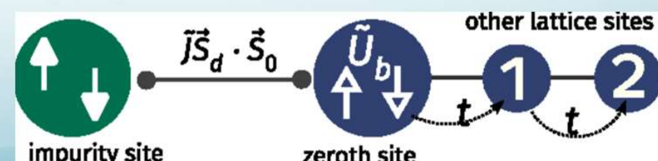


Fall in Kondo correlations between impurity and bath zeroth sites coincides with growth in pairing (holon-doublon) fluctuations between bath zeroth and first sites





Fall in Kondo correlations & growth in pairing (holon-doublon) fluctuations saturates as the MIT is approached. Shows that the MIT at $r=r_c=1/4$ is indeed abrupt.



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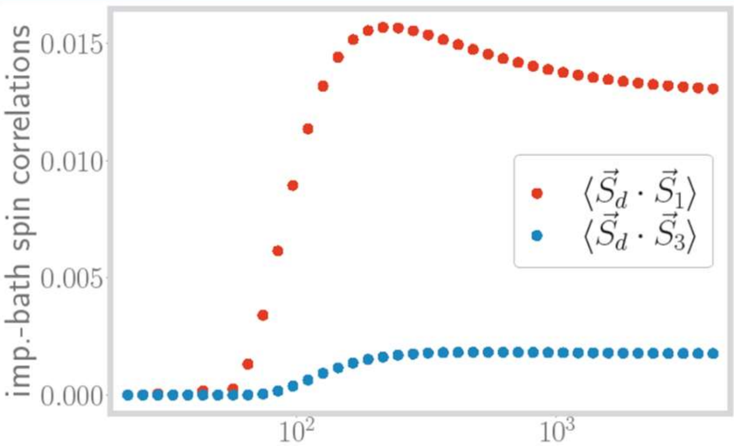
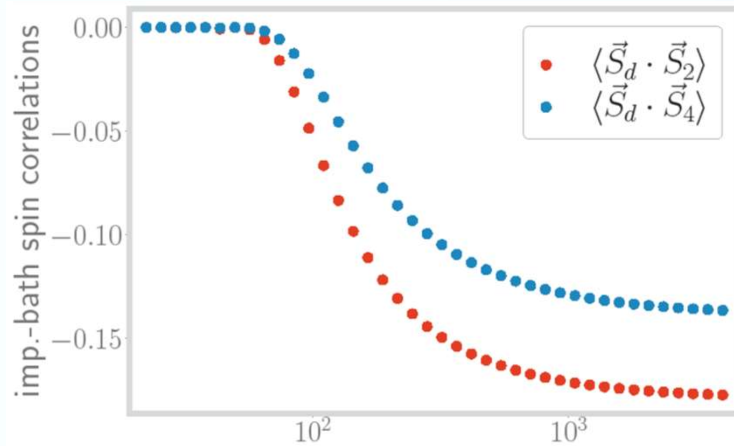
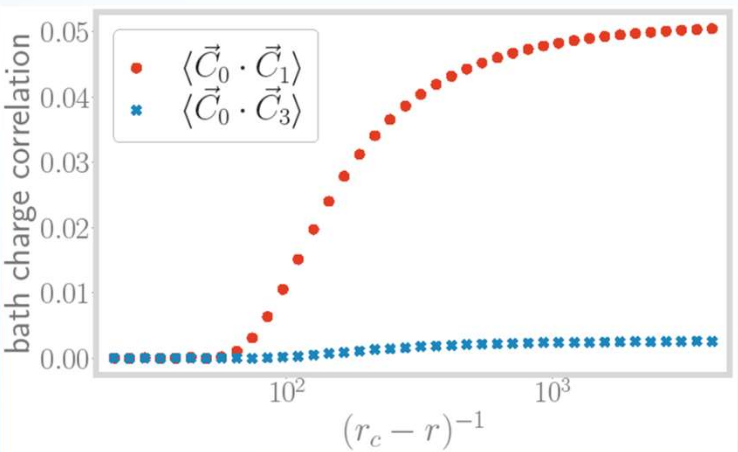


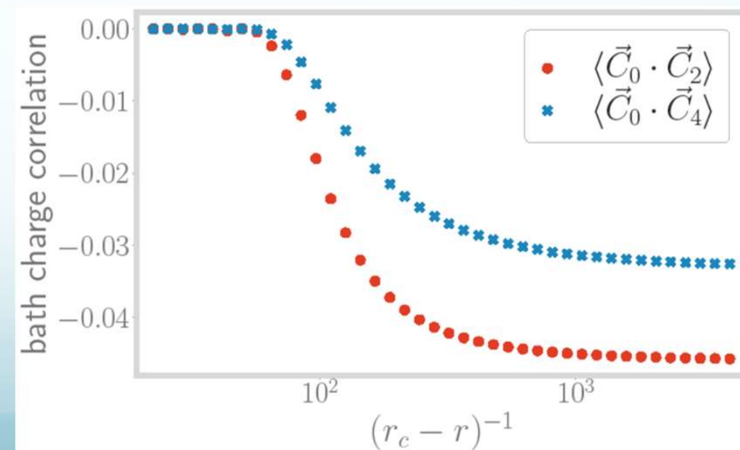
Fall in Kondo correlations between impurity and bath zeroth sites coincides with

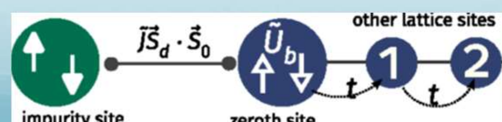
- growth in spin-spin correlations between impurity and further bath sites, and with alternation on odd & even sites,

- growth in pairing (holon-doublon) fluctuations between bath zeroth and further sites, and with opposite phases on odd & even sites

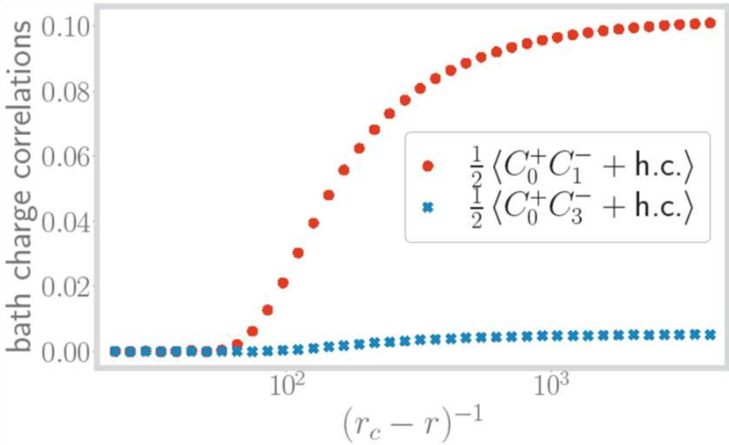


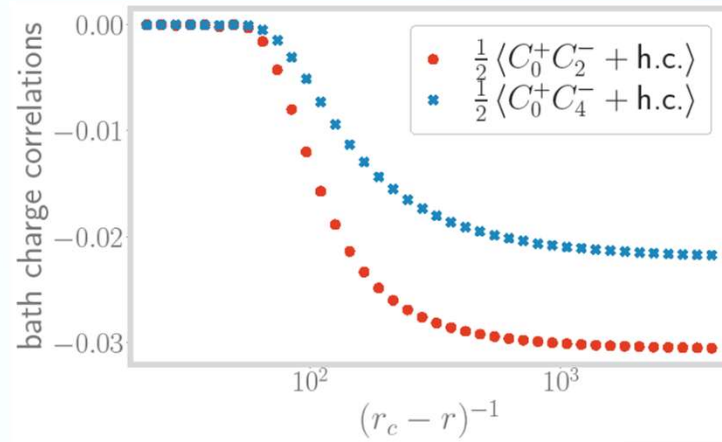






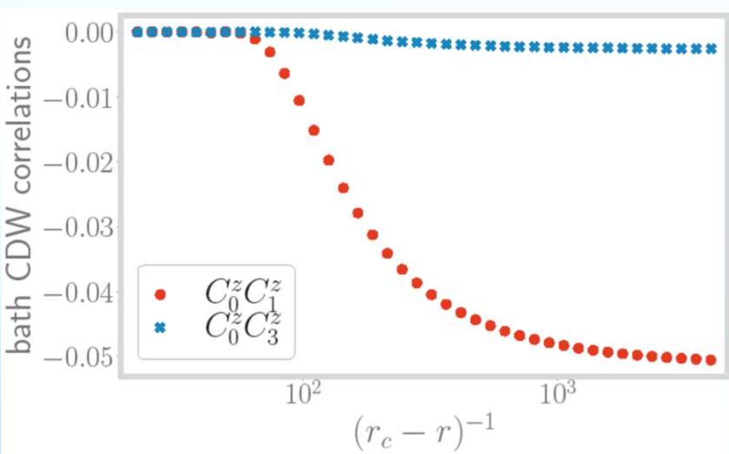
QCP at U_{c2}: MIT as breakdown of local Fermi liquid metallic phase

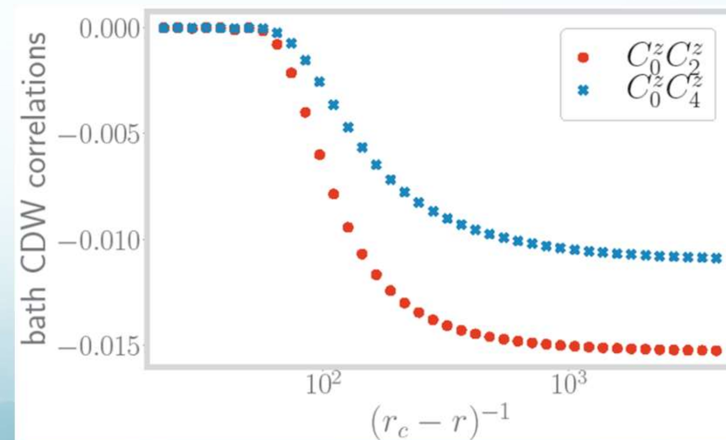


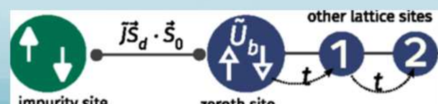


Fall in Kondo correlations between impurity and bath zeroth sites coincides with

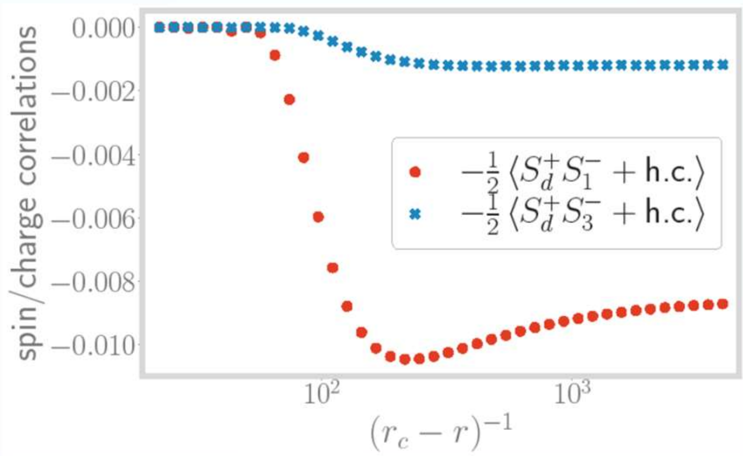
- growth in pairing (holon-doublon) fluctuations between bath zeroth and further sites, and with opposite phases on odd & even sites,
- similar growth observed in CDW correlations
- SU(2) symmetry observed in correlations





