Magnetic moments and non-Fermi liquid behavior in quasicrystals

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Next Generation Quantum Materials

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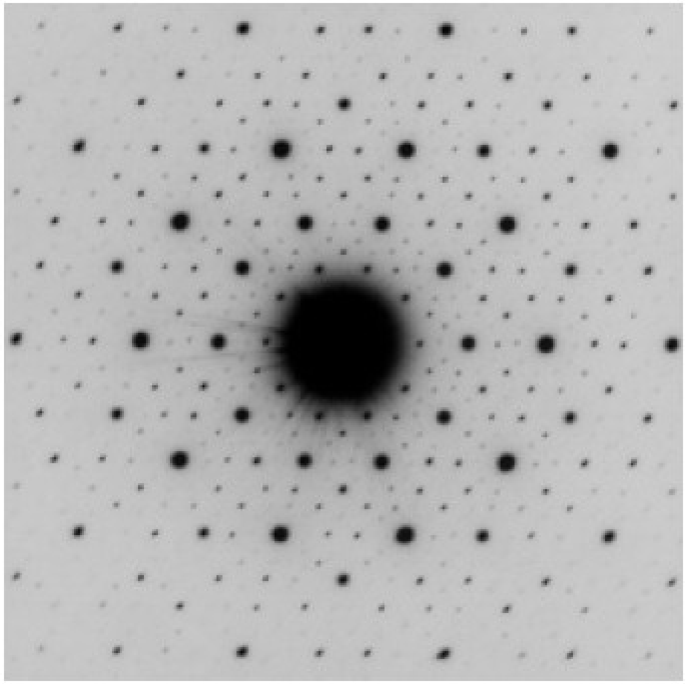
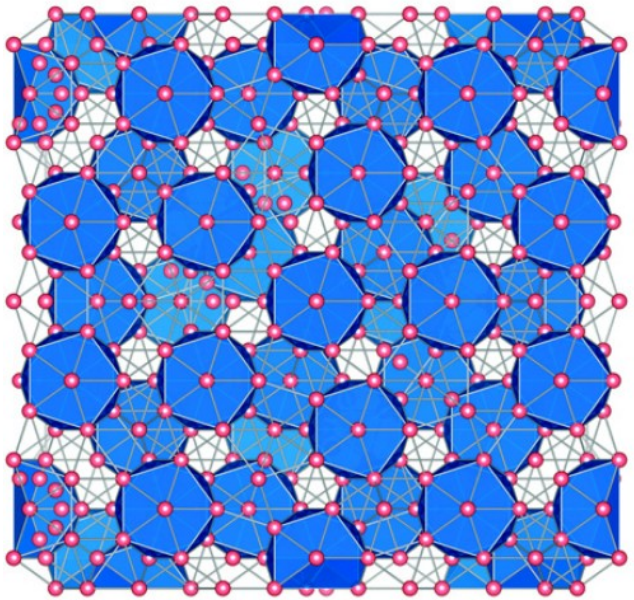
Outline

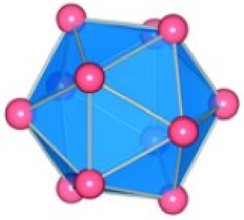
- **Introduction**
  - $Au_{51}Al_{34}Yb_{15}$ quasicrystal
  - Intrinsic NFL behavior in $Au_{51}Al_{34}Yb_{15}$
- **Tiling models and quasicrystals**
  - Geometrical and electronic properties
- **Kondo effect in metallic quasicrystals**
  - Power-law distribution of Kondo temperatures
  - NFL behavior
- **Conclusions**

$Au_{51}Al_{34}Yb_{15}$ quasicrystal

- Icosahedron QC (Tsai-type)
  - 12 Yb icosahedron
  - Projected positions of Yb atoms
- 10-fold symmetry diffraction pattern



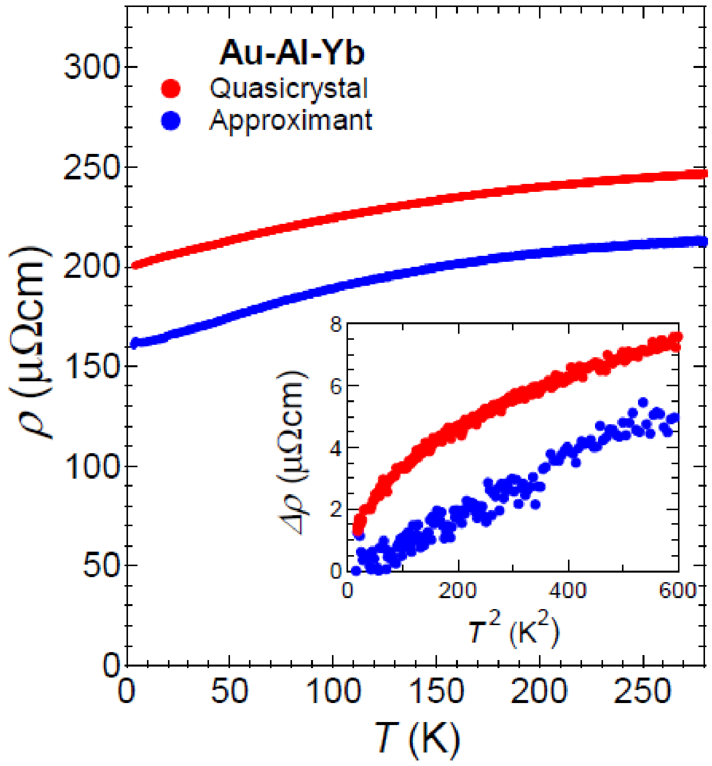




Ishimasa *et al.* Philos. Mag. 91, 4218 (2011)
Deguchi *et al.* Nat. Mater. **11**, 1013 (2012)
Watanuki *et al.* PRB **86**, 094201 (2012)

$Au_{51}Al_{34}Yb_{15}$ quasicrystal: a Heavy Fermion

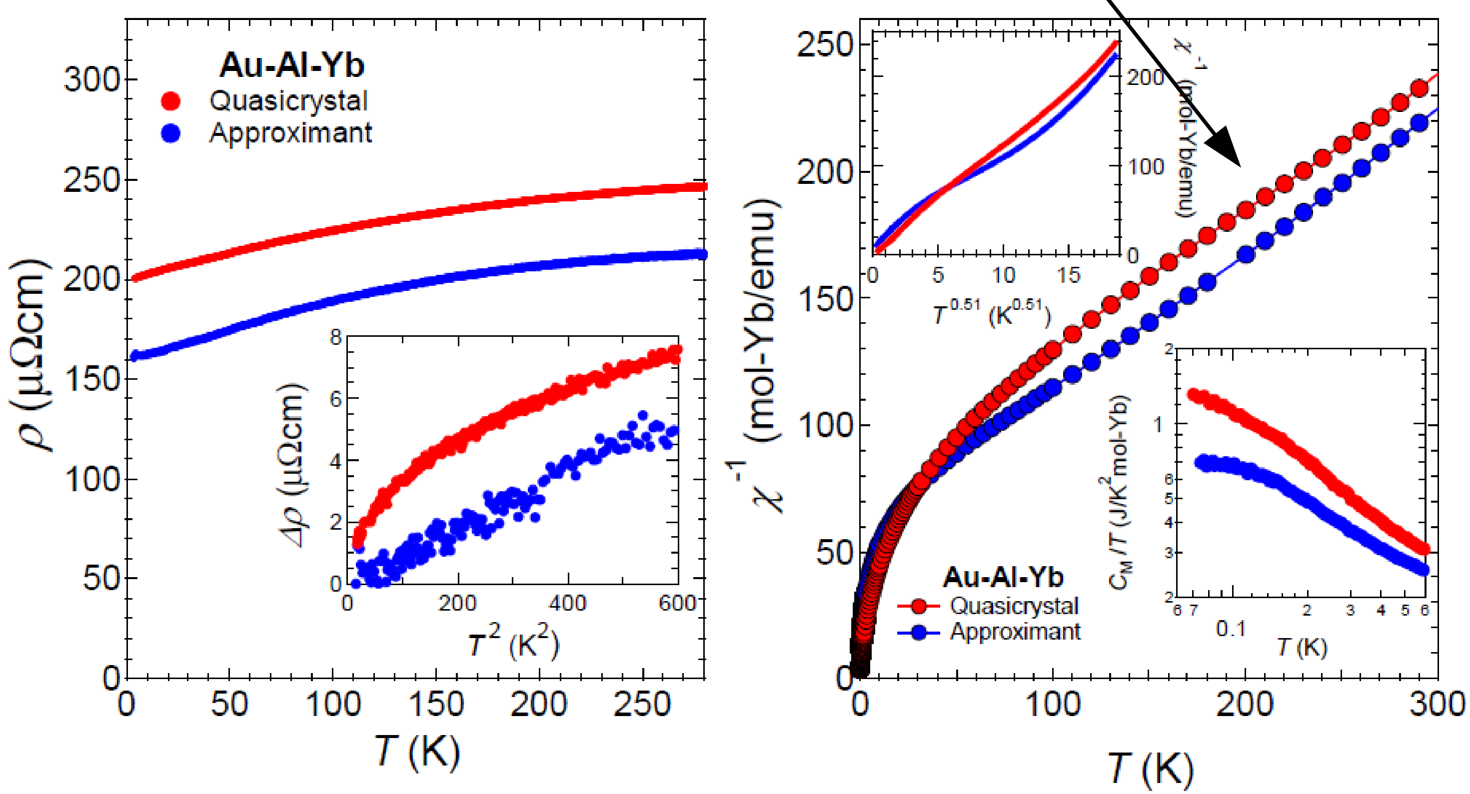
- Metallic system $\partial\rho\,(T)/\partial T > 0$



Deguchi *et al.* Nat. Mater. **11**, 1013 (2012)

$Au_{51}Al_{34}Yb_{15}$ quasicrystal: a Heavy Fermion

- Metallic system $\partial\rho\left(T\right)/\partial T>0$
- Local moments at high-T: Curie law with $\mu = 3.92\mu_B$
- Mixed-valence (2.61): Yb^{2+} (μ = 0) – Yb^{3+} ($\mu = 4.52\mu_B$)



Deguchi *et al.* Nat. Mater. **11**, 1013 (2012)

