Emergence in free and correlated fermions: from impurity models to the bulk

JRF-to-SRF Presentation

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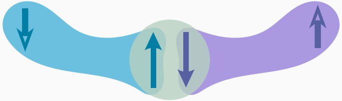
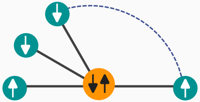
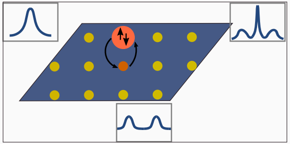
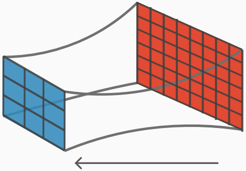




Summary of Work





Summary of Work

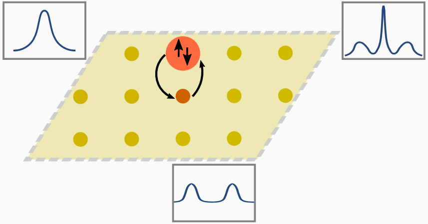
Completed Projects

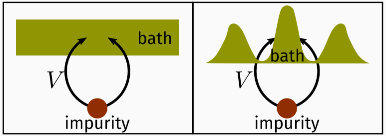
- ✓ Unveiling the Kondo cloud: Unitary renormalization-group study of the Kondo model
  Phys. Rev. B 105, 085119, arXiv:2111.10580v3
  A. Mukherjee, *Abhirup Mukherjee*, N. S. Vidhyadhiraja, A. Taraphder, and S. Lal
- ✓ Frustration shapes multi-channel Kondo physics: A star graph perspective
  under review at PRB, arXiv:2205.00790
  S. Patra, *Abhirup Mukherjee*, A. Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, S. Lal

Ongoing Projects

- ✓ Metal-insulator transition in an extended Anderson impurity model (*manuscript in preparation*)
- ✓ Holography and topology of entanglement scaling in free fermions (*manuscript in preparation*)
- ✓ URG-based auxiliary model approach to correlated systems (*ongoing*)

Local MIT in an extended Anderson impurity model



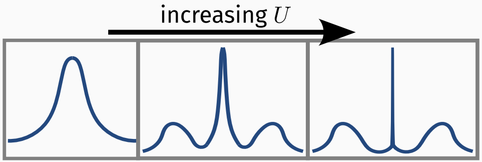


Introducing the extended Anderson impurity model

Introducing the extended Anderson impurity model

Standard Anderson impurity model

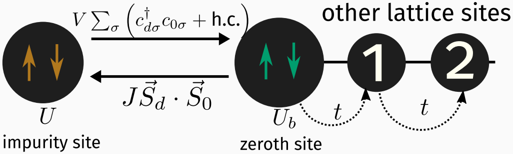
- no local-moment phase, $A(\omega)$ gapless
- cannot explain insulating phase of DMFT



Gap in spectral function requires additional physics!

Extended **Anderson impurity model**

- impurity-bath spin correlation: J
- bath zeroth site local correlation: U_b



Anderson 1961; Anderson 1978; Wilson et al. 1974; Nozieres 1974; Krishna-murthy et al. 1980; Andrei 1980; Tsvelick et al. 1983; Hewson 1993; Costi et al. 1990; Costi 2000; Kuramoto et al. 1987; Cox et al. 1988; Metzner et al. 1989; Georges et al. 1992; Parcollet et al. 2004; Maier et al. 2005; Kotliar et al. 2006; Ohashi et al. 2008.