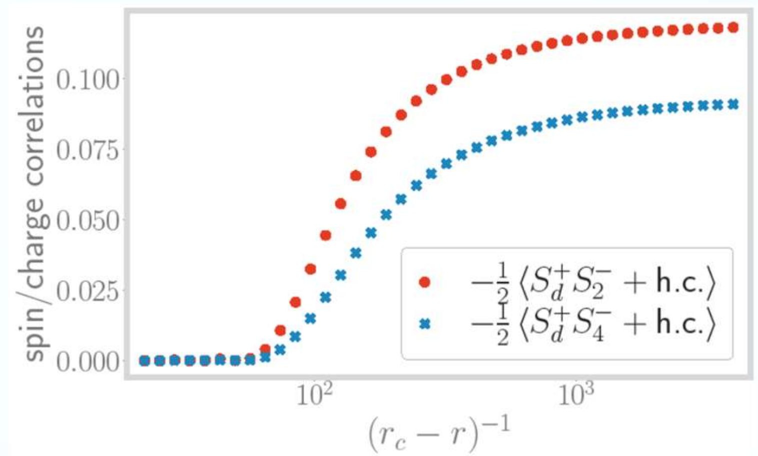


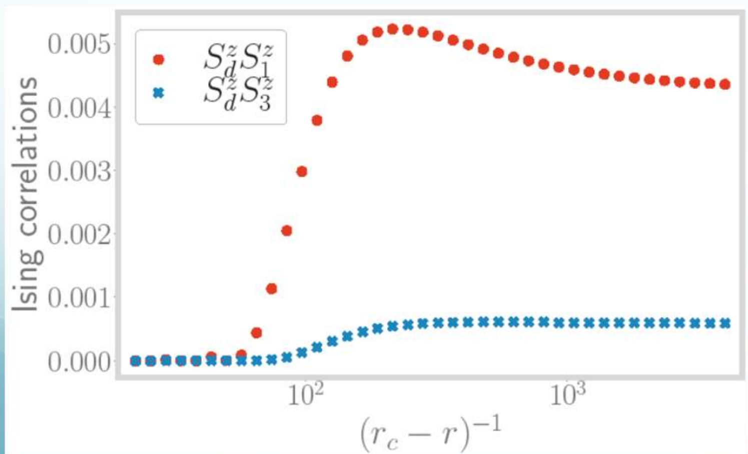
QCP at U_{c2}: MIT as breakdown of local Fermi liquid metallic phase

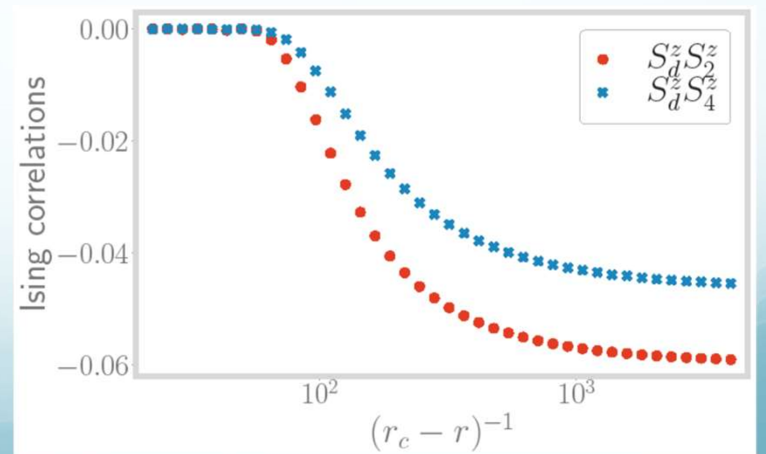


Fall in Kondo correlations between impurity and bath zeroth sites coincides with

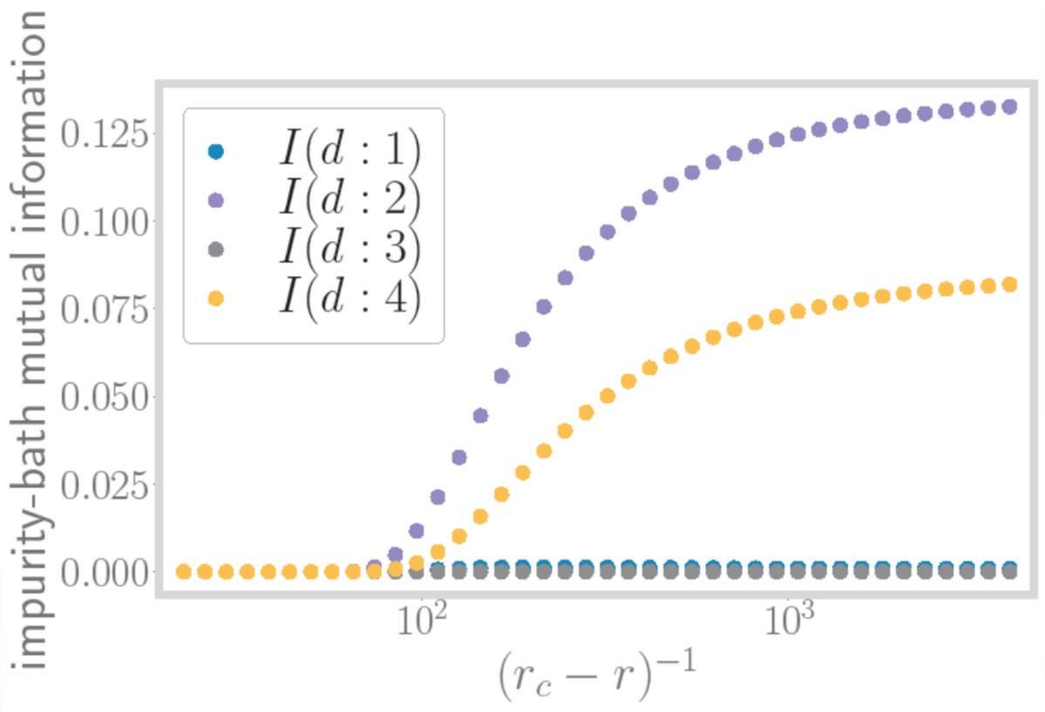
- growth in pairing spin-flip fluctuations between bath zeroth and further sites, and with opposite phases on odd & even sites,
- similar growth observed in SDW correlations
- SU(2) symmetry observed in correlations







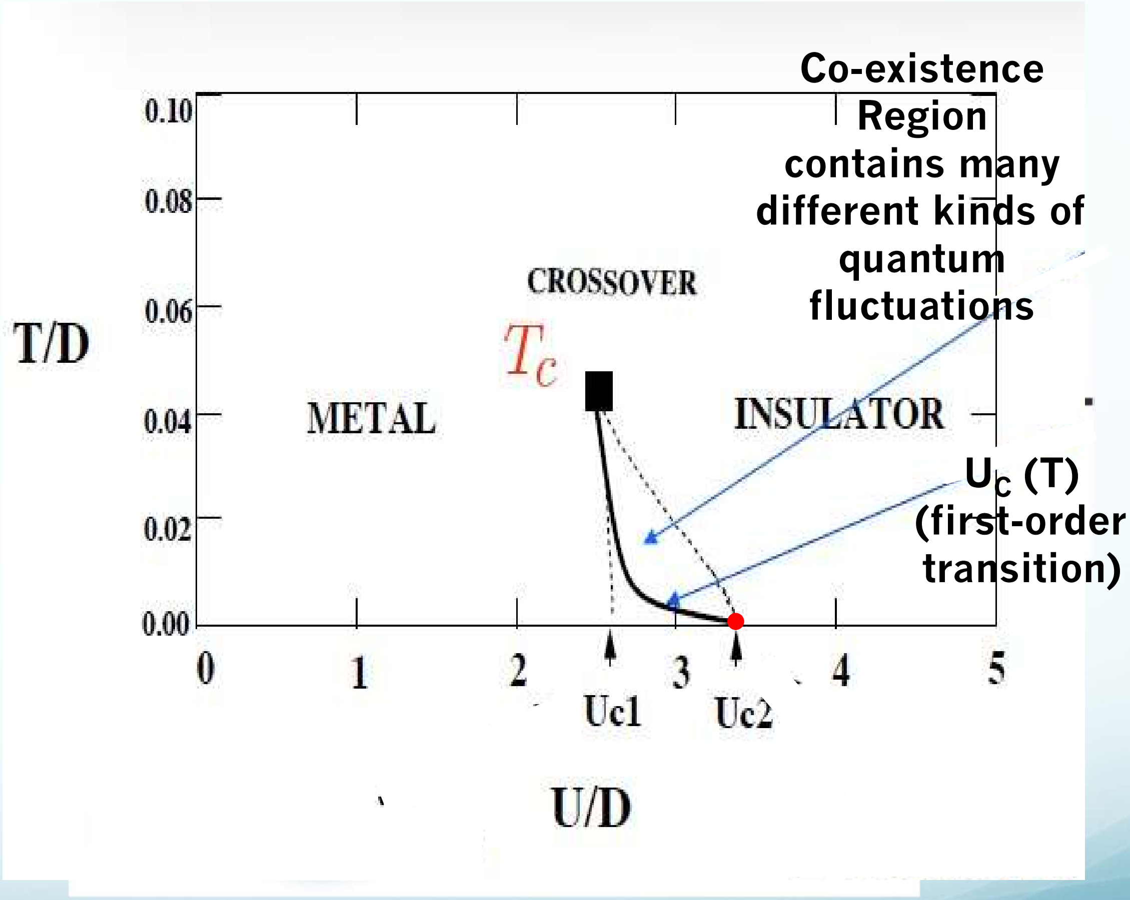
Spread of impurity-bath entanglement near the MIT

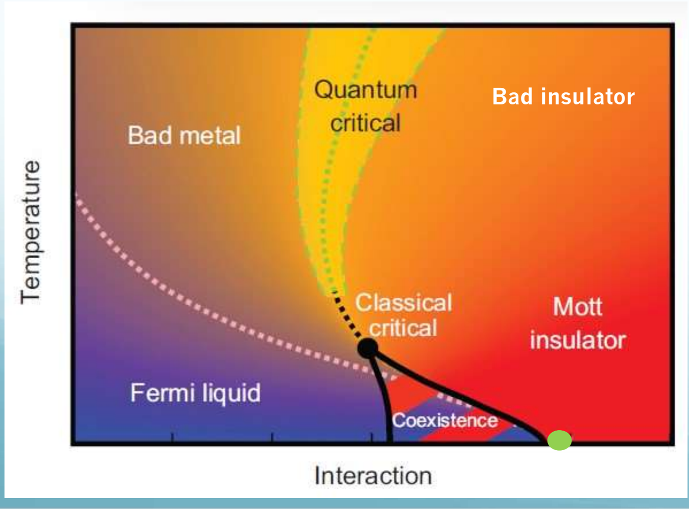


- Very close to the MIT (on the metallic side), the mutual information measure shows growth in quantum entanglement between the impurity (d) and other bath sites beyond the zeroth site.