$\theta_{CW}=-153\,K$

$\theta_{CW}=-117\,K$

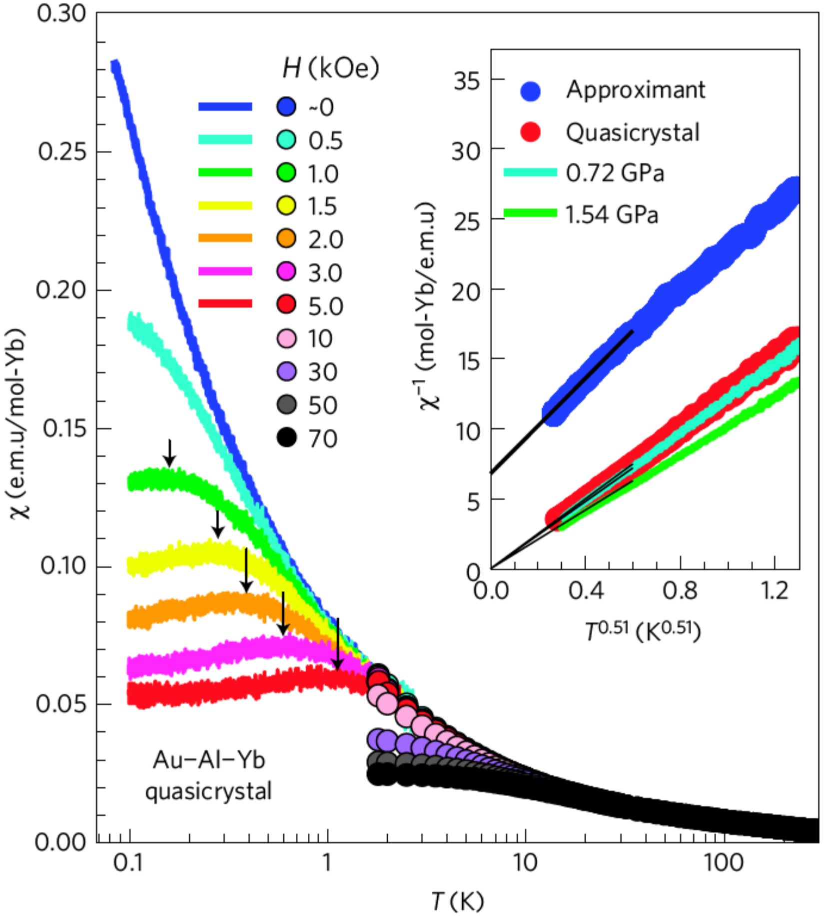
NFL behavior in the $Au_{51}Al_{34}Yb_{15}$ quasicrystal

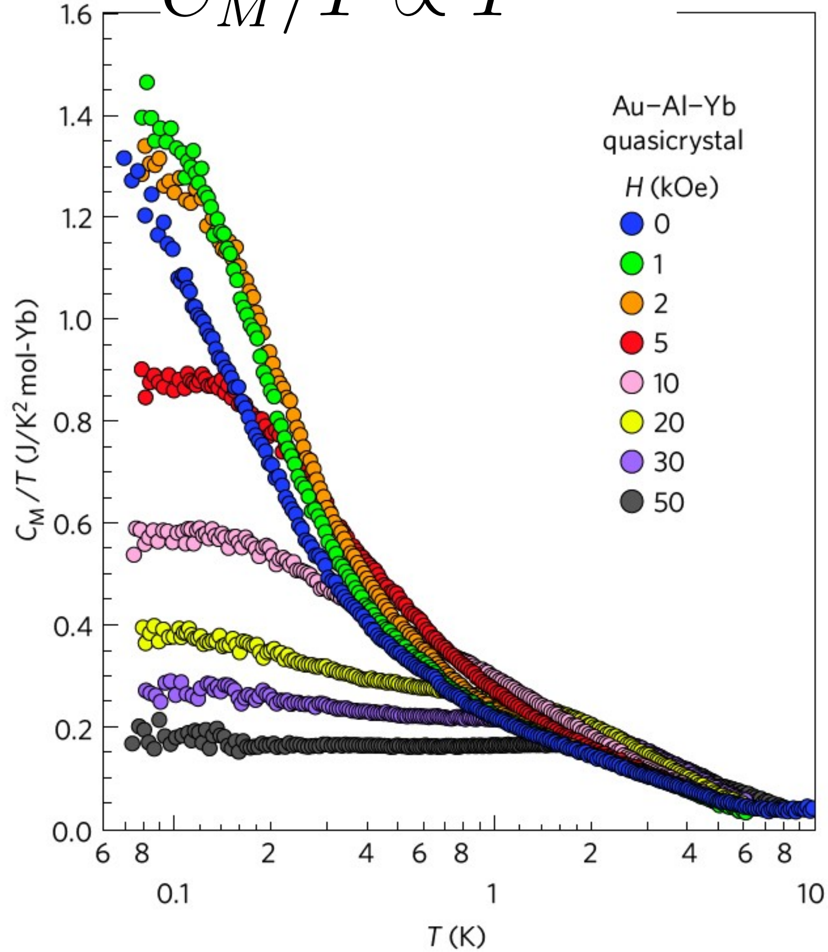
- NFL without tunning any parameter!

$$C_M/T \propto -\log(T)$$

$$C_M/T \propto T^{-0.66}$$

$$\chi \propto T^{-0.51} \quad \chi \propto T^{-0.55}$$

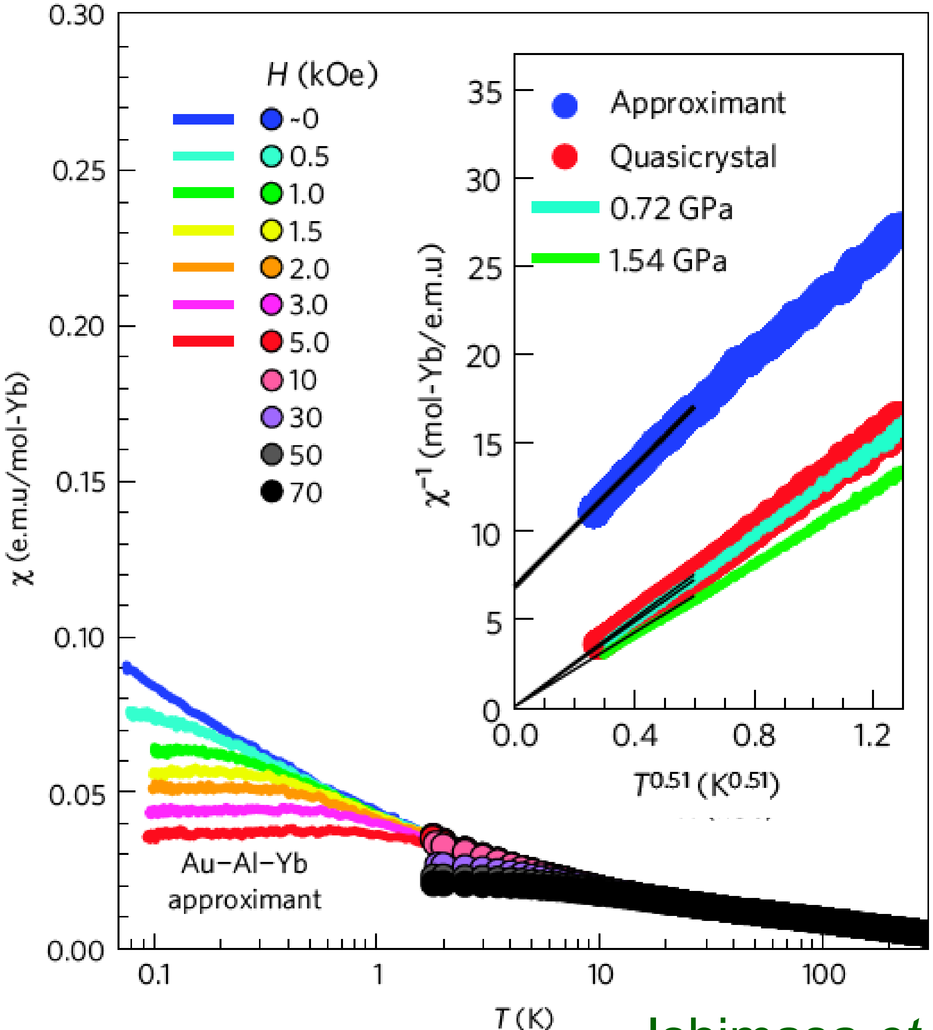


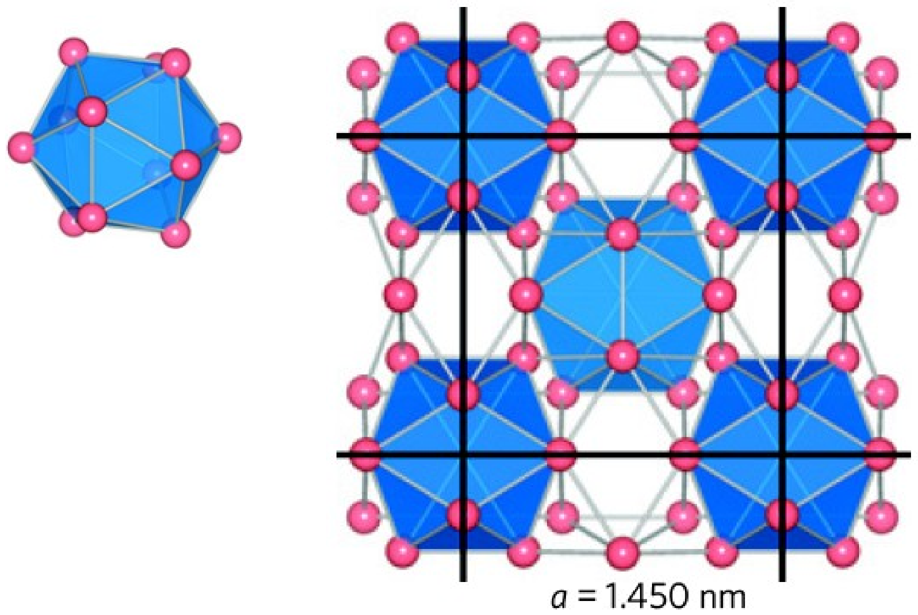


Deguchi *et al.* Nat. Mater. **11**, 1013 (2012)

Watanuki *et al.* PRB **86**, 094201 (2012)

NFL behavior in the 1/1 approximant?