Phase Diagram & Ground-States

Nature of the transition

Universal theory near the transition

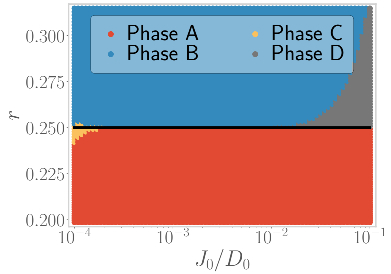
Insights into DMFT

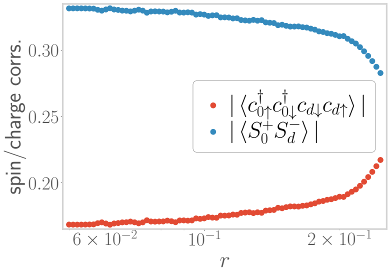
Phase Diagram & Nature of Ground-States

RG Phase diagram:

Local MIT in an extended Anderson impurity model

- Competition between J and U_b leads to phase transition from screened singlet phase at $|U_b| \leq 4J$ to unscreened local moment phase at $|U_b| > 4J$.
- Impurity spectral function becomes gapped beyond the critical point.
- Decoupling the impurity model leads to an effective model with the zeroth site as the correlated impurity, demonstrating the symmetry between the impurity and zeroth site.
- Geometric entanglement and mutual information track the transition by vanishing beyond the critical point.
- Subdominant pairing tendencies are observed near the quantum critical point.



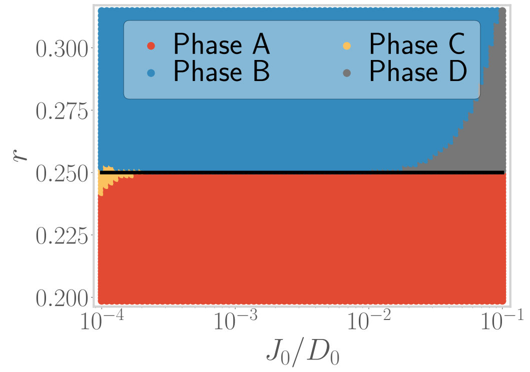


RG Phase Diagram

RG equations reveal critical point where J, V **become irrelevant**

1. orange phase: J is relevant: strong-coupling
2. blue phase: J is irrelevant: local moment
3. yellow phase: spin+charge liquid
4. gray phase: all couplings irrelevant

$r = -U_b / J$



Presence of a phase transition

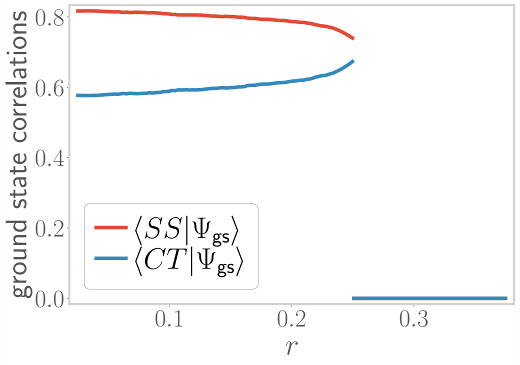
singlet ⟶ spin+charge liquid ⟶ local moment

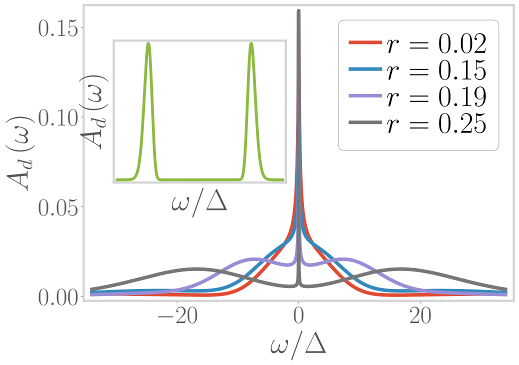
impurity spectral function gaps out

$r = -U_b/J$

$|SS\rangle = |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle$

$|CT\rangle = |2, 0\rangle + |0, 2\rangle$





Bath spectral function: towards self-consistency

- Decoupling the impurity site leads to an Anderson impurity model

$$H_{0+\text{rest}} = \underbrace{-\left(U_0 + U_b\right)\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2}_{\text{new correlated impurity}} \quad \underbrace{- t \sum_{\substack{j \in \text{n.n. of } 0, \\ \sigma}} \left(c^\dagger_{0\sigma} c_{j\sigma} + \text{h.c.}\right)}_{\text{hopping between new impurity \& new bath}} \quad \underbrace{- t \sum_{\langle i,j \rangle} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right)}_{\text{K.E. of new bath}}$$