QCP at U_{c2}: MIT as breakdown of local Fermi liquid metallic phase

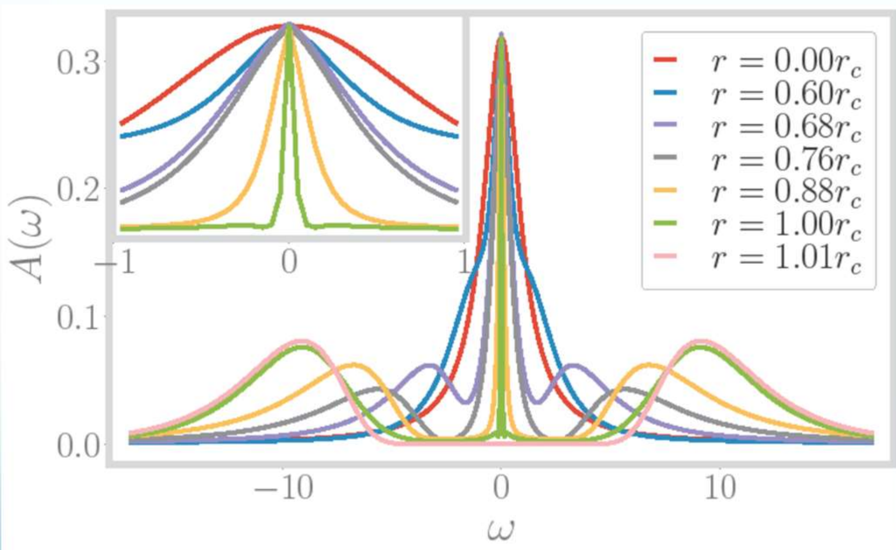
- Critical quantum fluctuations in spin & holon-doublon sectors should be visible in co-existence region for T>0.
- However, may be feeble, easier to sense in the region above T_C
- Observed in some organics (Furukawa, Nat. Phys., 2015)

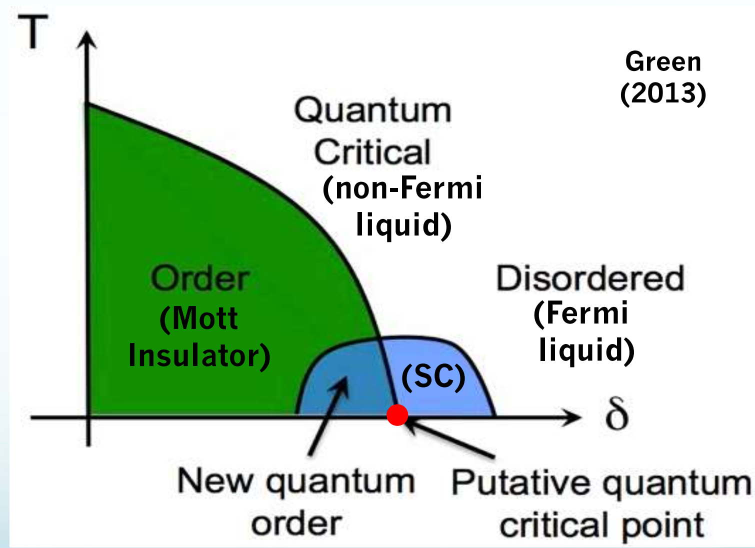




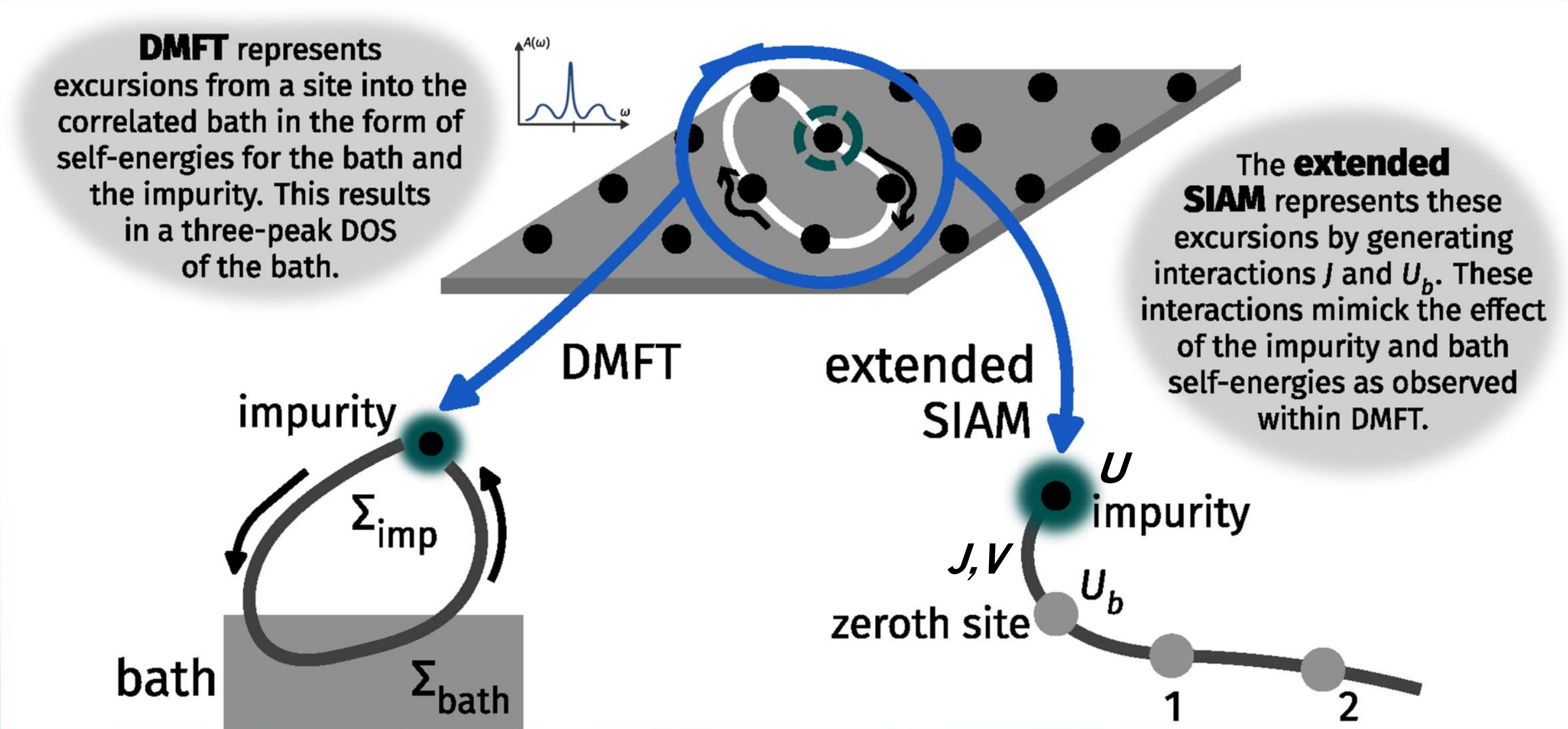
(Terletska et al, PRL 2011; Vucicevic et al, PRB 2013)

Conclusions & Outlook





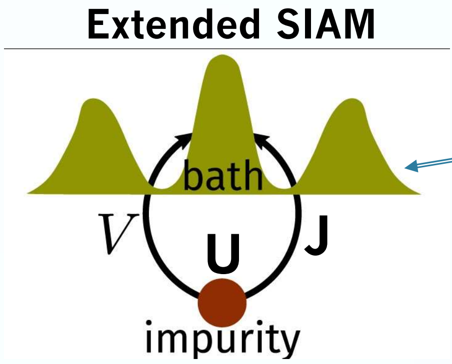
Mott MIT & DMFT : Our approach

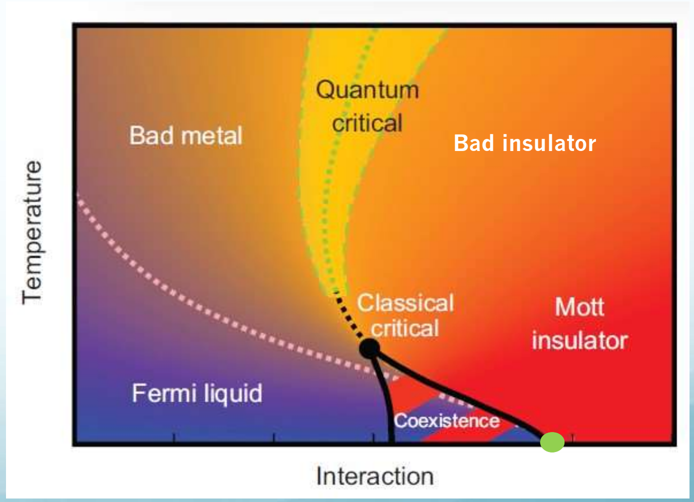


Conclusions

- Extended SIAM captures phenomenology of Mott MIT observed in DMFT for Bethe lattice.
- Key ingredient: competition of
  (i) Kondo screening physics of impurity (J), &
  (ii) local attractive correlations (U_b) in bath.
- Enhancement of local holon-doublon (pairing) fluctuations in bath destroys Kondo cloud.
- Provides explanation for coexistence of Mott insulating and metallic phases at T>0.
- Mott criticality involves a NFL with long-ranged spin-exchange and holon-doblon fluctuations in the conduction bath.

➤ Local moment Mott Insulating phase appears at a continuous transition.

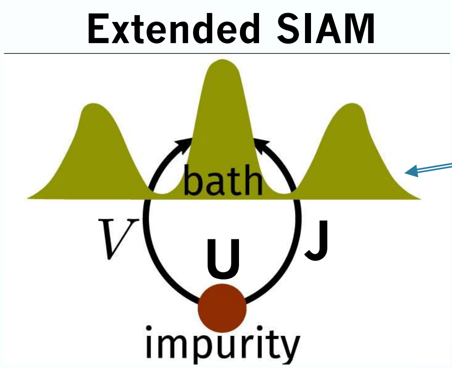


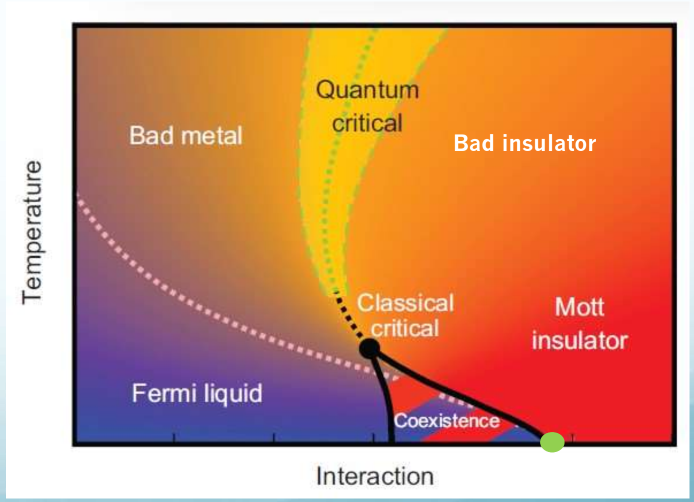


(Terletska et al, PRL 2011; Vucicevic et al, PRB 2013)

Conclusions

- Coexistence arises from a clear separation of energy scales, namely
  - U_{c1} : emergence of (doubly degenerate) local moment states in low-energy spectrum by turning single-particle hybridization (V) RG irrelevant; appearance of the metastable insulating solution.
  - Leads to formation of a "pre-formed" gap in the impurity spectral function of the J-U_b effective Kondo impurity model.
  - Corresponds to abrupt Mott-Hubbard transition where the metastable insulating solution turns unstable, and the gap closes.





(Terletska et al, PRL 2011; Vucicevic et al, PRB 2013)

Conclusions

- Coexistence arises from a clear separation of energy scales, namely

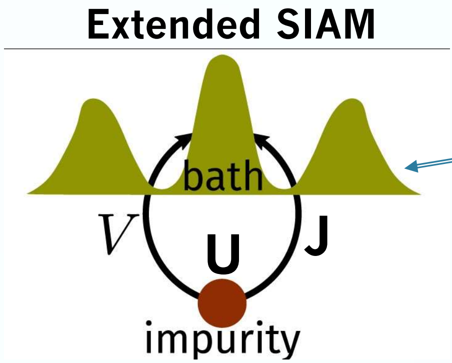
➢ U_{c2} : raising of the singlet ground state energy till it becomes degenerate with the (doubly degenerate) local moment states.

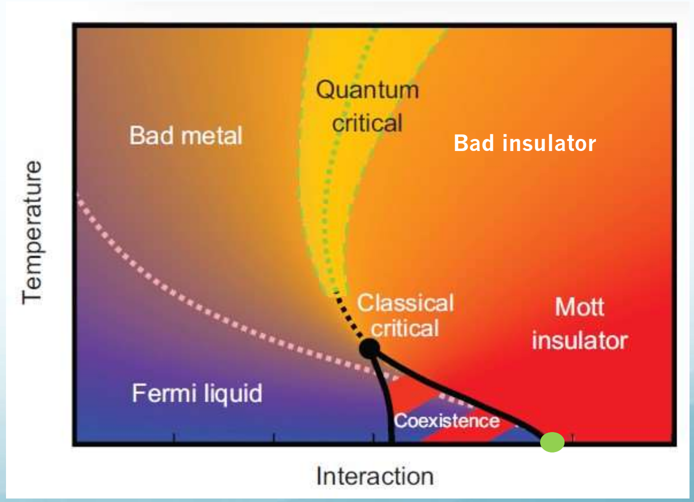
➢ Leads to weakening & destruction of the Kondo screening (spin-flip exchange scattering) of the impurity by the bath zeroth site. RG irrelevance of J

➢ Leads to increase in long-range spin correlations between impurity and other conduction bath sites, and holon-doublon correlations between bath zeroth and other bath sites.