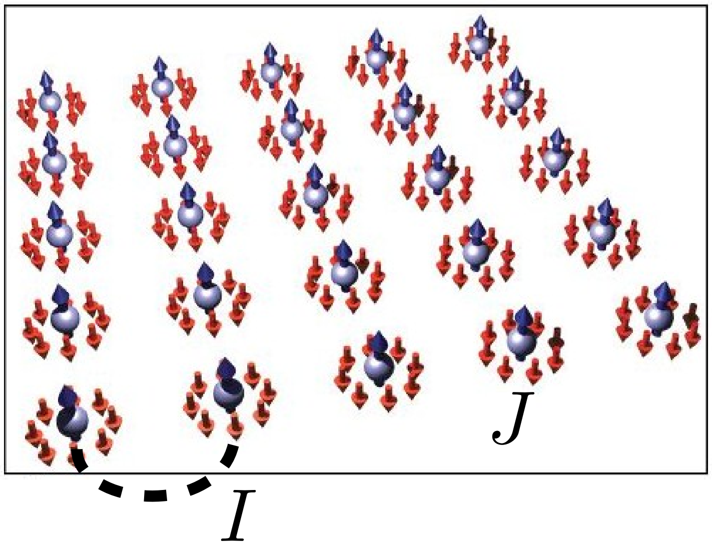


Electronic state of the light electrons: critical vs. Bloch

Ishimasa *et al.*, Philos. Mag. 91, 4218 (2011)
Deguchi *et al.* Nat. Mater. **11**, 1013 (2012) (No)
Watanuki *et al.* PRB **86**, 094201 (2012) (Yes, but ≠)

Quantum critical point scenario

- NFL behavior observed in several other Heavy Fermions
- Proximity to Quantum Critical Point
- Tuning of external parameter: field, doping, pressure, ...



$J/I \gg 1$

Kondo screening and Fermi liquid

$J/I \ll 1$

Magnetic order

Quantum critical point scenario

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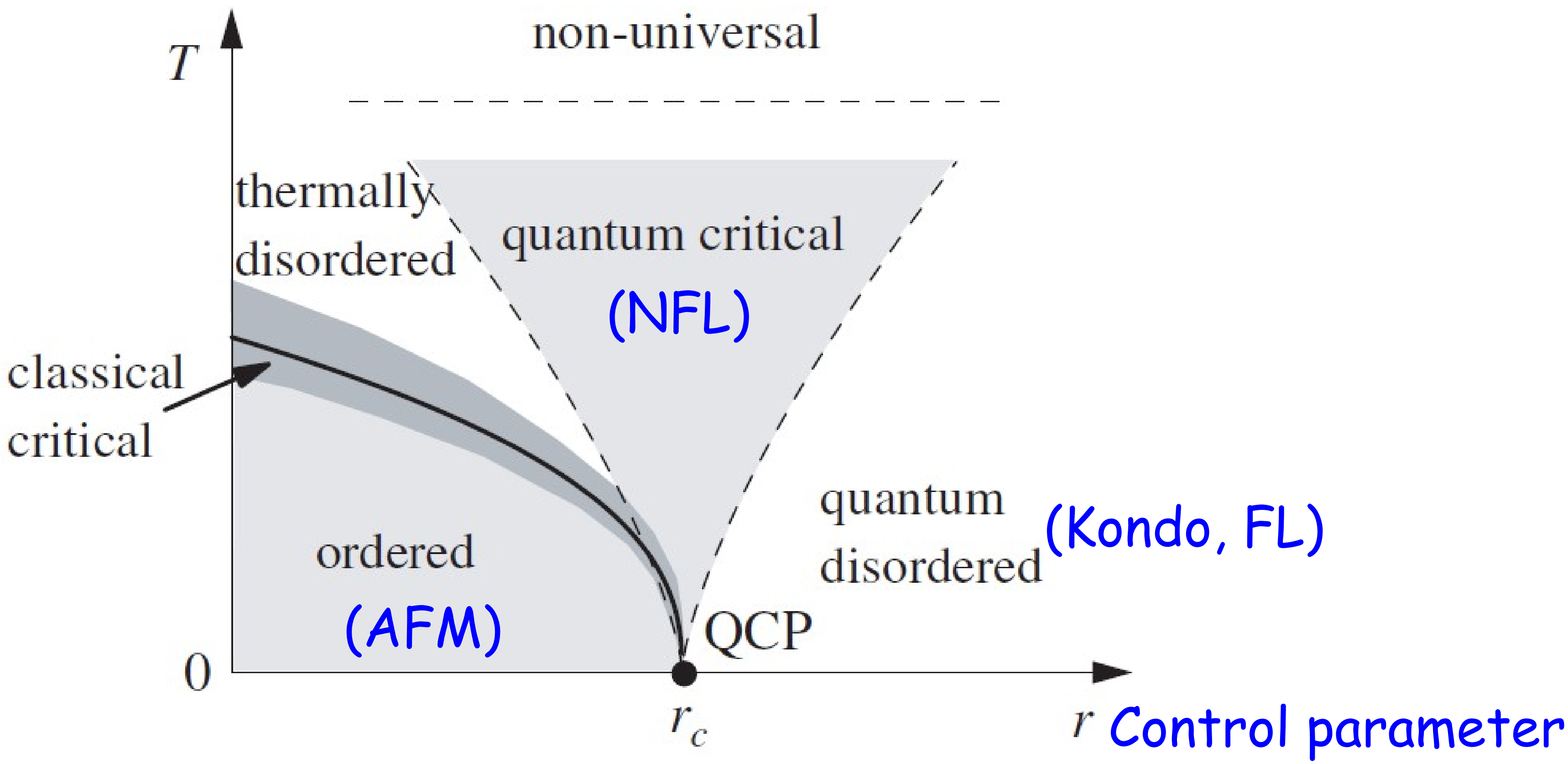

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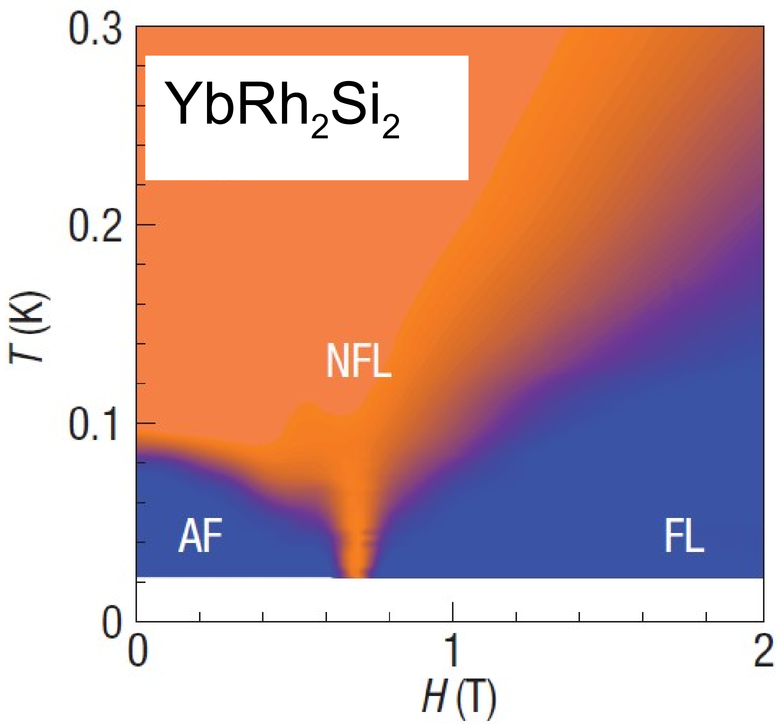
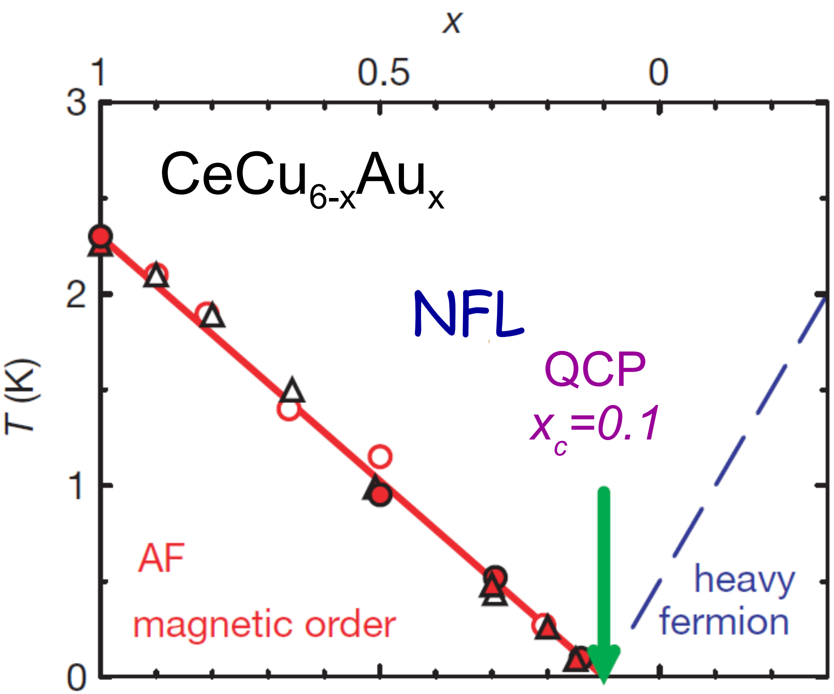


Clusters *et al.*, Nature, **424**, 524 (2003)



Schröder *et al.*, Nature, **407**, 351 (2000)

Intrinsic NFL: $Au_{51}Al_{34}Yb_{15}$ quasicrystal

- Conventional QCP approaches:
  - Quantum valence criticality

    Watanabe *et al.* J. Phys. Soc. Jpn. **82**, 083704 (2013)
  - Fermion condensation quantum phase transition

    Shaginyan *et al.* PRB **87**, 245122 (2013)
- *Parameter* driven QCP (pressure, doping, field): Fine-tuning
- Quasicrystalline environment of the light electrons considered only minimally