- correlated, dominant spin-flip processes lead to repulsive $U_{\text{eff}} = U_0 + U_b \sim J^*/8$

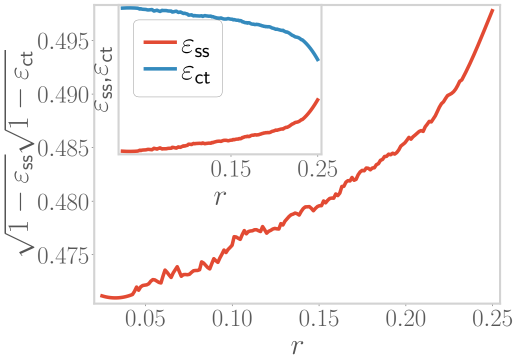
- J symmetrises the two sites, leading to similar spectral functions $\longrightarrow$ essence of self-consistency

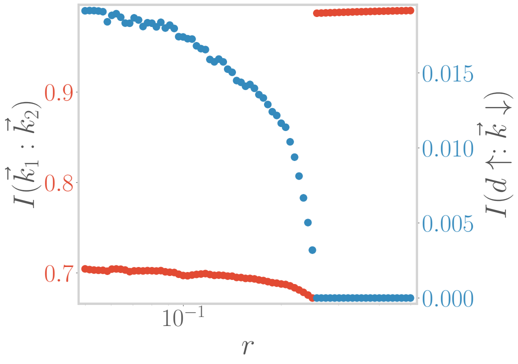
Entanglement as a probe for the transition

Geometric entanglement: $\varepsilon(\psi_1, \psi_2) = 1 - |\langle\psi_1|\psi_2\rangle|^2$

$\longrightarrow \sqrt{1 - \varepsilon_{SS}}\sqrt{1 - \varepsilon_{CT}}$ is maximised, then vanishes

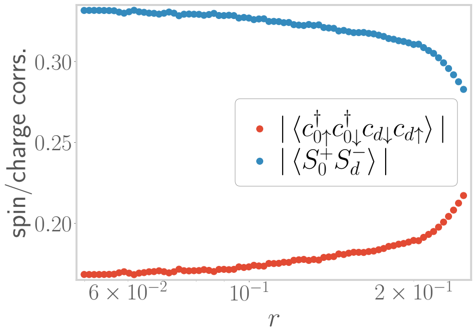
Mutual information between impurity and cloud vanishes

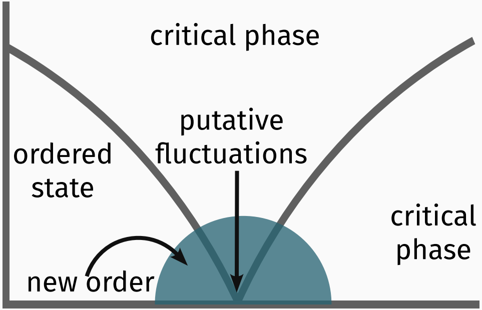




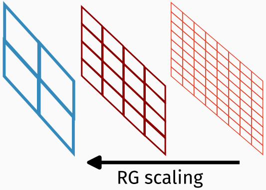
Presence of subdominant pair fluctuations

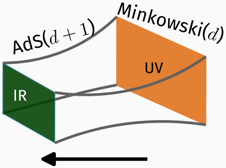
- **pairing tendencies** observed near the quantum critical point
- might lead to **superconductivity** with doping
- seen in cuprates, heavy-fermions materials, pnictides, etc





Entanglement scaling in free fermions: holography & topology





Creating subsystems

Free Dirac fermions on torus: $k_x^n = \frac{2\pi}{L_x} n, \quad n \in \mathbb{Z};$ define **sparsity** $= \Delta n = 1$

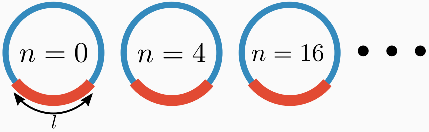
Simplest choice: the entire set

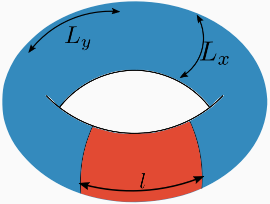
sparsity = 1 $\longrightarrow n \in \{-N, -(N-1), -(N-2), \dots, -1, 0, 1, \dots, N-2, N-1, N\}$