➢ Leads to breakdown of the local Fermi liquid metal, and its replacement by a non-Fermi liquid.

➢ Corresponds to Brinkman-Rice continuous transition where the Landau quasiparticle residue (essentially the Kondo screening energy scale) vanishes, and the metallic ground state is rendered unstable towards the local moment insulating ground states.





(Terletska et al, PRL 2011; Vucicevic et al, PRB 2013)

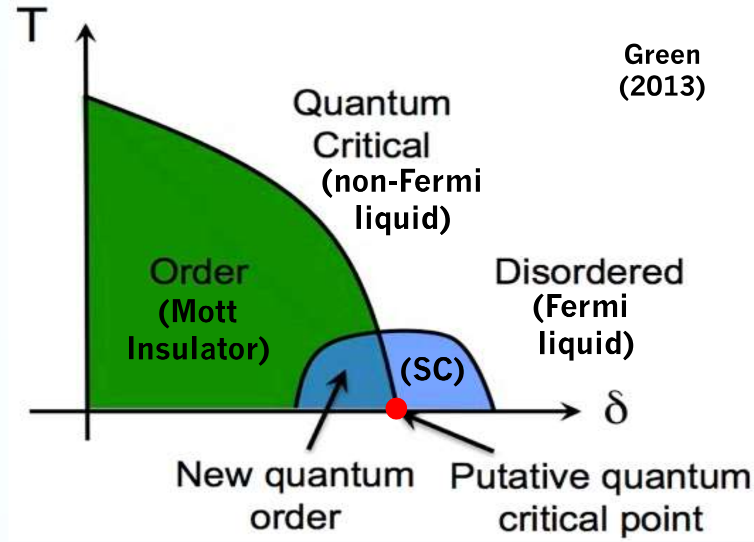
Outlook

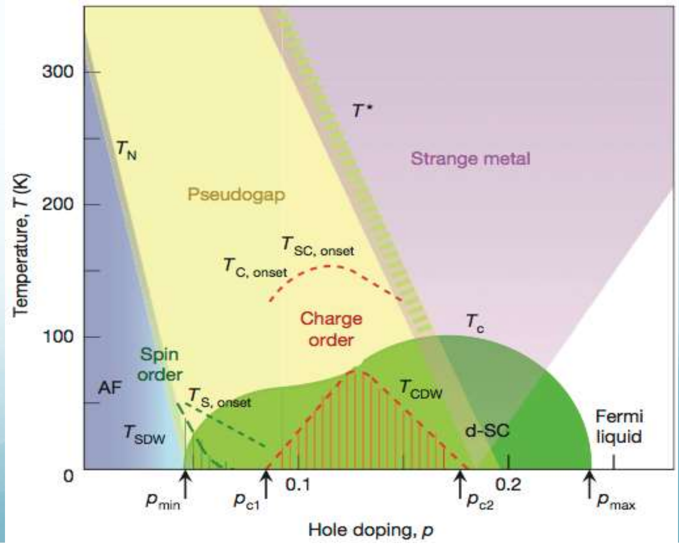
- Is this a generic mechanism for MIT leading to/away from Mott insulators?

- Can doping away from ½-filling lead to
  - a true QCP at which the NFL is revealed?
  - condensation of the enhanced pairing fluctuations (in neighbourhood of MIT) into a superconducting phase?

- Could a coexistence region (of insulator and metal) with critical quantum fluctuations of various kinds in it be an indication of the pseudogap phenomena observed in the cuprates?

- Suggestion of intimate connection within the (seemingly complex?) arrangement of phases in such phase diagrams?






EPQM
Thanks!

The Unitary Renormalisation group method

The General Idea

- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple states lying at high energy / high momenta
- Obtain sequence of Hamiltonians and hence extract scaling equations for couplings

$$H_j \;\xrightarrow{\;U_j\;}\; H_{j-1}$$

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

The Unitary Renormalization Group Method

Select a UV-IR Scheme

UV shell $\vec{k}_N$ (zeroth RG step)

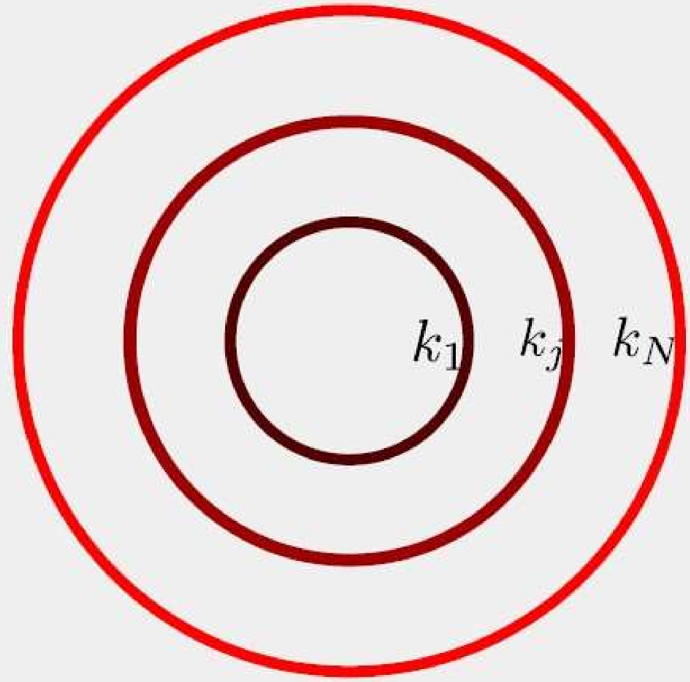
$\vdots$

$\vec{k}_j$ $\left(j^{\text{th}}\text{ RG step}\right)$

$\vdots$

IR shell $\vec{k}_1$ (Fermi surface)

Implemented for finite but large systems. Size can be increased systematically for conclusions in thermodynamic limit.



Isotropic dispersion $\epsilon(k) = \frac{\hbar^2 k^2}{2m}$ assumed for conduction electrons in the Kondo problem.

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

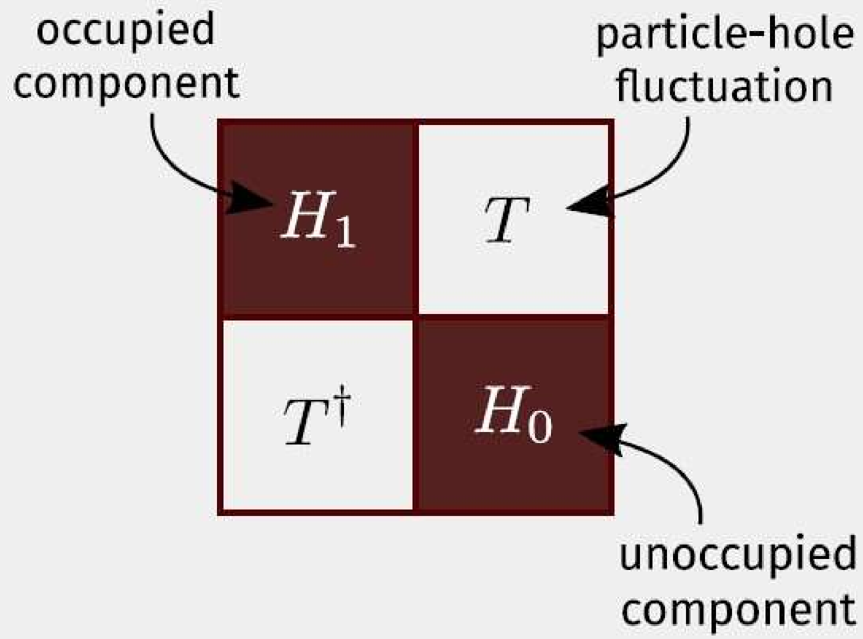
Write Hamiltonian in single electron Fock basis (n_j) of $\left\{\vec{k}_j, \sigma\right\}$

$$n_j = c^\dagger_{k_j,\sigma} c_{k_j,\sigma}$$

$$H_{(j)} = H_1 \hat{n}_j + H_0 \left(1 - \hat{n}_j\right) + c_j^\dagger T + T^\dagger c_j$$

$$2^{j-1}\text{-dim.} \longrightarrow \begin{cases} H_1, H_0 \longrightarrow \text{diagonal parts} \\ T \longrightarrow \text{off-diagonal part} \end{cases}$$

(j) : j^{th} RG step



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

The Unitary Renormalization Group Method

Rotate Hamiltonian such that off-diagonal blocks vanish

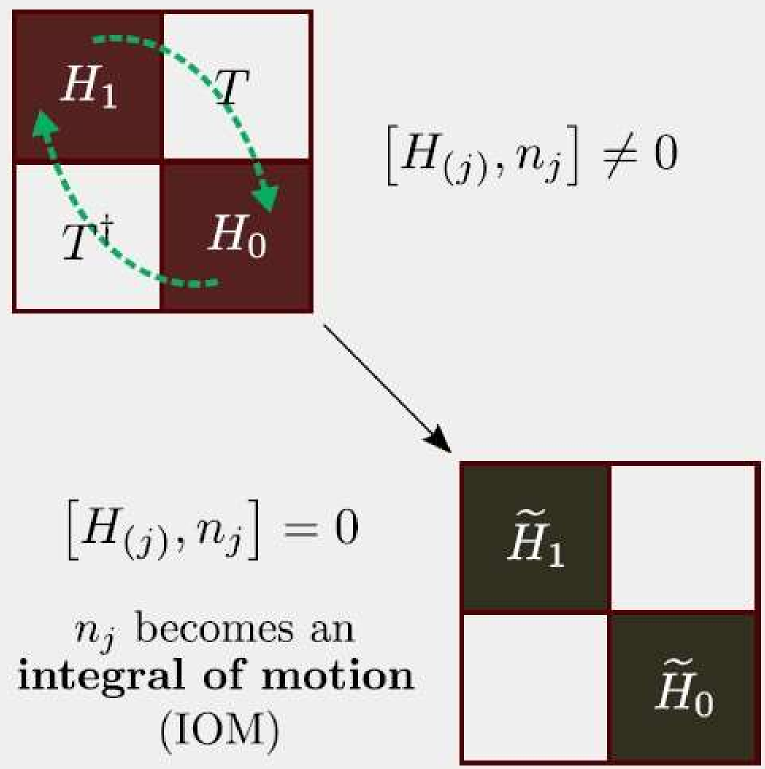
$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

$$U_{(j)} = \frac{1}{\sqrt{2}}\left(1 - \eta_{(j)} + \eta^{\dagger}_{(j)}\right)$$

$$\left.\eta^{\dagger}_{(j)} = \frac{1}{\hat{\omega}_{(j)} - H_D} c^{\dagger}_j T \right\} \rightarrow \text{many-particle rotation}$$