Our Goal: Study the Kondo problem in a quasicrystal

Outline

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- **Tiling models and quasicrystals**
  - Geometrical and electronic properties
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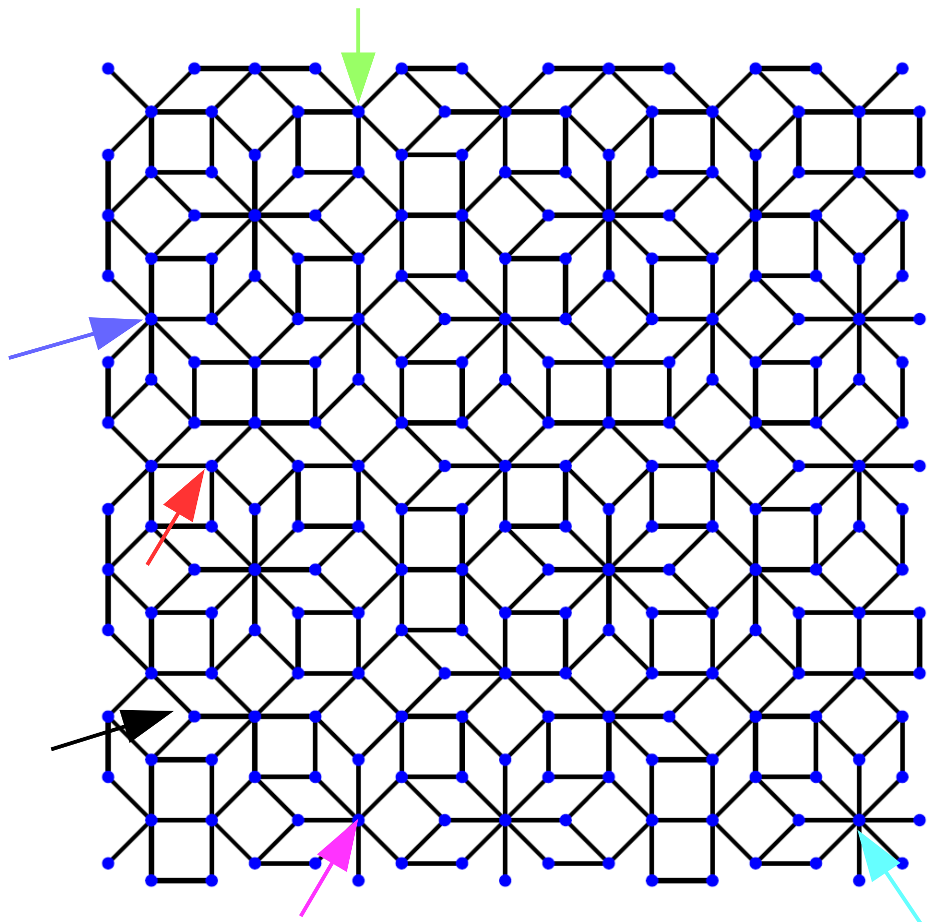
  - Power-law distribution of Kondo temperatures
  - NFL behavior
- **Conclusions**

Octagonal tiling (Ammann-Beenker)

- 2D quasicrystal. Easier to handle and akin to 3D quasicrystals
- Periodic approximants to the $N_a \to \infty$ quasicrystal
- Local environments with quasiperiodic order: z = 3,4,5,6,7,8

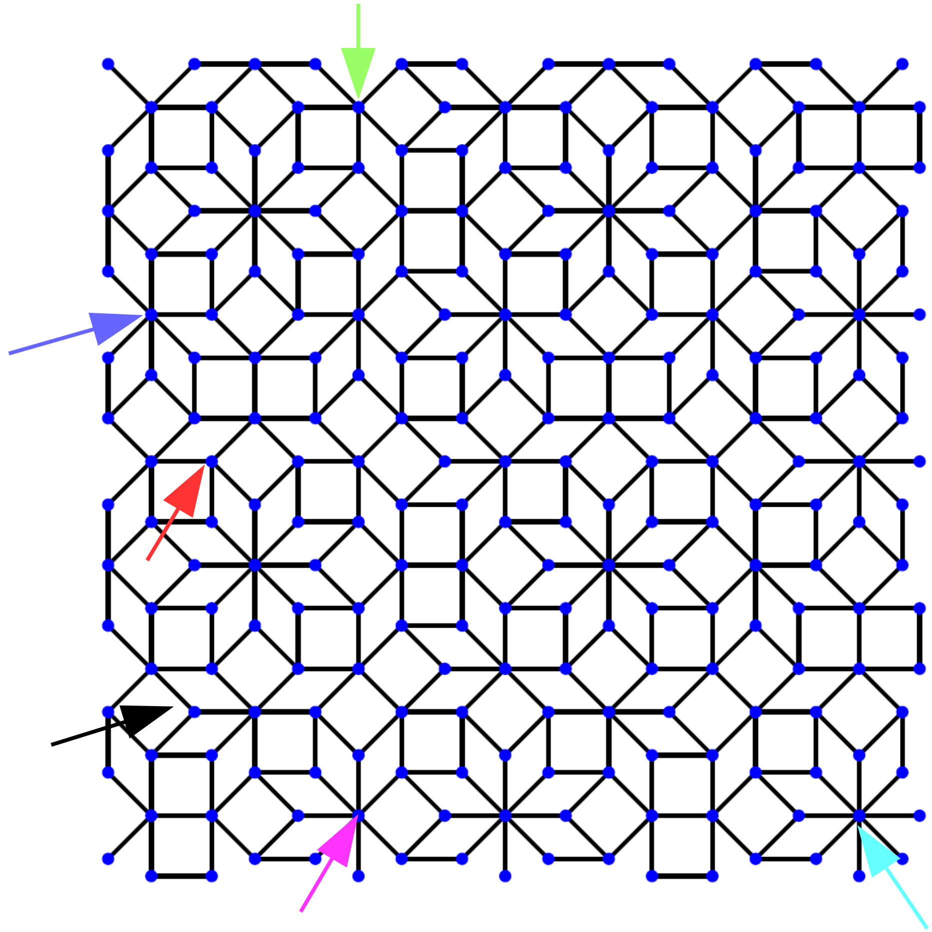


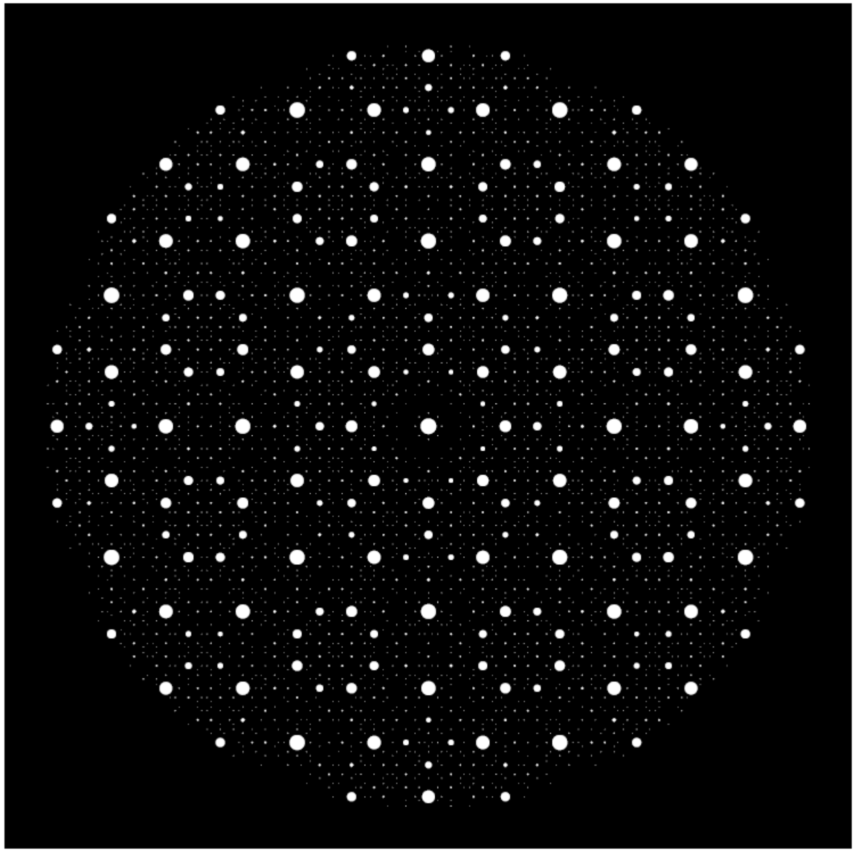
$$\sqrt{2} = 1 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \cfrac{1}{2 + \ddots}}}}.$$

$$N_a = 7,\ 41,\ 239,\ 1393,\ \ldots$$

Octagonal tiling (Ammann-Beenker)

- Local environments with quasiperiodic order: z = 3,4,5,6,7,8
- *8*-fold symmetry: Equiprobable orientation of local environments