Coarser choices: increase sparsity

sparsity = 2 $\longrightarrow n \in \{-N, -(N-2), -(N-4), \dots, -2, 0, 2, \dots, N-4, N-2, N\}$

sparsity = 4 $\longrightarrow n \in \{-N, -(N-4), -(N-8), \dots, -4, 0, 4, \dots, N-8, N-4, N\}$





Subsystem entanglement entropy: Entanglement hierarchy

$$S_{A_z(j)} = f_z(j) c \alpha L_x - c \log \left| 2 \sin \left(\pi f_z(j) \phi \right) \right|$$

$$i < j, \quad S_{i \cup j} = \begin{cases} S_i, & z > 0 \\ S_j, & z < 0 \end{cases}$$

- presents a **hierarchy** of entanglement $\longrightarrow$ EE distributed across RG steps
  RG transformation $\longrightarrow$ reveals entanglement
- distribution of entanglement also present in **multipartite** entanglement

Calabrese et al. 2004; Casini et al. 2005; Arias et al. 2015; Chen et al. 2017; Murciano et al. 2020.

Mutual information = distance

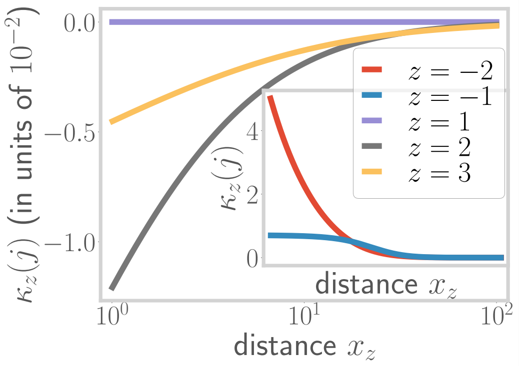
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

Define distances using mut. info.

$$x_z(j) = \log t_z(j), \quad y_z(j) = \log t_z(j \pm 1)$$

$$v_z(j) \equiv \Delta y_z(j)/\Delta x_z(j), \quad v' = \Delta v_z(j)/\Delta x_z(j)$$

Curvature as well: $\kappa_z(j) = \dfrac{v_z'(j)}{[1 + v_z(j)^2]^{\frac{3}{2}}}$



Van Raamsdonk 2010; Lee et al. 2016; Mukherjee et al. 2022; Lee 2010; Lee 2014; Qi 2013; Lee et al. 2016; Mukherjee et al. 2020a; Mukherjee et al. 2020b; Ryu et al. 2006b; Ryu et al. 2006a; Nozaki et al. 2012.

RG evolution = emergent distance

- Distances and curvature can be related to an RG **beta function**
- Amounts to an **explicit demonstration** of the holographic principle
- Sign of curvature is **topological**, can be written in terms of winding numbers

Maldacena 1999; Ryu et al. 2006a; Holzhey et al. 1994.

Topological nature of geometry-independent term

$$S_{A_z(j)} = f_z(j)c\alpha L_x - \underbrace{c\log\left|2\sin\left(\pi f_z(j)\phi\right)\right|}_{=Q(\phi),\text{geometry-independent term}}$$

- $Q(\phi)$ is periodic in the flux ϕ, $\phi = 1$ transports a charge across Fermi surface
- pole structure of $\left(\sin\frac{\pi}{4} - |\sin\left(\pi f_z(j)\right)\phi|\right)^{-1}$ counts number of states $\longrightarrow$ tracks Luttinger volume
- Luttinger volume is topological, so is $Q(\phi)$; $Q(\phi)$ can be expressed in terms of winding numbers

Luttinger et al. 1960; Luttinger 1960; Oshikawa 2000; Seki et al. 2017; Mukherjee et al. 2020a; Heath et al. 2020.