H_D : Diagonal part of H (contains single-particle dispersion and self-energies) ; $\hat{\omega}_{(j)}$ tracks energyscale of quantum fluctuations being resolved

$$\left\{\eta_{(j)}, \eta^{\dagger}_{(j)}\right\} = 1$$

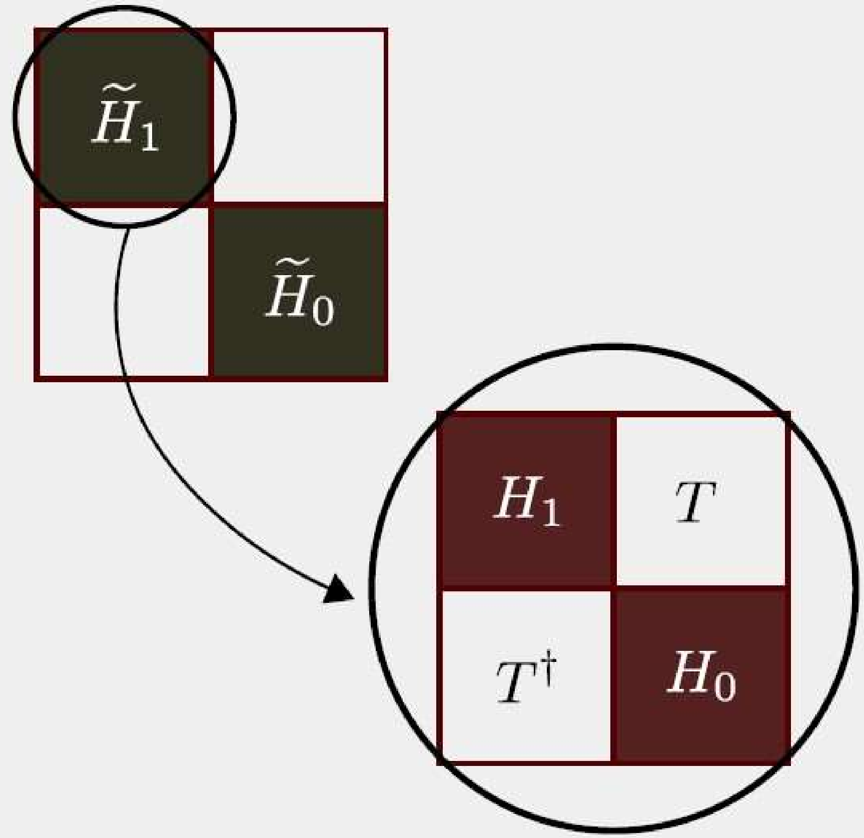


Repeat with renormalised Hamiltonian

$$H_{(j-1)} = \widetilde{H}_1\hat{n}_j + \widetilde{H}_0\left(1 - \hat{n}_j\right)$$

$$\widetilde{H}_1 = H_1\hat{n}_{j-1} + H_0\left(1 - \hat{n}_{j-1}\right) + c^\dagger_{j-1}T + T^\dagger c_{j-1}$$

The new Hamiltonian obtained can also have quantum fluctuations within it.



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

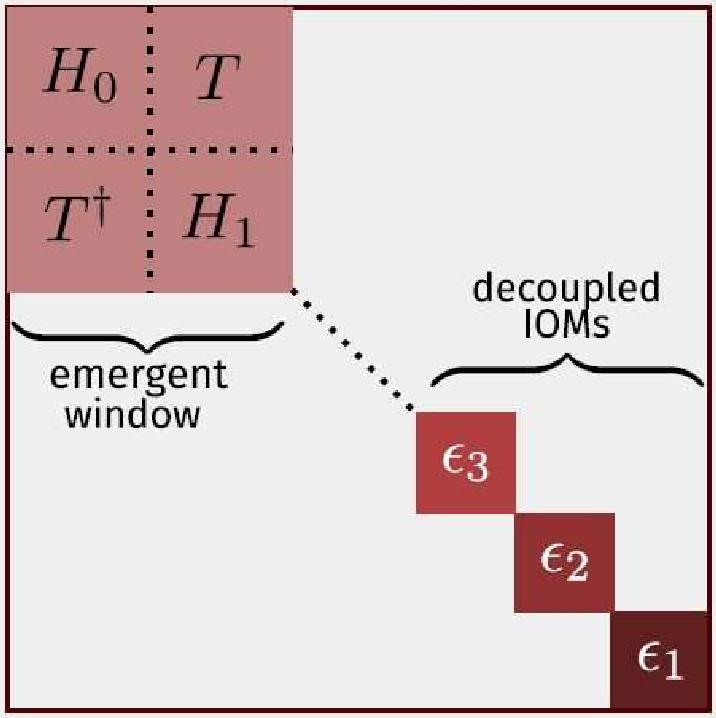
RG Equations and Stable Fixed Point

$$\Delta H_{(j)} = \left(\hat{n}_j - \frac{1}{2}\right)\left\{c_j^\dagger T, \eta_{(j)}\right\}$$

$$\eta_{(j)}^\dagger = (\hat{\omega}_{(j)} - H_D)^{-1} c_j^\dagger T$$

Fixed point: $\hat{\omega}_{(j*)} - (H_D)^* = 0$

Stopping point reached as no further rotations can be made. ω **attains an eigenvalue of** H**.**

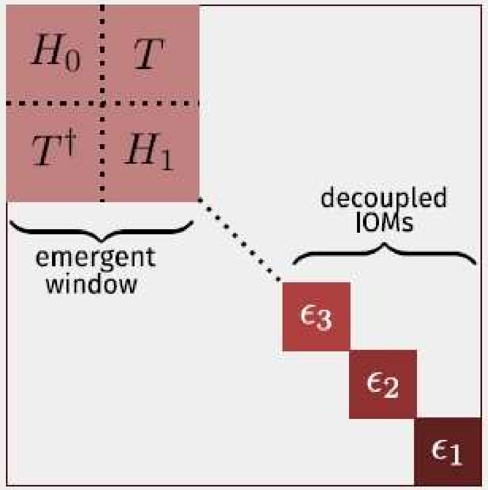


Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

THE UNITARY RENORMALIZATION GROUP METHOD

Novel Features of the Method

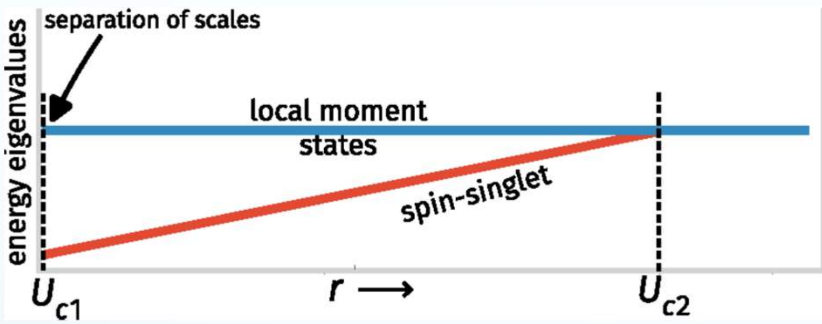
- $T = 0$ **method : Quantum fluctuation scale** $\hat{\omega}$ tracks all orders of renormalisation
- Finite-valued fixed points for finite systems - leads to **emergent degrees of freedom**
- **Spectrum-preserving** unitary transformations - partition function does not change, sum rules satisfied
- Tractable low-energy effective Hamiltonians - allow **renormalised perturbation theory** around them; studying the **entanglement content** of the ground state wavefunction is also possible sometimes

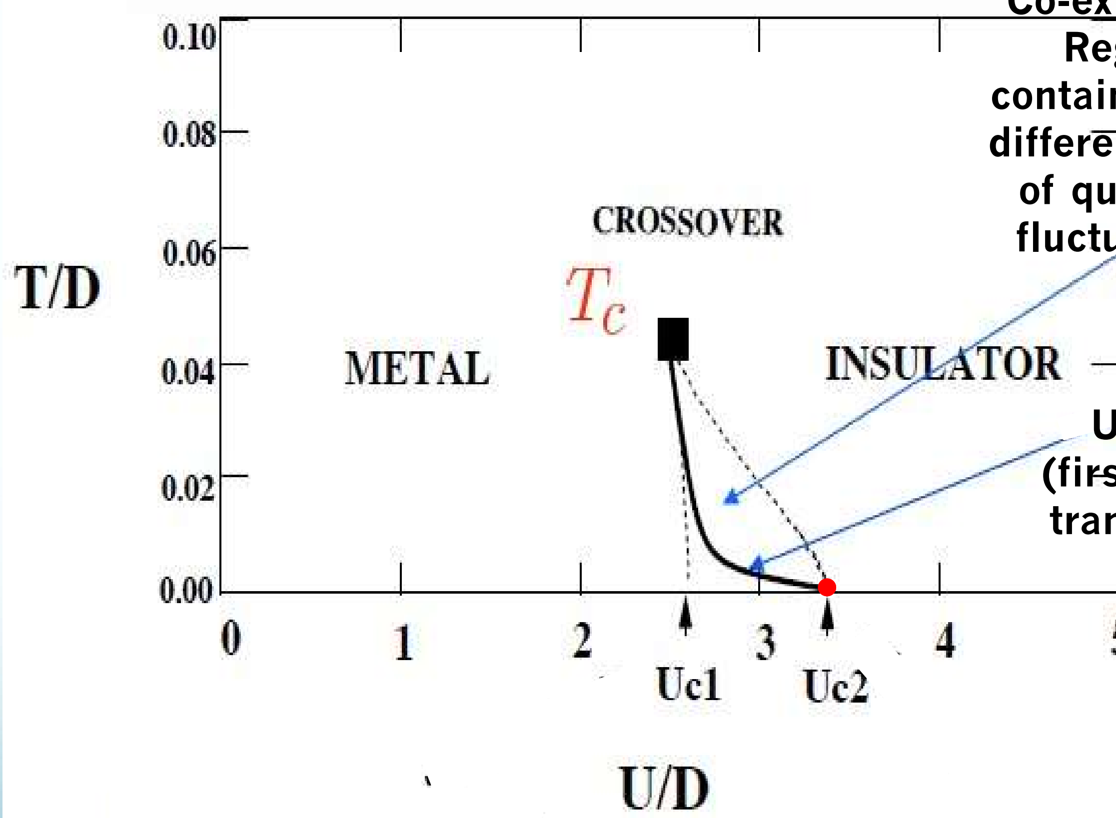


URG TREATMENTS OF OTHER PROBLEMS

- MIT of the 2D Hubbard model at half-filling (New J. Phys. **22**, 063007 (2020))
- MIT of the hole-doped 2D Hubbard model (New J. Phys. **22**, 063008 (2020) & arXiv:2003.06118)
- The Cooper Pair Insulator and the BCS superconductor (Physical Review B **104**, 144514 (2021))
- The 1D Hubbard Model & the spin-1/2 XXZ chain (JHEP **04** (2021) 148)
- The spin-1/2 Heisenberg antiferromagnet on the 2D Kagome lattice (New J. Phys. **21**, 023019 (2019))
- Phenomenology of a single band of correlated electrons with translation invariance (Nuclear Physics B **960**, 115163 (2020))
- The Sachdev-Ye model of disordered and correlated electrons (Nuclear Physics B **960**, 115163 (2020))

A closer look at the physics of U_{c1}

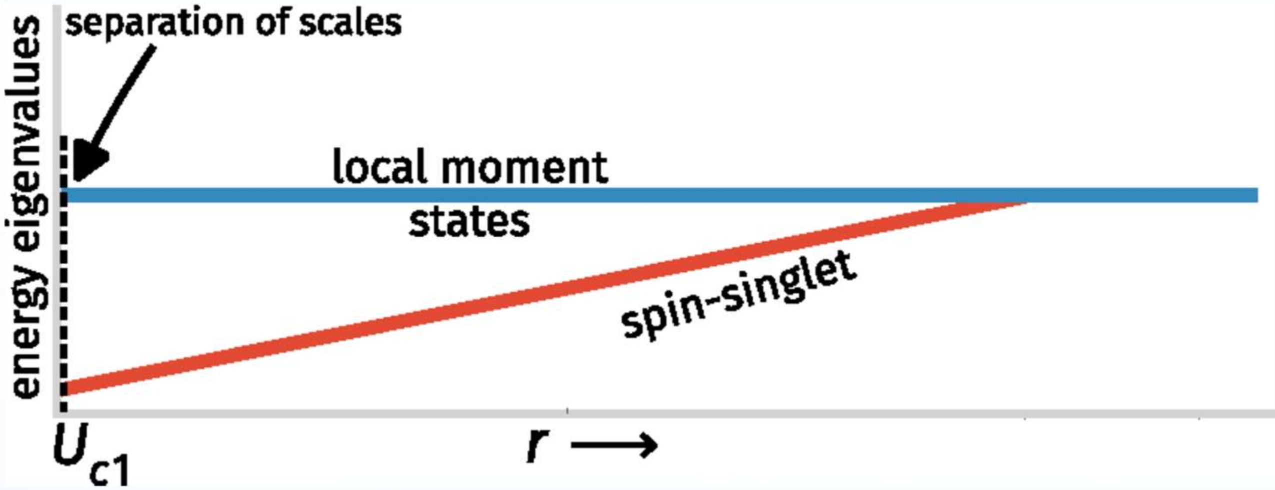


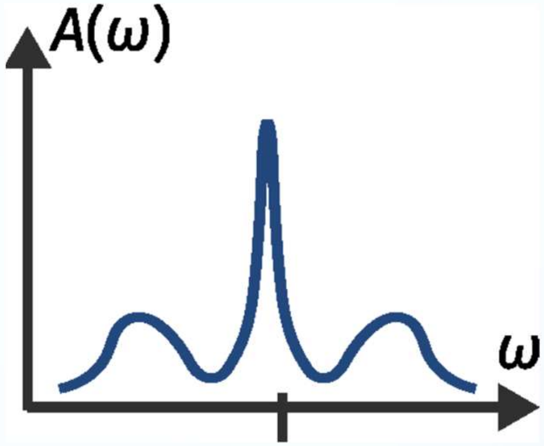


Co-existence Region contains many different kinds of quantum fluctuations

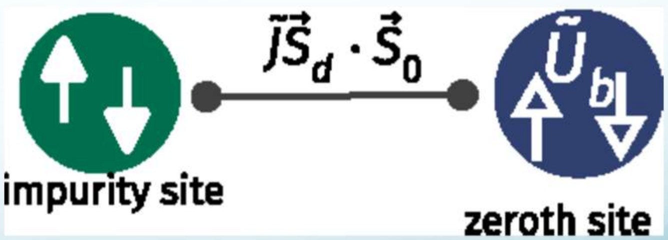
U_C (T) (first-order transition)