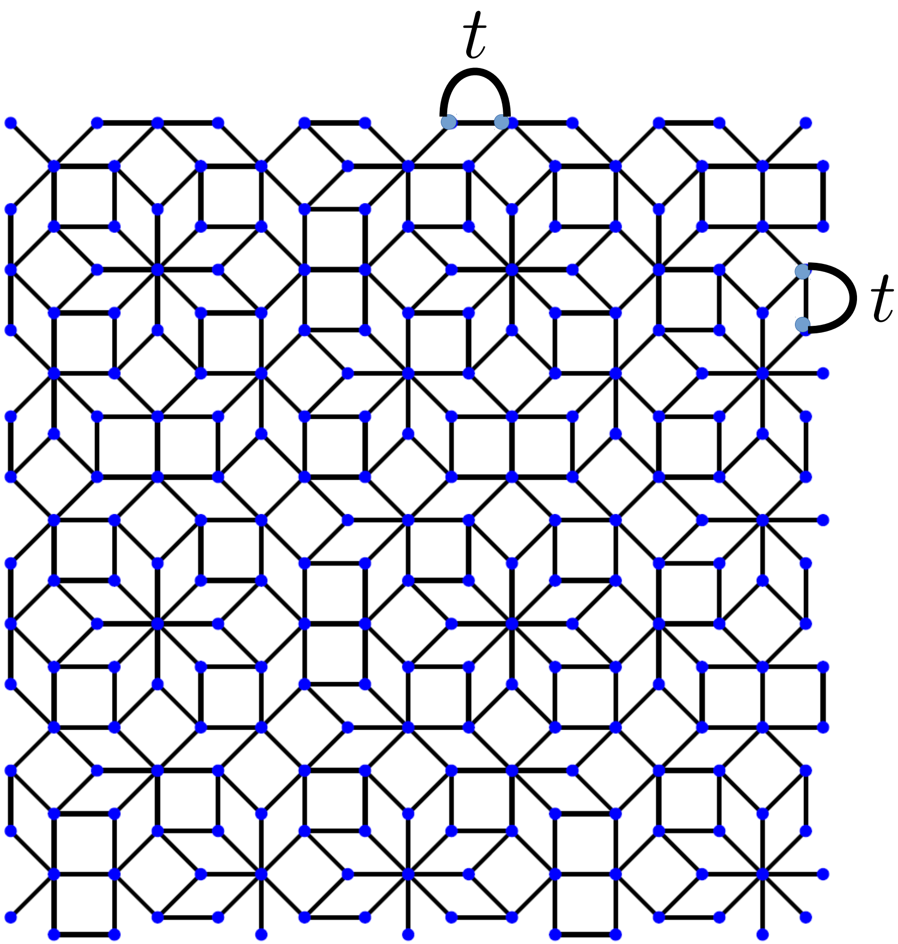




Octagonal tiling – Electronic properties

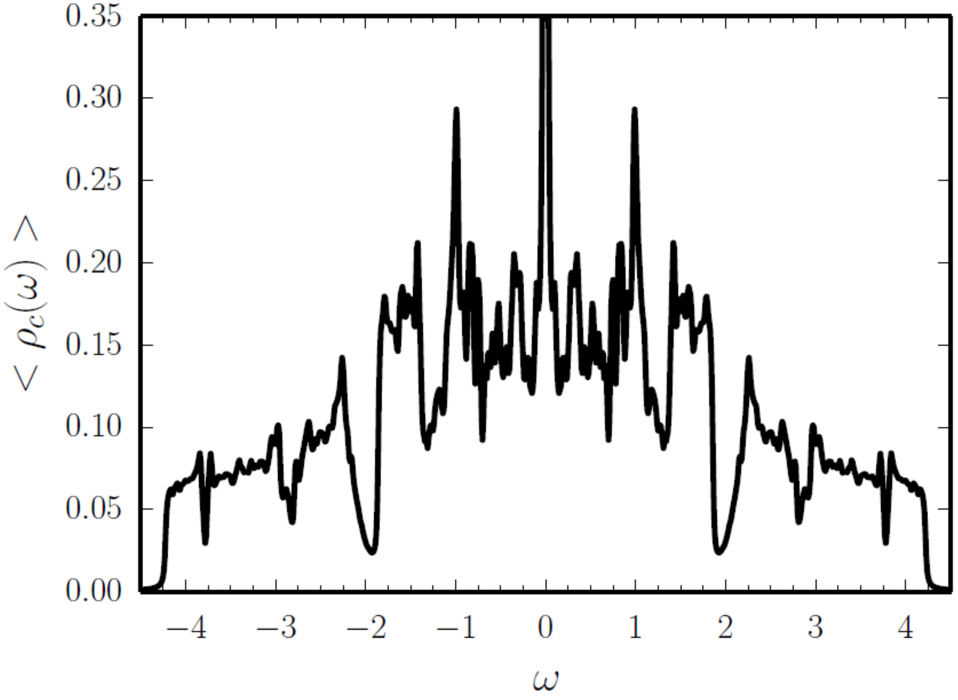
- Nearest neighbor tight-biding model. Non-interacting electrons hopping in a *quasiperiodic* potential

$$\mathcal{H}_c = -t \sum_{\langle ij \rangle, \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right)$$



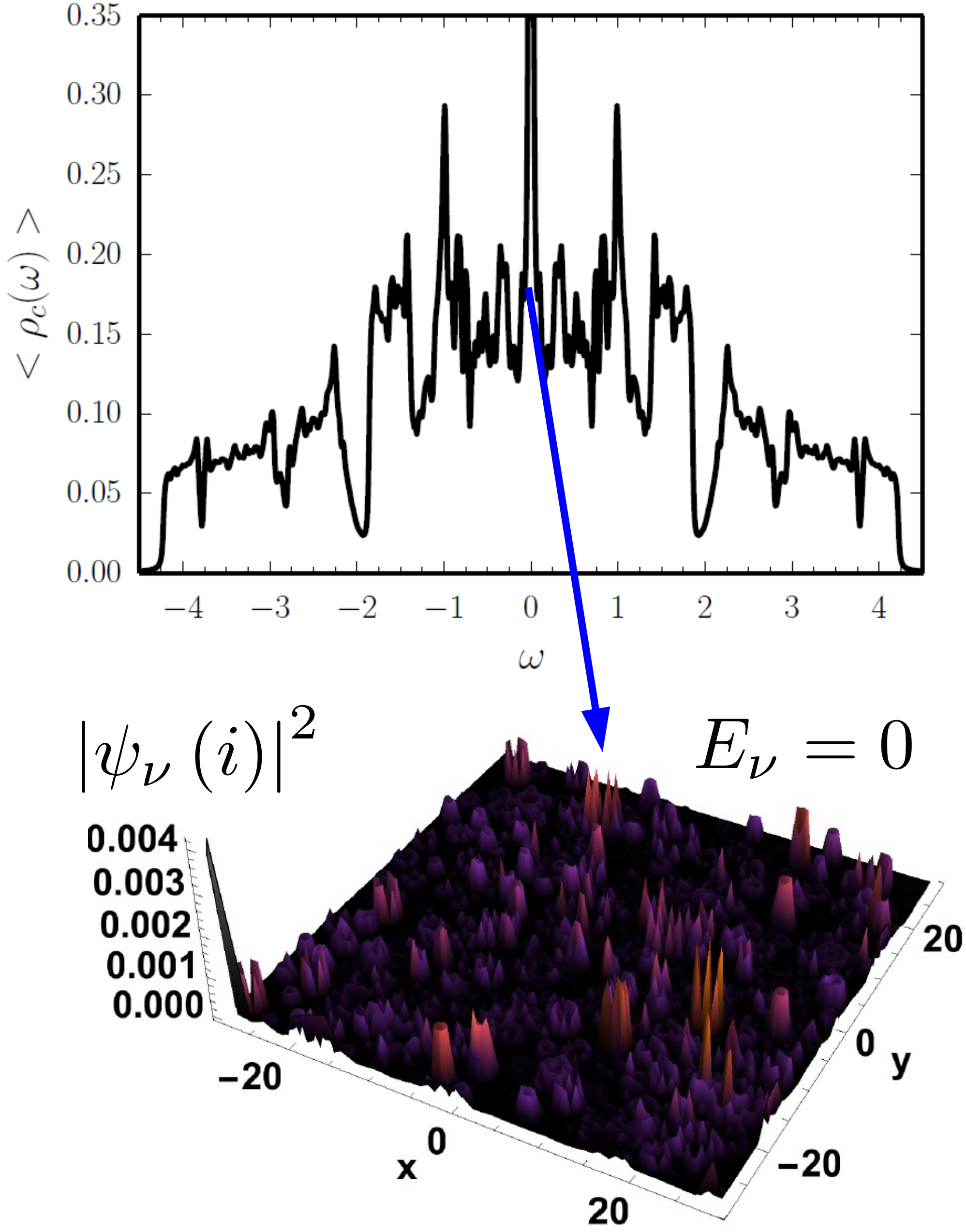
- Socolar, PRB **39**, 10519 (1989)
- Duneau, J. Phys. A **22**, 4549 (1989)
- Benza/Sire, PRB **44**, 10343 (1991)
- Grimm/Schreiber, in Quasicrystals—Structure and Physical Properties
- Jagannathan/Piéchon, Philos. Mag. **87**, 2389 (2007)
- ...

Octagonal tiling – DOS and wave function



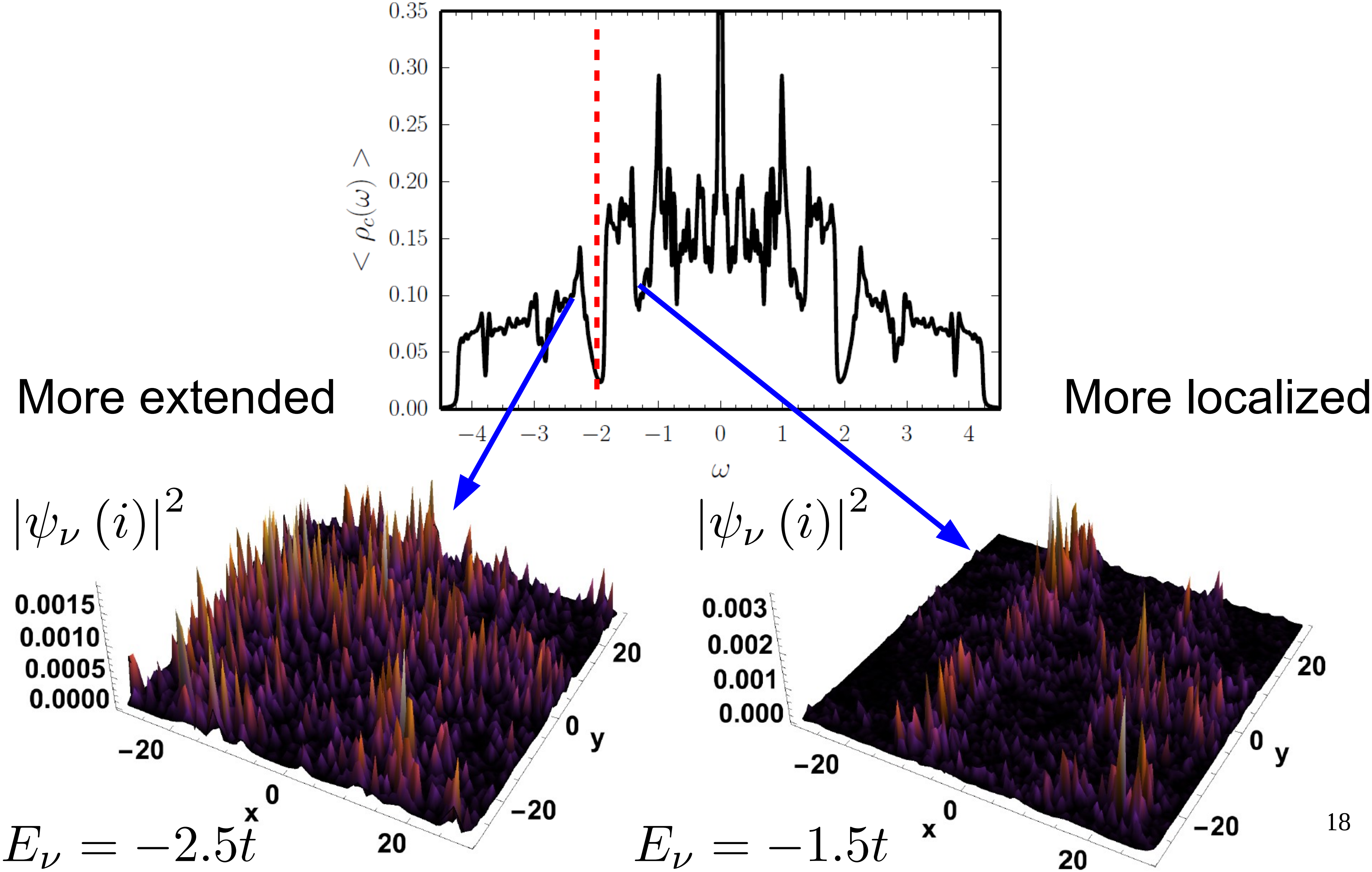
- Spiked: several “Bragg peaks”
- Particle-hole symmetric