Future Prospects

Future Prospects

- Better model can be obtained by taking multiple impurities and general impurity filling
- novel auxiliary model method can used for studying other models of strong-correlations as well as topologically active or flat band systems
- The URG can be applied to heavy-fermion materials towards a study of phase diagram and unconventional superconductivity, as well as Kondo insulators
- Interacting systems in a magnetic field is also a potential area of study, specifically fractional Chern insulators (e.g. the fractional quantum hall effects)

Acknowledgements

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References

- Affleck, Ian (1995). “Conformal field theory approach to the Kondo effect”. In: *Acta Phys.Polon.B* 26.1869.
- Affleck, Ian and Andreas W.W. Ludwig (1991). “Critical theory of overscreened Kondo fixed points”. In: *Nuclear Physics B* 360.2, pp. 641–696. ISSN: 0550-3213.
- Affleck, Ian and Andreas WW Ludwig (1993). “Exact conformal-field-theory results on the multichannel Kondo effect: Single-fermion Green’s function, self-energy, and resistivity”. In: *Physical Review B* 48.10, p. 7297.
- Anderson, P. W. (1961). “Localized Magnetic States in Metals”. In: *Phys. Rev.* 124 (1), pp. 41–53.
- — (1978). “Local moments and localized states”. In: *Rev. Mod. Phys.* 50 (2), pp. 191–201.
- Anderson, PW (1970). “A poor man’s derivation of scaling laws for the Kondo problem”. In: *Journal of Physics C: Solid State Physics* 3.12, p. 2436.
- Andrei, N. (1980). “Diagonalization of the Kondo Hamiltonian”. In: *Phys. Rev. Lett.* 45 (5), pp. 379–382.
- Andrei, N, K Furuya, and J H Lowenstein (1983). “Solution of the Kondo problem”. In: *Rev. Mod. Phys.* 55, p. 331.
- Arias, Raúl E, David D Blanco, and Horacio Casini (2015). “Entanglement entropy as a witness of the Aharonov–Bohm effect in QFT”. In: *Journal of Physics A: Mathematical and Theoretical* 48.14, p. 145401.
- Bulla, R, A C Hewson, and Th Pruschke (1998). “Numerical renormalization group calculations for the self-energy of the impurity Anderson model”. In: *Journal of Physics: Condensed Matter* 10.37, pp. 8365–8380.
- Calabrese, Pasquale and John Cardy (2004). “Entanglement entropy and quantum field theory”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2004.06, P06002.
- Casini, H, C D Fosco, and M Huerta (2005). “Entanglement and alpha entropies for a massive Dirac field in two dimensions”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2005.07, P07007–P07007.
- Chen, Xiao et al. (2017). “Two-cylinder entanglement entropy under a twist”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2017.4, p. 043104.
- Costi, T. A. (2000). “Kondo Effect in a Magnetic Field and the Magnetoresistivity of Kondo Alloys”. In: *Phys. Rev. Lett.* 85 (7), pp. 1504–1507.
- Costi, T.A. and A.C. Hewson (1990). “A new approach to the calculation of spectra for strongly correlated systems”. In: *Physica B: Condensed Matter* 163.1, pp. 179–181. ISSN: 0921-4526.
- Cox, D. L. and N. Grewe (1988). “Transport properties of the Anderson lattice”. In: *Zeitschrift für Physik B Condensed Matter* 71.3, pp. 321–340.
- Emery, V. J. and S. Kivelson (1992). “Mapping of the two-channel Kondo problem to a resonant-level model”. In: *Phys. Rev. B* 46 (17), pp. 10812–10817.
- Gan, J (1994). “On the multichannel Kondo model”. In: 6.24, pp. 4547–4568.
- Georges, Antoine and Gabriel Kotliar (1992). “Hubbard model in infinite dimensions”. In: *Physical Review B* 45.12, p. 6479.
- Goldhaber-Gordon, D. et al. (1998). “Kondo effect in a single-electron transistor”. In: *Nature* 391.6663, pp. 156–159. ISSN: 1476-4687.
- Heath, Joshuah T and Kevin S Bedell (2020). “Necessary and sufficient conditions for the validity of Luttinger’s theorem”. In: *New Journal of Physics* 22.6, p. 063011.
- Hewson, A. C. (1993). *The Kondo Problem to Heavy Fermions*. Cambridge University Press.
- Holzhey, Christoph, Finn Larsen, and Frank Wilczek (1994). “Geometric and renormalized entropy in conformal field theory”. In: *Nuclear Physics B* 424.3, pp. 443–467. ISSN: 0550-3213.
- Kondo, Jun (1964). “Resistance minimum in dilute magnetic alloys”. In: *Progress of theoretical physics* 32.1, pp. 37–49.