Co-existence within extended SIAM: physics at U_{c1}





- U_{C1} is when the side peaks get separated from the sharp central Kondo resonance, i.e., appearance of near-zeroes in the impurity spectral function as RG irrelevant single-particle hybridization (V) vanishes



- Singlet ground state stabilized; local Fermi liquid with (local) Landau qp excitations

Excited state QPT at U_{c1}: emergence of degenerate local moment states

$|\uparrow_d 0_0\rangle + |0_d \uparrow_0\rangle$

Mixing of spin & charge states on impurity site (RG relevant V)

$|\downarrow_d 0_0\rangle + |0_d \downarrow_0\rangle$

Splitting $\propto \sqrt{U^2 + V^2}$

$|\uparrow_d 0_0\rangle - |0_d \uparrow_0\rangle$

Degenerate Delocalised states

$|\downarrow_d 0_0\rangle - |0_d \downarrow_0\rangle$

Excited states before U_{C1}

RG irrelevance of V at U_{c1}

$|0_d \uparrow_0\rangle$

No mixing of spin & charge states on Impurity site

$|0_d \downarrow_0\rangle$

Splitting ~ U

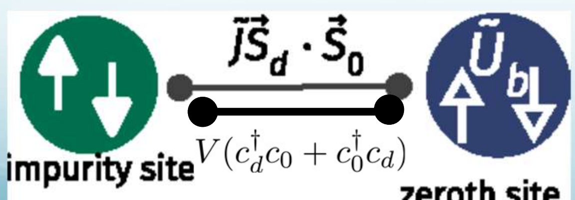
$|\uparrow_d 0_0\rangle$

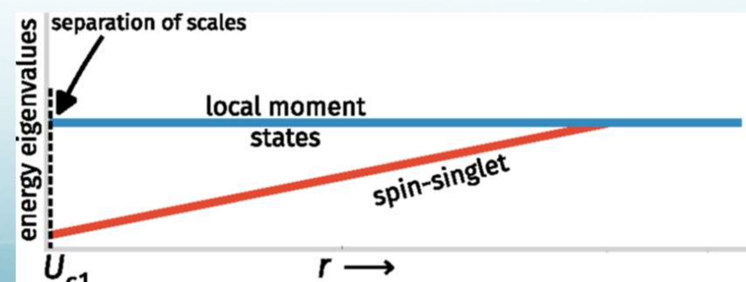
Degenerate Local Moment states

$|\downarrow_d 0_0\rangle$

Excited states after U_{C1}

(Similar states exist with doublon on 0th bath site.)





Excited state QPT at U_{c1}: emergence of degenerate local moment states

Excited states before U_{C1}

$|\uparrow_d 0_0\rangle + |0_d \uparrow_0\rangle$ | $|\downarrow_d 0_0\rangle + |0_d \downarrow_0\rangle$

Splitting $\propto \sqrt{U^2 + V^2}$

Mixing of spin & charge states on impurity site (RG relevant V)

$|\uparrow_d 0_0\rangle - |0_d \uparrow_0\rangle$ | $|\downarrow_d 0_0\rangle - |0_d \downarrow_0\rangle$

Degenerate Delocalised states

RG irrelevance of V at U_{c1}

Excited states after U_{C1}

$|0_d \uparrow_0\rangle$ | $|0_d \downarrow_0\rangle$

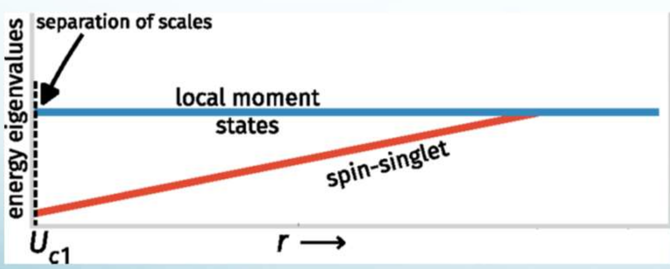
Splitting ~ U

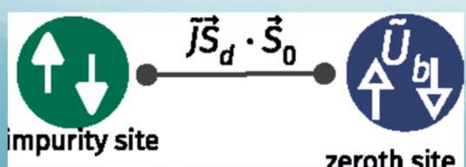
No mixing of spin & charge states on Impurity site

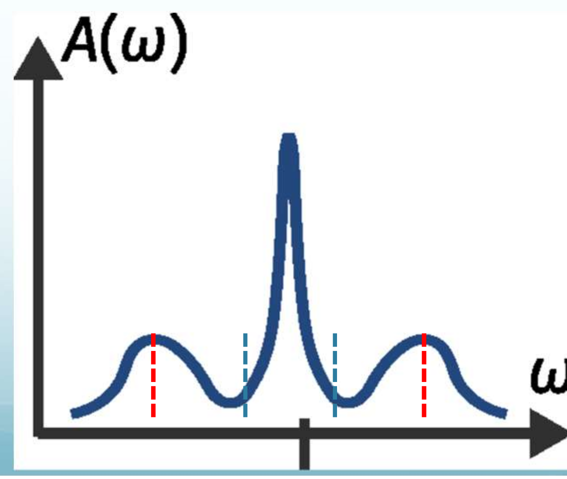
$|\uparrow_d 0_0\rangle$ | $|\downarrow_d 0_0\rangle$

Degenerate Local Moment states

(Similar states exist with doublon on 0th bath site.)







$|\uparrow_d 0_0\rangle$ $|\downarrow_d 0_0\rangle$ — Local moment states on impurity site

$|0_d \uparrow_0\rangle$ $|0_d \downarrow_0\rangle$ — Holon-Doublon states on impurity site

- LM states are at edges of central peak, holon-doublon excited states well within Hubbard side bands.

Excited state QPT at U_{c1}: emergence of degenerate local moment states

$|\uparrow_d 0_0\rangle + |0_d \uparrow_0\rangle$ **Mixing of spin & charge states on impurity site (RG relevant V)** $|\downarrow_d 0_0\rangle + |0_d \downarrow_0\rangle$

Splitting $\propto \sqrt{U^2 + V^2}$

Degenerate Delocalised states

$|\uparrow_d 0_0\rangle - |0_d \uparrow_0\rangle$ $|\downarrow_d 0_0\rangle - |0_d \downarrow_0\rangle$

Excited states before U_{c1}

RG irrelevance of V at U_{c1}

$|0_d \uparrow_0\rangle$ **No mixing of spin & charge states on Impurity site** $|0_d \downarrow_0\rangle$

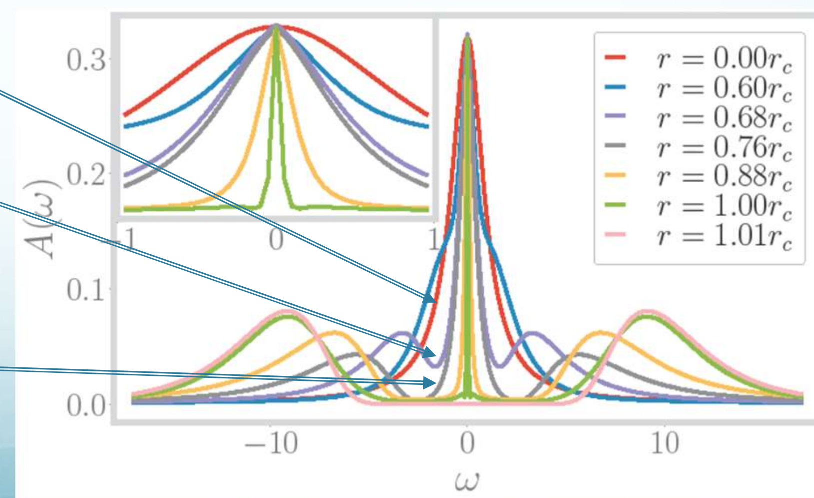
Splitting ~ U

Degenerate Local Moment states

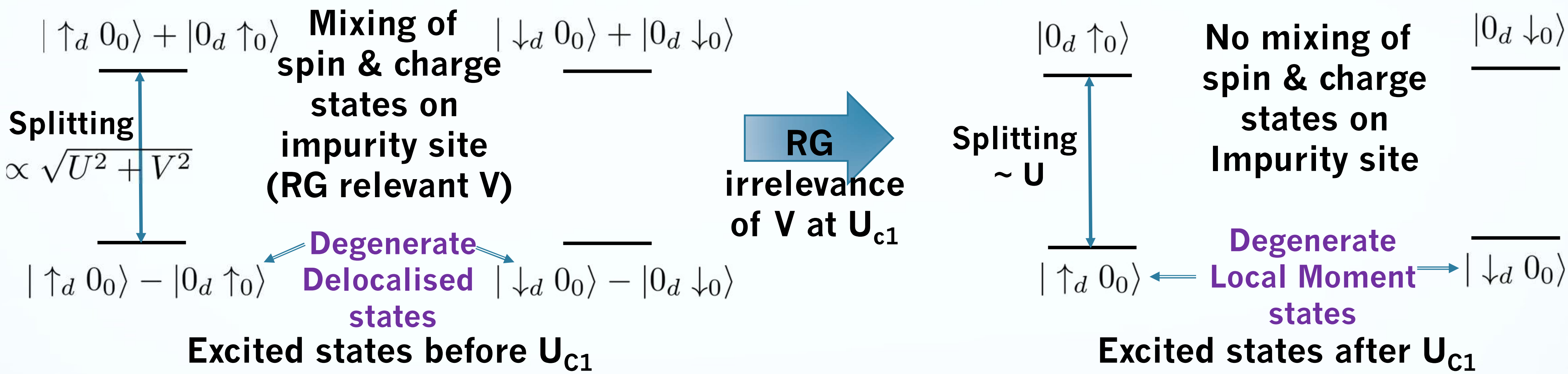
$|\uparrow_d 0_0\rangle$ $|\downarrow_d 0_0\rangle$

Excited states after U_{c1}

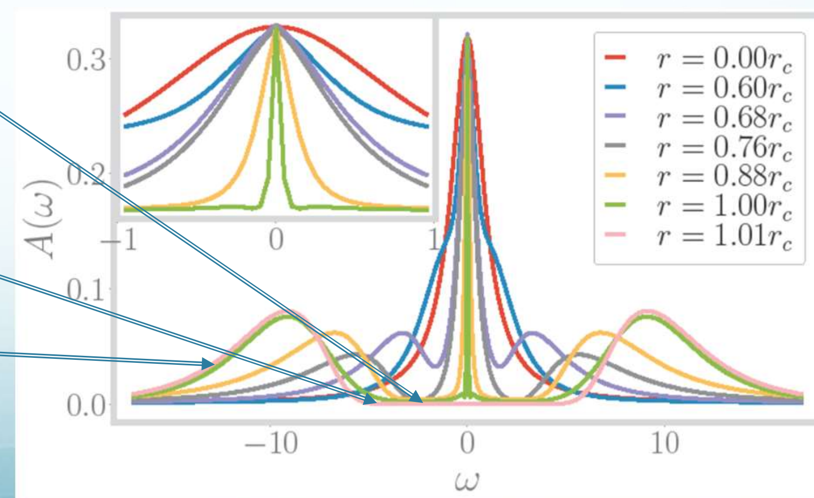
- Broad Kondo resonance (red & blue curves) for $U < U_{C1}$ includes V-mixed states in imp. spec.func.
- $U \sim U_{C1}$: RG irrelevance of V & increased splitting between Local Moment and holon-doublon excited states (purple curve).
- Depletion of spectral weight at intermediate frequencies & isolation of Kondo peak from Hubbard side bands (grey curve).