Octagonal tiling – DOS and wave function

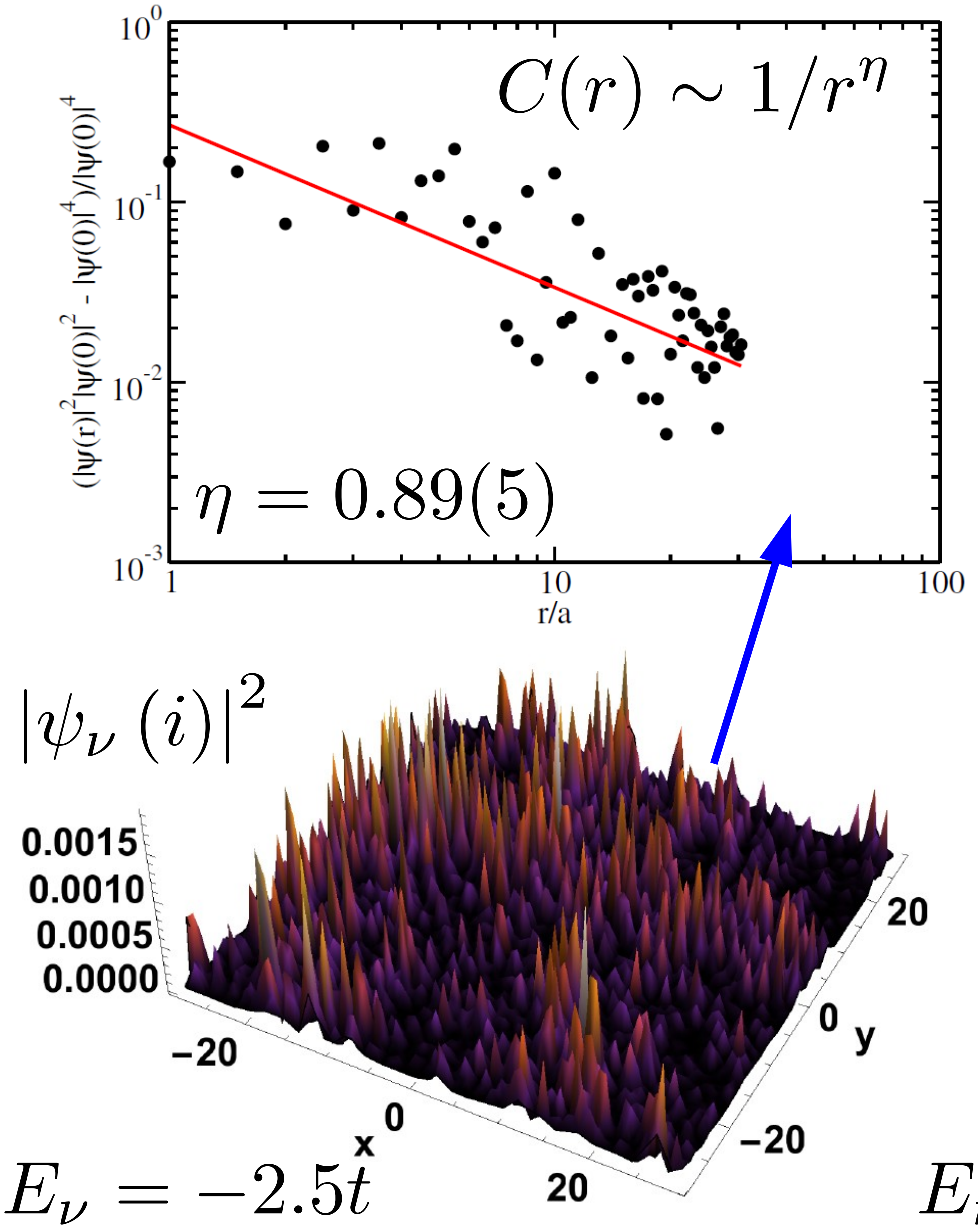


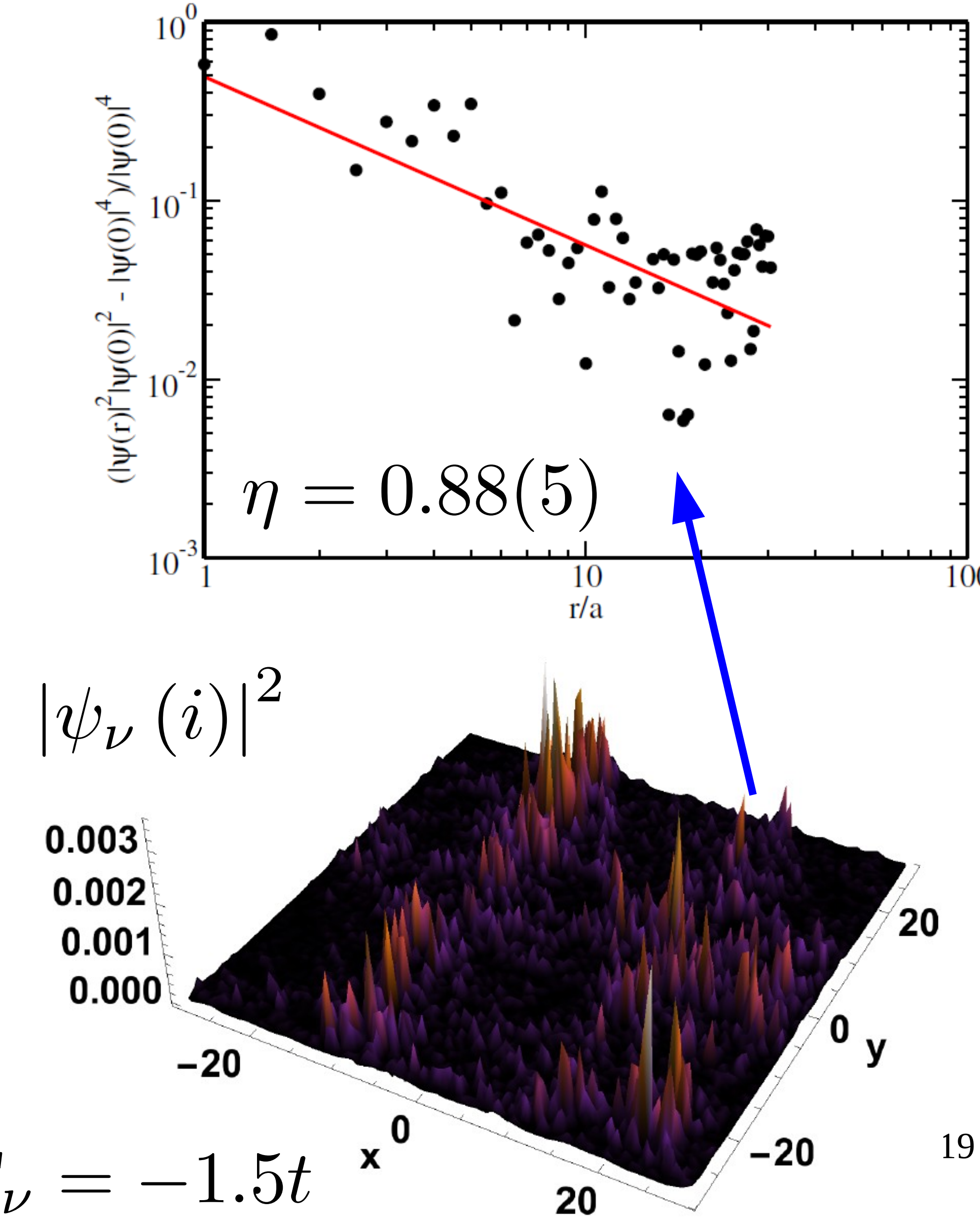
Localized states around the *z=8* sites. Special feature of the tiling

Octagonal tiling – DOS and wave function



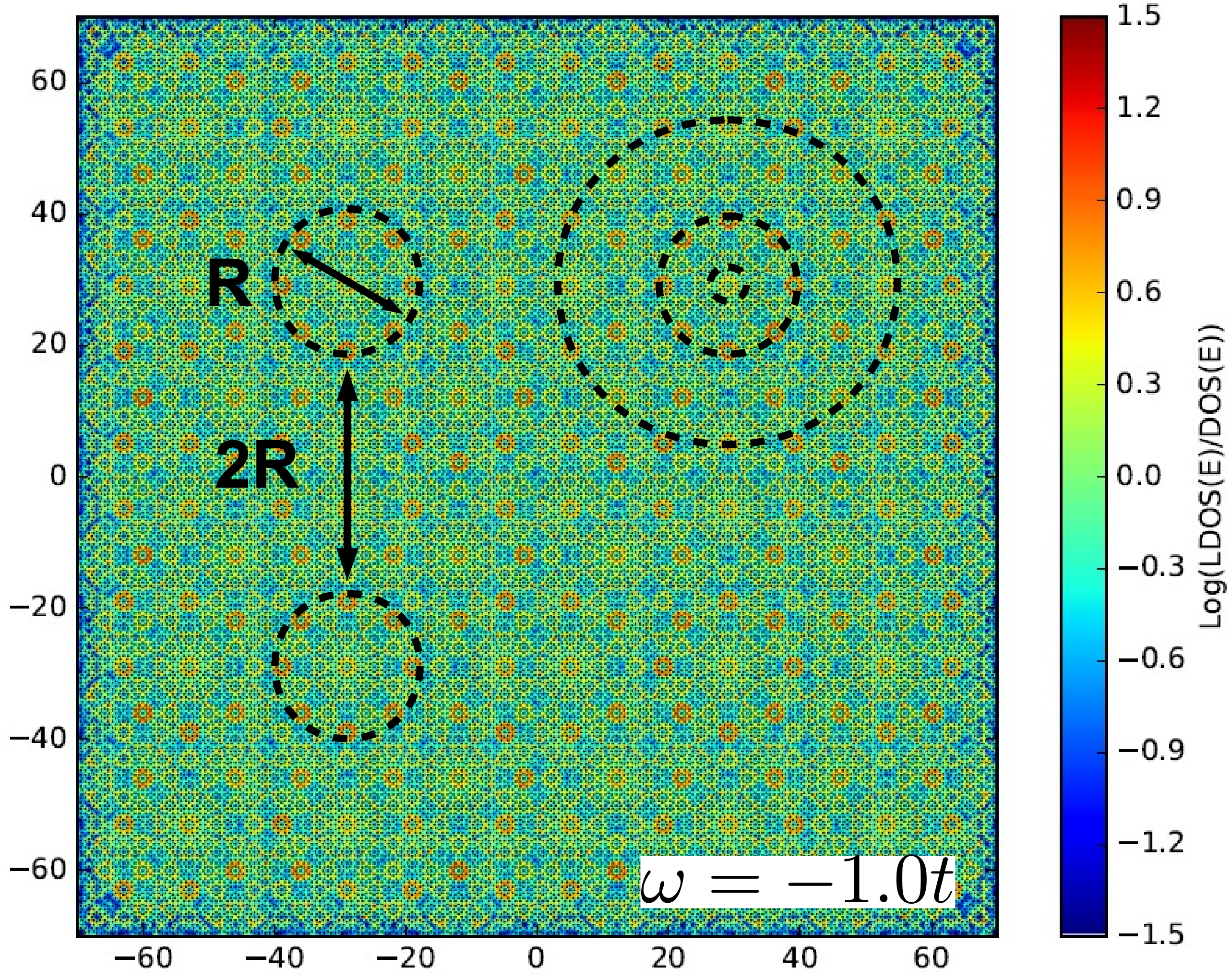
Octagonal tiling – Critical wave function