References

- Kotliar, G. et al. (2006). "Electronic structure calculations with dynamical mean-field theory". In: *Rev. Mod. Phys.* 78 (3), pp. 865–951.
- Krishna-murthy, H. R., J. W. Wilkins, and K. G. Wilson (1980). "Renormalization-group approach to the Anderson model of dilute magnetic alloys. I. Static properties for the symmetric case". In: *Phys. Rev. B* 21 (3), pp. 1003–1043.
- Kuramoto, Y and T Watanabe (1987). "Theory of momentum-dependent magnetic response in heavy-fermion systems". In: *Proceedings of the Yamada Conference XVIII on Superconductivity in Highly Correlated Fermion Systems*. Elsevier, pp. 80–83.
- Lee, Ching Hua and Xiao-Liang Qi (2016). "Exact holographic mapping in free fermion systems". In: *Physical Review B* 93.3, p. 035112.
- Lee, Sung-Sik (2010). "Holographic description of quantum field theory". In: *Nuclear Physics B* 832.3, pp. 567–585.
- — (2014). "Quantum renormalization group and holography". In: *Journal of High Energy Physics* 2014.1, p. 76.
- Luttinger, JM (1960). "Fermi surface and some simple equilibrium properties of a system of interacting fermions". In: *Physical Review* 119.4, p. 1153.
- Luttinger, Joaquin Mazdak and John Clive Ward (1960). "Ground-state energy of a many-fermion system. II". In: *Physical Review* 118.5, p. 1417.
- Maier, Thomas et al. (2005). "Quantum cluster theories". In: *Rev. Mod. Phys.* 77 (3), pp. 1027–1080.
- Maldacena, Juan (1999). "The large-N limit of superconformal field theories and supergravity". In: *International journal of theoretical physics* 38.4, pp. 1113–1133.
- Metzner, Walter and Dieter Vollhardt (1989). "Correlated Lattice Fermions in $d = \infty$ Dimensions". In: *Phys. Rev. Lett.* 62 (3), pp. 324–327.
- Mukherjee, Anirban and Siddhartha Lal (2020a). "Unitary renormalisation group for correlated electrons-I: a tensor network approach". In: *Nuclear Physics B* 960, p. 115170.
- — (2020b). "Unitary renormalisation group for correlated electrons-II: insights on fermionic criticality". In: *Nuclear Physics B* 960, p. 115163.
- — (2022). "Superconductivity from repulsion in the doped 2D electronic Hubbard model: an entanglement perspective". In: *Journal of Physics: Condensed Matter* 34.27, p. 275601.
- Murciano, Sara, Paola Ruggiero, and Pasquale Calabrese (2020). "Symmetry resolved entanglement in two-dimensional systems via dimensional reduction". In: *Journal of Statistical Mechanics: Theory and Experiment* 2020.8, p. 083102.
- Nozaki, Masahiro, Shinsei Ryu, and Tadashi Takayanagi (2012). "Holographic geometry of entanglement renormalization in quantum field theories". In: *Journal of High Energy Physics* 2012.10, p. 193.
- Nozieres, P (1974). "A "Fermi-liquid" description of the Kondo problem at low temperatures". In: *Journal of Low Temperature Physics* 17, p. 31.
- Nozières, Ph. and Blandin, A. (1980). "Kondo effect in real metals". In: *J. Phys. France* 41.3, pp. 193–211.
- Ohashi, Takuma et al. (2008). "Finite Temperature Mott Transition in Hubbard Model on Anisotropic Triangular Lattice". In: *Phys. Rev. Lett.* 100 (7), p. 076402.
- Oshikawa, Masaki (2000). "Topological approach to Luttinger's theorem and the Fermi surface of a Kondo lattice". In: *Physical Review Letters* 84.15, p. 3370.
- Parcollet, O., G. Biroli, and G. Kotliar (2004). "Cluster Dynamical Mean Field Analysis of the Mott Transition". In: *Phys. Rev. Lett.* 92 (22), p. 226402.
- Qi, Xiao-Liang (2013). "Exact holographic mapping and emergent space-time geometry". In: *arXiv preprint arXiv:1309.6282*.
- Ryu, Shinsei and Tadashi Takayanagi (2006a). "Aspects of holographic entanglement entropy". In: *Journal of High Energy Physics* 2006.08, p. 045.
- — (2006b). "Holographic derivation of entanglement entropy from the anti–de sitter space/conformal field theory correspondence". In: *Physical review letters* 96.18, p. 181602.