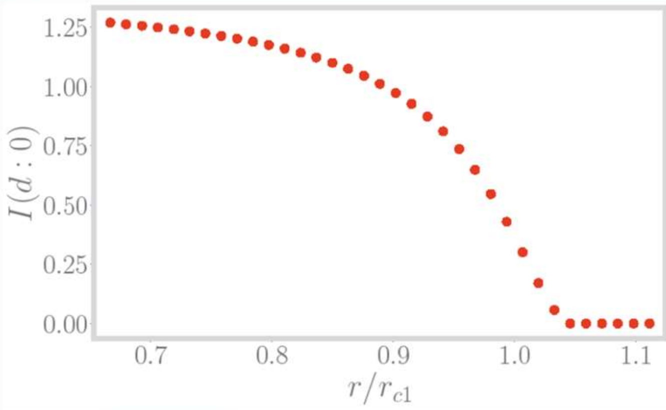
Excited state QPT at U_{c1}: emergence of degenerate local moment states



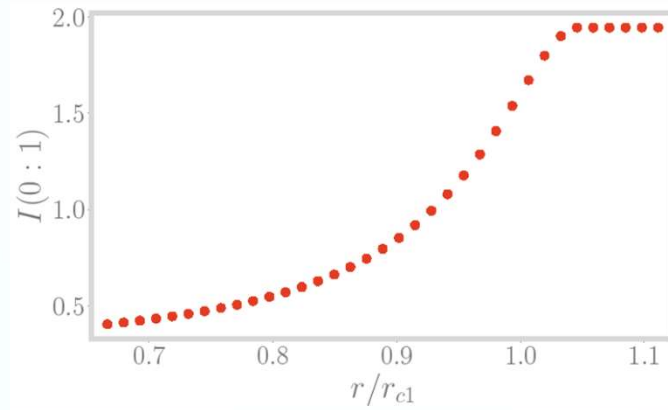
- Increasing U beyond U_{C1} opens optical gap (yellow & green curves).
- Optical gap merges into insulating gap (pink curve) for $U>U_{C2}$.
- Hubbard side bands contain holon-doublon states on impurity site hybridizing into conduction bath.

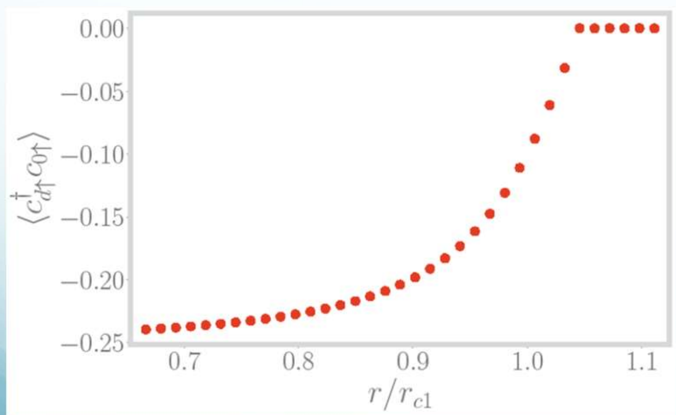


Delocalisation-localisation transition of excited states at U_{C1}

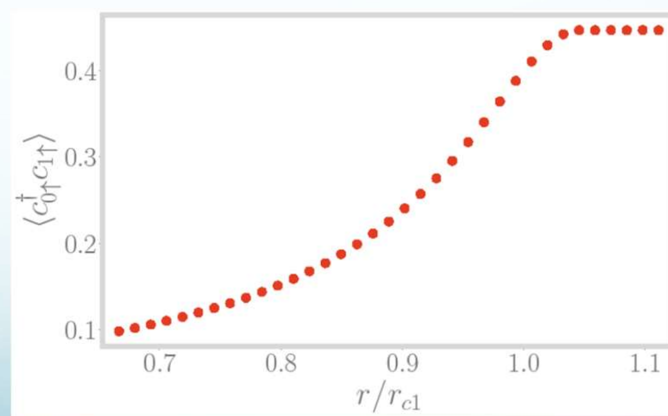


- Entanglement between impurity & bath in certain excited states vanishes, stabilising local moments in the eigenspectrum.

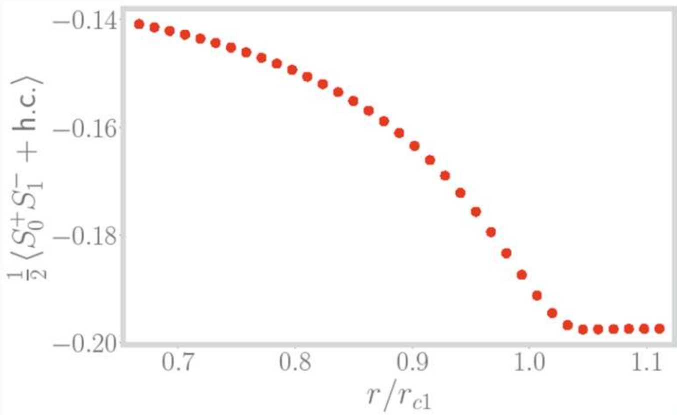


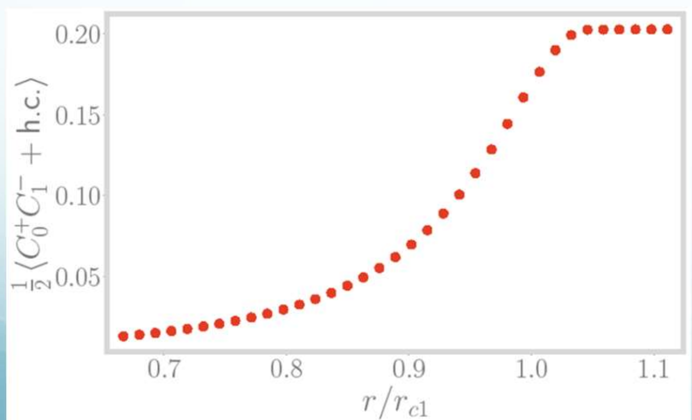


- Coincides with vanishing of single-particle hybridisation between impurity and bath & increase in the bath.

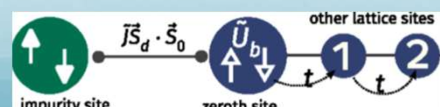


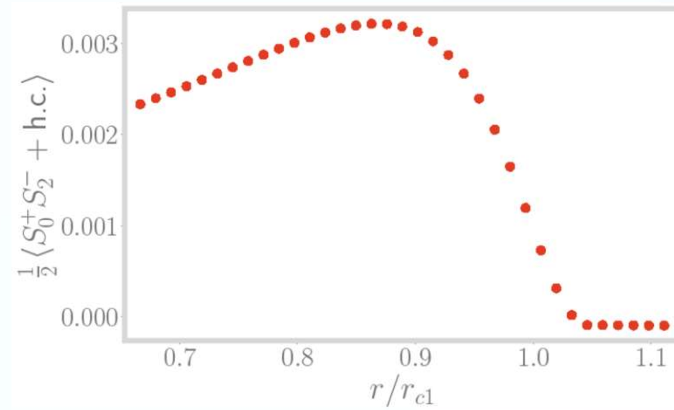
Delocalisation-localisation transition of excited states at U_{C1}

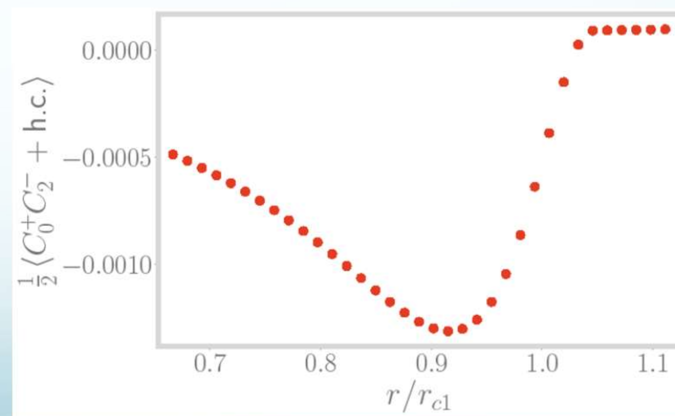




- Entanglement between impurity & bath in certain excited states vanishes, stabilising local moments in the eigenspectrum.
- Coincides with vanishing of single-particle hybridisation between impurity and bath.
- Coincides with increase in spin and charge correlations in the bath.