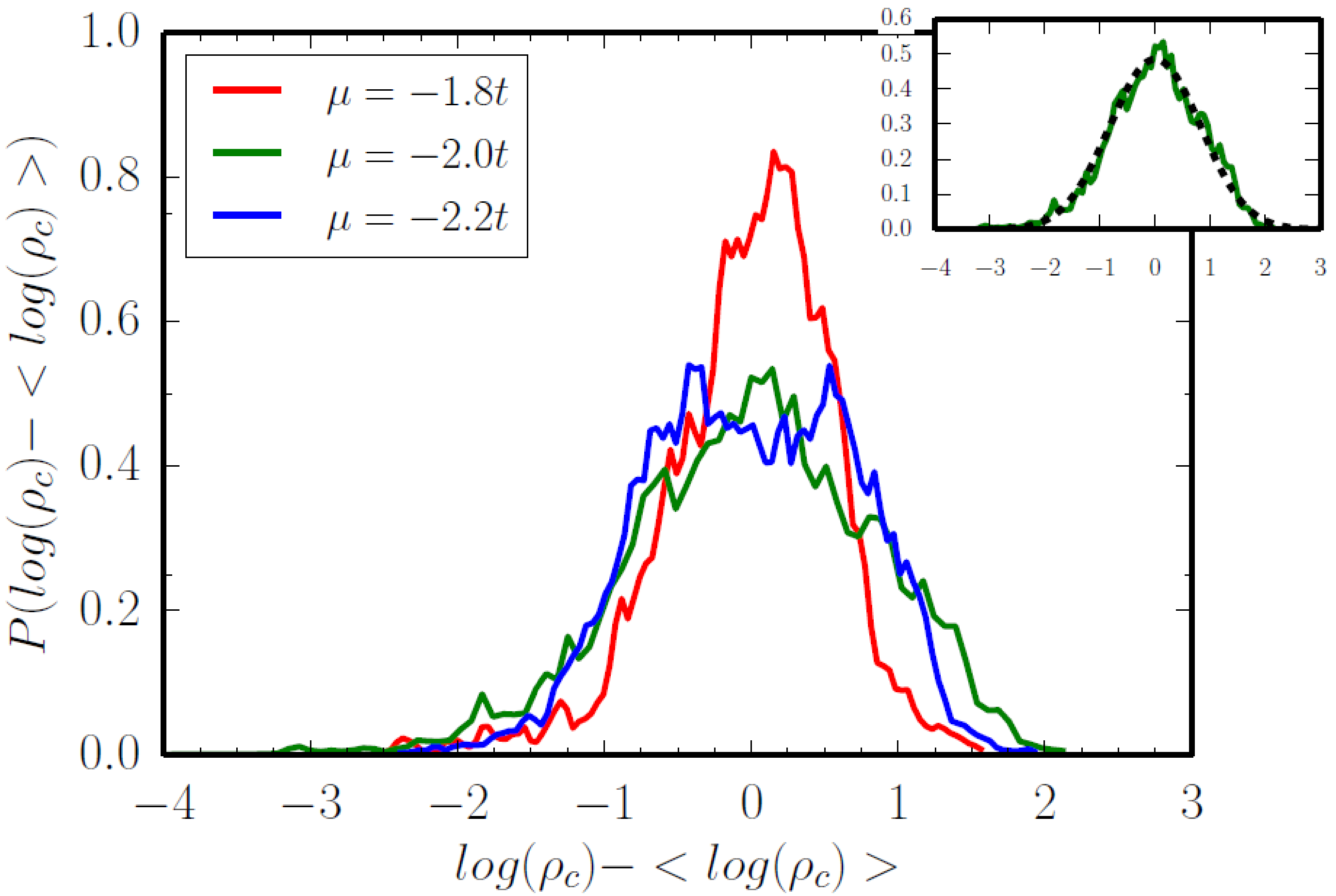
Octagonal tiling – Local density of states

- “Translation invariance” (Conway theorem): identical regions of size R are spaced ~ 2R apart



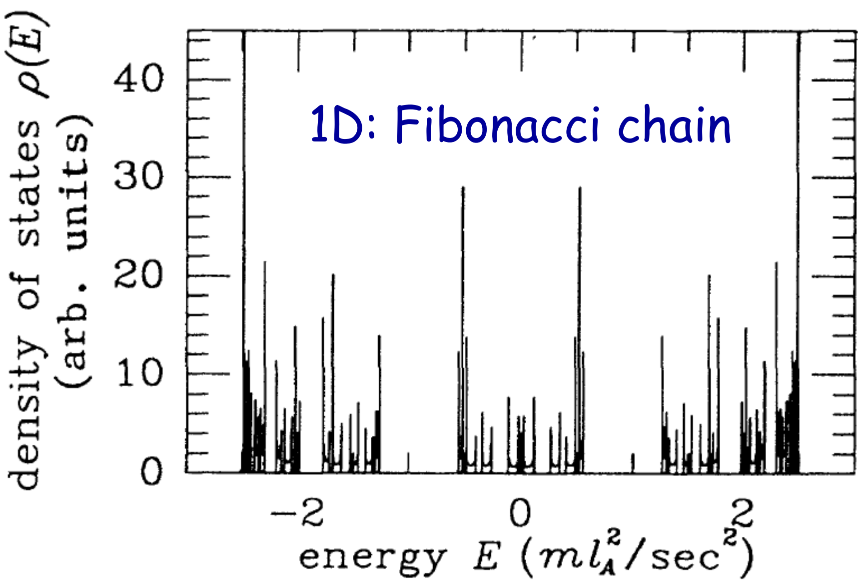
Octagonal tiling – Density of states

- LDOS is site dependent
- Log-normal distribution envelope in real space (fixed μ)

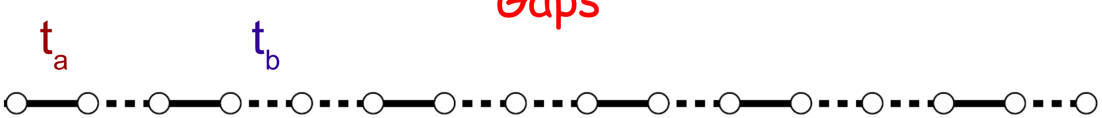


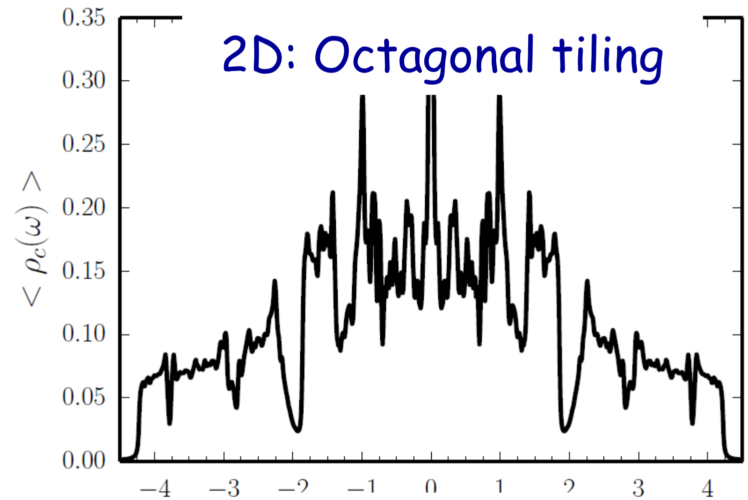
Density of states in different tilings

- DOS becomes less “spiky” as the dimension increases

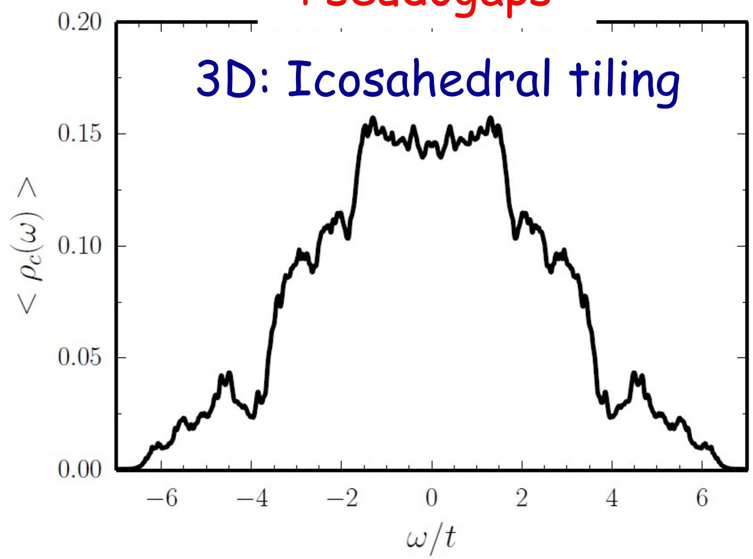


Gaps





Pseudogaps



Newman, PRB **43**, 10915 (1991)
Zijlstra/Janssen, EPL **52**, 578 (2000)

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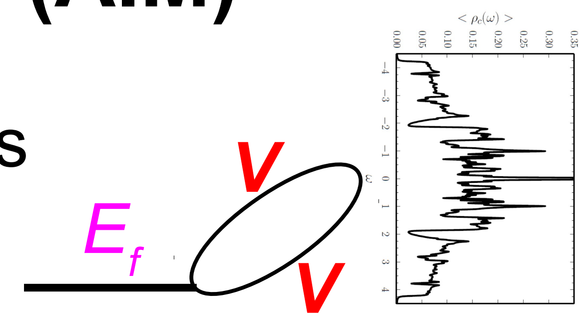
Anderson impurity model (AIM)