References

- Sakai, Osamu, Yukihiro Shimizu, and Tadao Kasuya (1989). "Single-Particle and Magnetic Excitation Spectra of Degenerate Anderson Model with Finite f–f Coulomb Interaction". In: *Journal of the Physical Society of Japan* 58.10, pp. 3666–3678. eprint: `https://doi.org/10.1143/JPSJ.58.3666`.
- Seki, Kazuhiro and Seiji Yunoki (2017). "Topological interpretation of the Luttinger theorem". In: *Physical Review B* 96.8, p. 085124.
- Tsvelick, A M and P B Wiegmann (1983). "Exact results in the theory of magnetic alloys". In: *Adv. in Phys.* 32, p. 453.
- Tsvelick, A. M. and P. B. Wiegmann (1985). "Exact solution of the multichannel Kondo problem, scaling, and integrability". In: *Journal of Statistical Physics* 38.1, pp. 125–147. ISSN: 1572-9613.
- V. Borzenets, Ivan et al. (2020). "Observation of the Kondo screening cloud". In: *Nature* 579.7798, pp. 210–213. ISSN: 1476-4687.
- Van Raamsdonk, Mark (2010). "Building up spacetime with quantum entanglement". In: *General Relativity and Gravitation* 42.10, pp. 2323–2329.
- Wilson, Kenneth G. (1975). "The renormalization group: Critical phenomena and the Kondo problem". In: *Rev. Mod. Phys.* 47 (4), pp. 773–840.
- Wilson, Kenneth G. and J. Kogut (1974). "The renormalization group and the ϵ-expansion". In: *Physics Reports* 12.2, pp. 75 –199.

Further Details

Theory for the single-channel Kondo cloud

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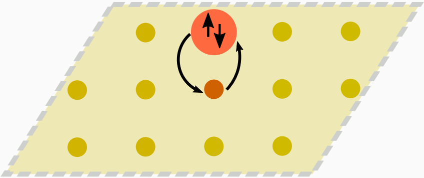
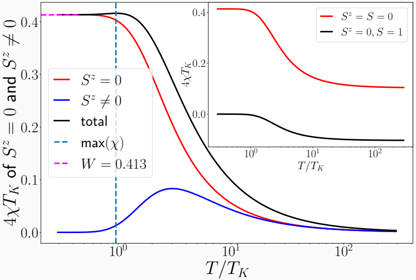
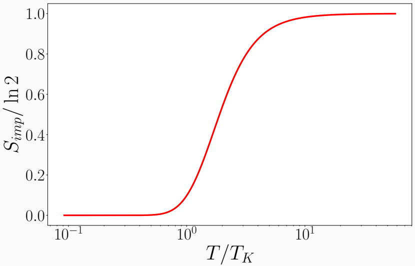


Theory for the single-channel Kondo cloud

✓ spectral function & magnetic susceptibility





✓ local Fermi liq. & orthogonality catastrophe

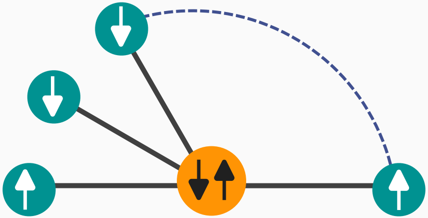
✓ thermal entropy

Kondo 1964; Wilson 1975; Andrei et al. 1983; Hewson 1993; Nozieres 1974; Anderson 1970; Tsvelick et al. 1983; Affleck et al. 1993; Goldhaber-Gordon et al. 1998; V. Borzenets et al. 2020; Sakai et al. 1989; Costi et al. 1990; Nozaki et al. 2012; Affleck 1995.