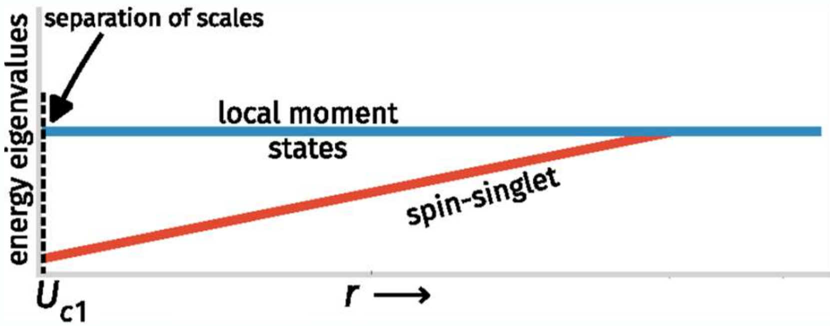


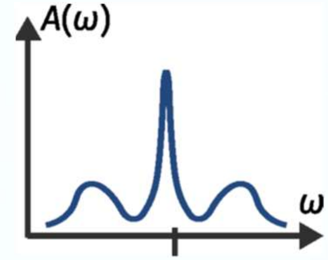


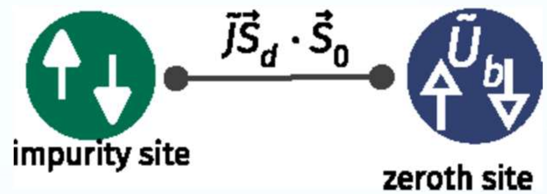


Excited state QPT at U_{c1}: emergence of degenerate local moment states

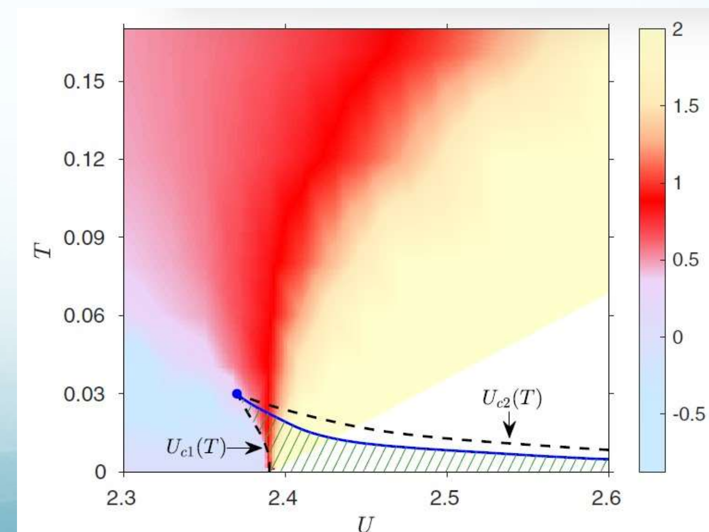
Degenerate Local Moment states



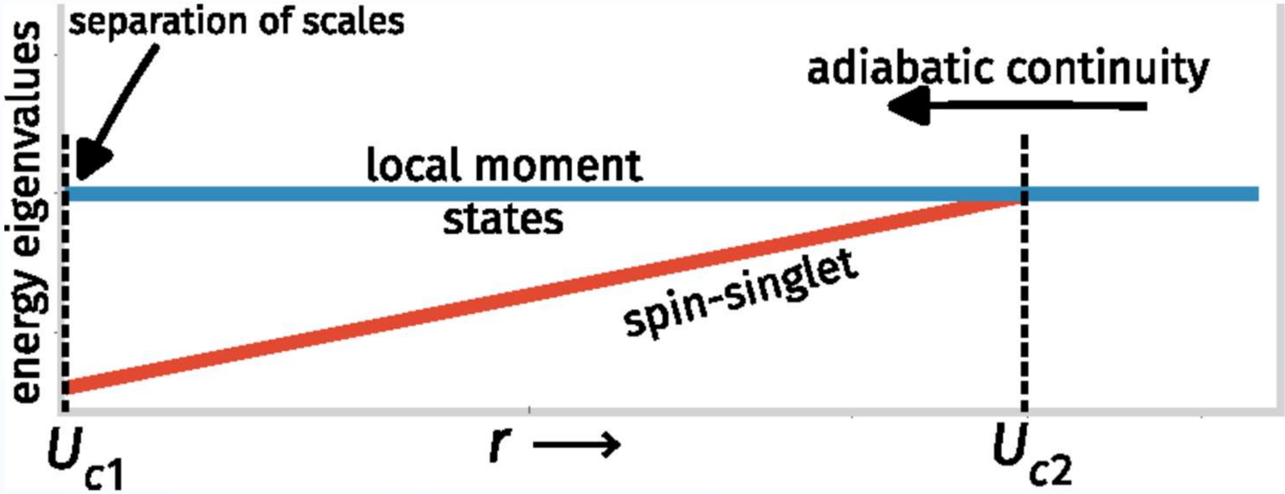


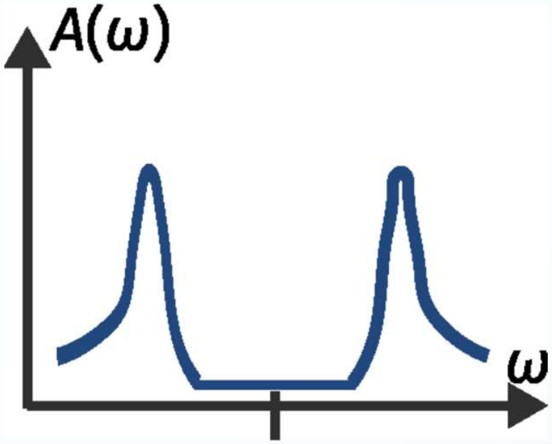


- U_{C1}: Degenerate local moment excited states emergent in J-U_b effective theory
- V leads to delocalisation ("thermalization") of local moment (excited) states into bath.
- Vanishing of V corresponds to excited state quantum phase transition (ESQPT)
- Localisation of charge on the impurity site: Insulating solution of DMFT is stabilised
- Signatures picked up in CTQMC-DMFT & NRG-DMFT (Dobrosavljevic et al 2014 & 2015, Eisenlohr et al, 2020)
- Observed in some organic materials (Furukawa, Nat. Phys., 2015)

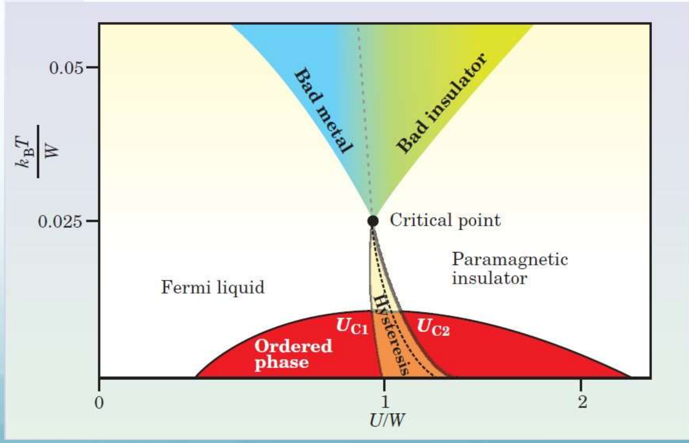


Co-existence by starting with an insulating state



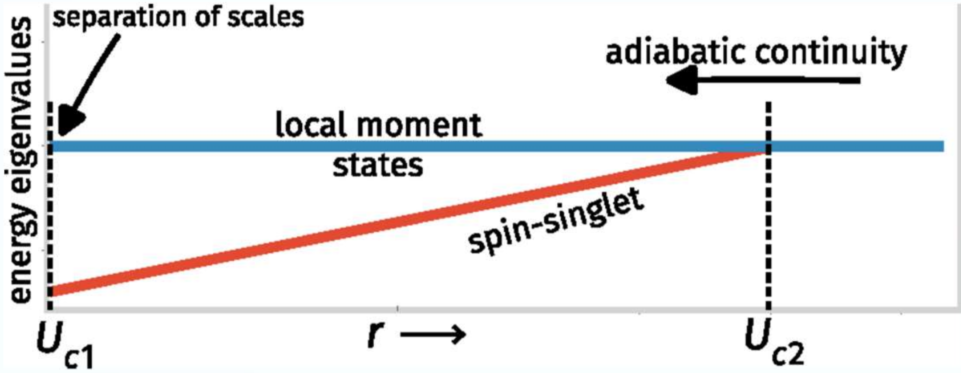


- Lowering U adiabatically through U_{C2} : passage into spectrally gapped degenerate local moment excited states
- Signals co-existence of insulating & metallic solutions at T>0, by taking into account entropy from degeneracy of LM solutions

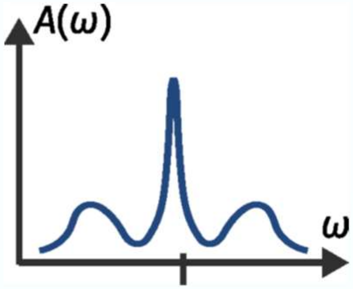


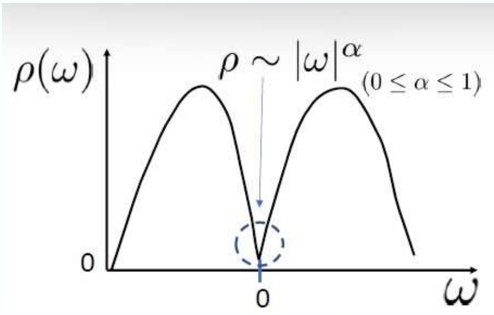
Kotliars & Vollhardt, Physics Today, 2004

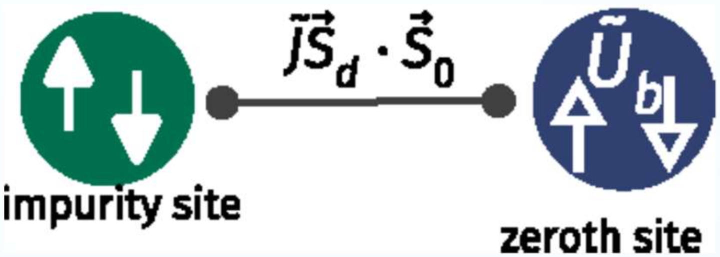
Co-existence from insulating state: pseudogapped Anderson model at U_{c1}

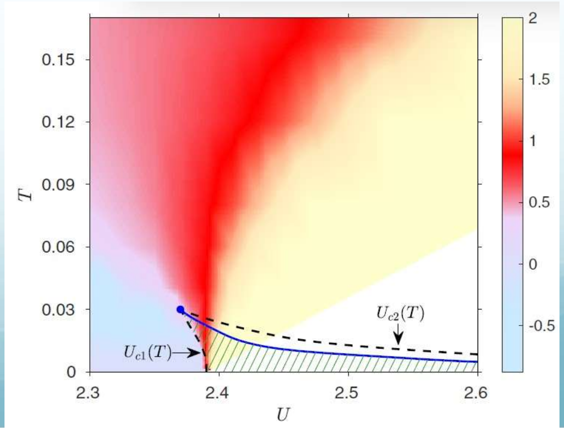


- $U \rightarrow U_{C1}$ + with insulating solution: e-DOS on bath zeroth site shrunk to pseudogap ($\rho \sim |\omega|^{\alpha}$)
- Effective pseudogapped Anderson model: screening of impurity emergent for $0 < \alpha < \frac{1}{2}$
- Observed by Eisenlohr et al., 2020

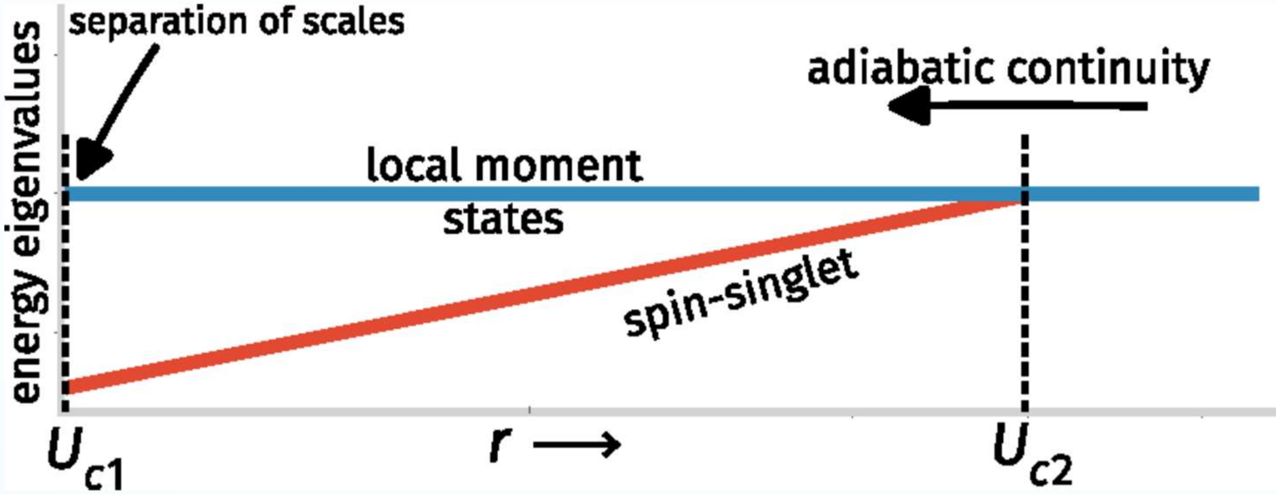


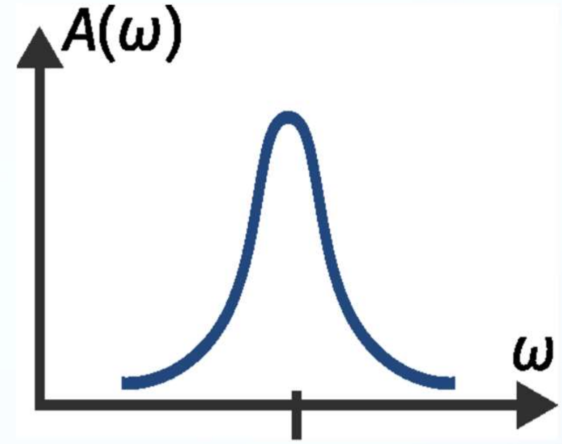






Exiting the co-existence region from insulating state





- $U < U_{C1}$: (degenerate) LM excited states rendered metastable
- System relaxes to singlet ground state