Role of degeneracy in the multi-channel Kondo problem

arXiv:2205.00790

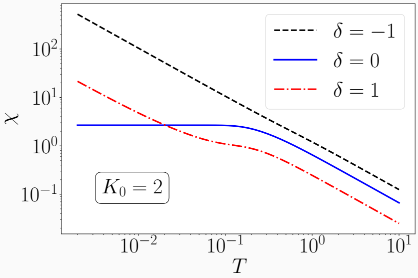
Siddhartha Patra, **Abhirup Mukherjee**, Anirban Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, Siddhartha Lal

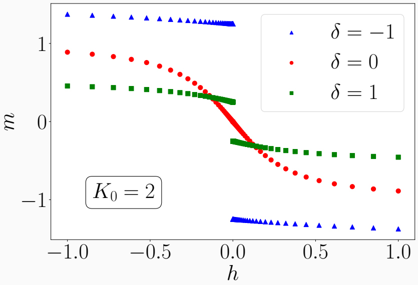


Role of degeneracy in the multi-channel Kondo problem

✓ Intermediate-coupling RG fixed point Hamiltonian and **degenerate** ground states

✓ Degree of compensation, magnetization and susceptibility show **incomplete screening**



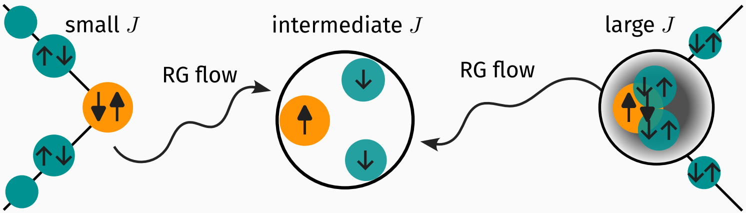


Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

Role of degeneracy in the multi-channel Kondo problem

✓ Local **marginal Fermi liquid** within the low-energy excitations of the bath

✓ **Duality** relations constrain the RG flows of the MCK model



Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

Holography and topology of entanglement scaling in free fermions

Future Prospects

Improvements to the auxiliary model

- Better model can be obtained by using multiple impurities
- Allows entangled liquid-like insulating phases
- Might also provide k–space resolution
  - partial gapping of Fermi surface?
  - pseudogap phases
- Introducing general impurity filling
  - new phases?
  - dominant pair fluctuations?

A novel auxiliary model approach

- Using local impurity models to create bulk lattice models (Bloch's theorem)

$$H_{\text{bulk}} = \sum_i H_{\text{local}}(i), \quad \Psi_{\text{bulk}}(\vec{k}) \sim \sum_i e^{i\vec{k}\cdot\vec{r}_i} \Psi_{\text{local}}(i)$$

- Relates bulk correlation functions to those of the auxiliary model

- phase transition in the extended AIM $\longrightarrow$ phase transition inthe bulk model, **metal-insulator transition** in Hubbard-Heisenberg model

A novel auxiliary model approach

- Should be useful for studying other models of strong-correlations
    - periodic Anderson/Kondo models
    - Heisenberg models
- Another potential application: topologically active systems:
    - Fractional quantum hall systems
- Extend the formalism towards higher order Greens functions
    - two-particle Greens functions, doublon-holon correlations
    - can provide more info on the MIT

Heavy-fermion materials

- Materials with very high quasiparticle masses

- Outstanding questions exist about the nature of phases and phase transitions
  - microscopic justification of certain phases
  - theory for the strange metal excitations
  - microscopic justification for the origin of unconventional superconductivity

- the URG, MERG and auxiliary model methods should prove useful