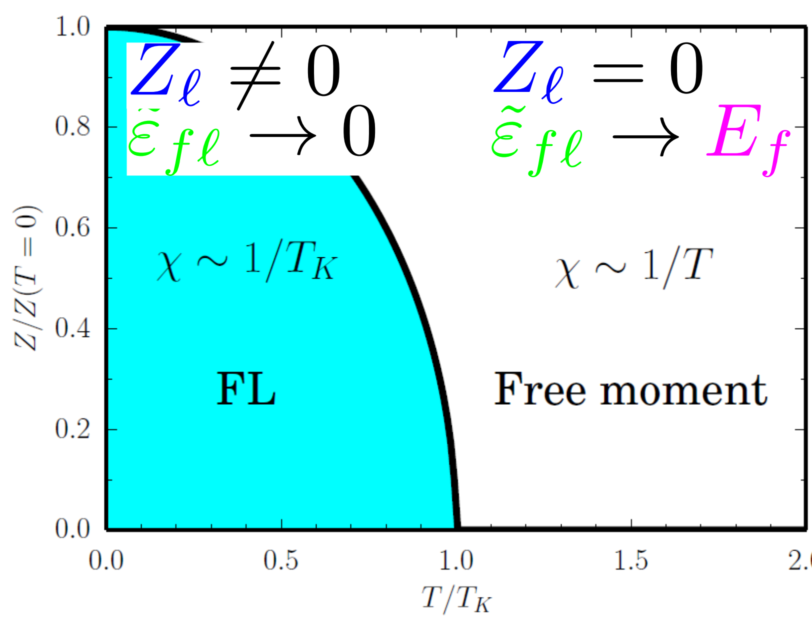
- Localized *f*-orbital hybridizes with *c*-electrons
- $U \to \infty$ AIM: Mixed-valence ($n_f \leq 1$)
- Slave-boson MF approach at *T=0*

$$\mathcal{H} = \mathcal{H}_c + \tilde{\varepsilon}_{f\ell} \sum_{\sigma} n_{f\sigma} + V\sqrt{Z_\ell} \sum_{\sigma} \left(f^{\dagger}_{\ell\sigma} c_{\ell\sigma} + c^{\dagger}_{\ell\sigma} f_{\ell\sigma} \right) + (\tilde{\varepsilon}_{f\ell} - E_f)(Z_\ell - 1)$$

- Low-energy description

$$\tilde{V} = V\sqrt{Z_\ell} \qquad J = 2V^2/\left|E_f\right|$$

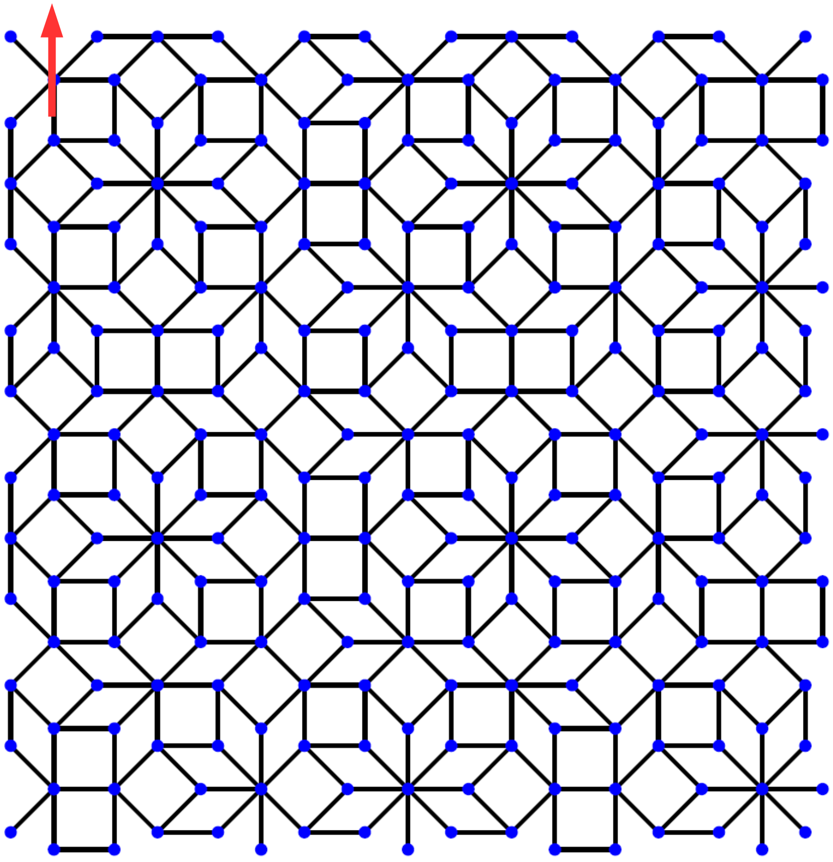
$$T_K^{\ell} = D\exp\left[-\frac{\pi}{2}\frac{\Delta'_{f\ell}(0) + |E_f|}{\Delta''_{f\ell}(0)}\right]$$



Read/Newns, J. Phys. C **16**, L1055 (1983)
Coleman, PRB **29**, 3035 (1984)

Kondo impurities in a quasicrystal

- Quasicrystal → Different environments: $\Delta_{f\ell}(\omega) = V^2 G^c_{\ell\ell}(\omega)$
- One Kondo impurity at each site. N_a values of T_K: $P(T_K)$



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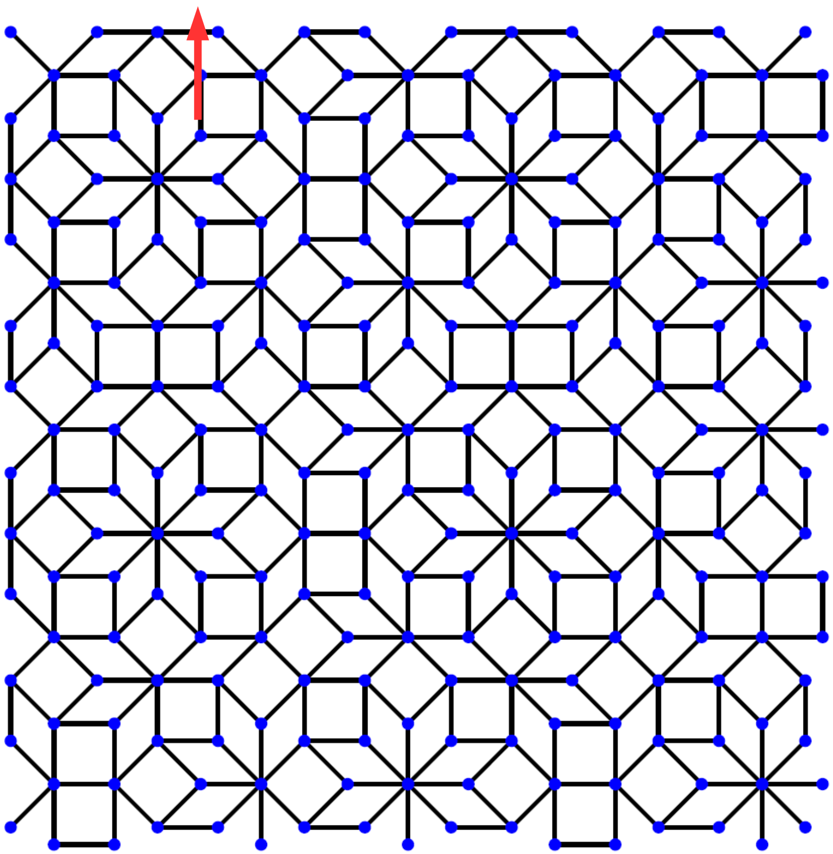

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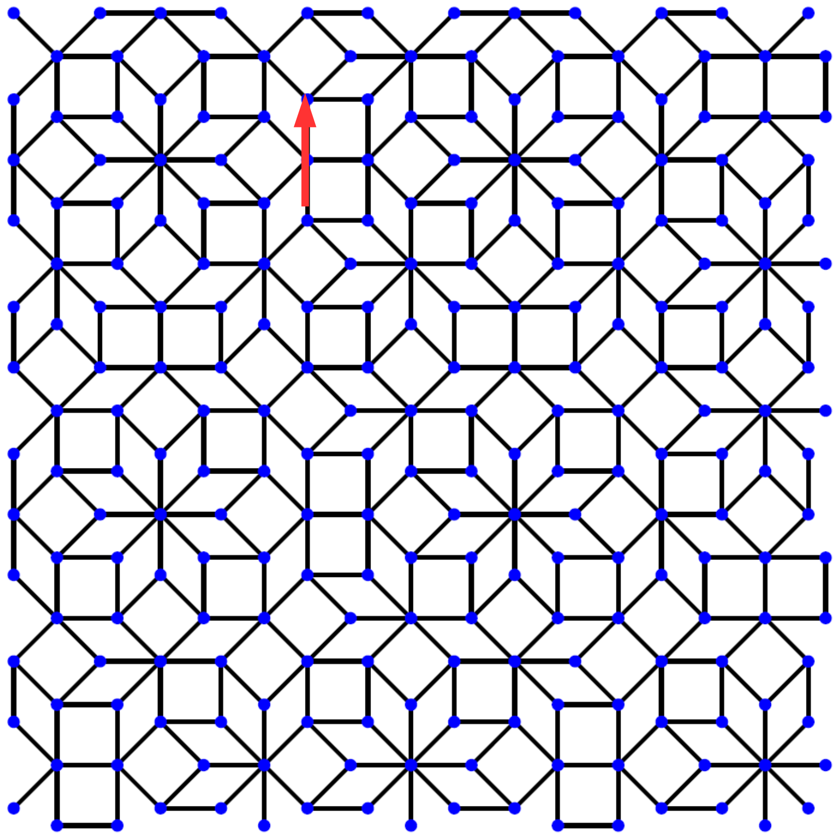
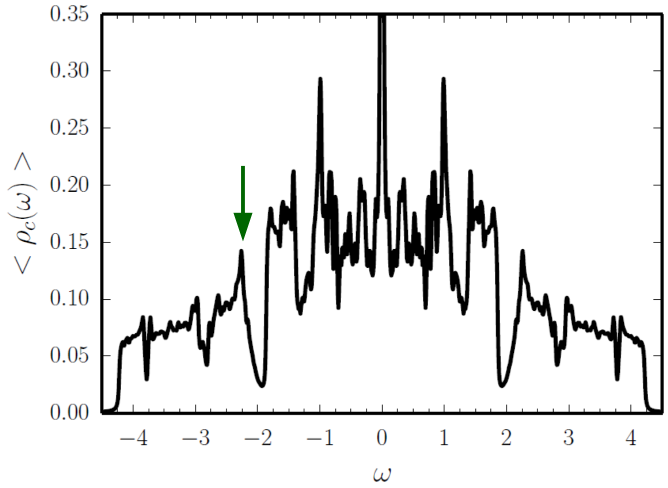
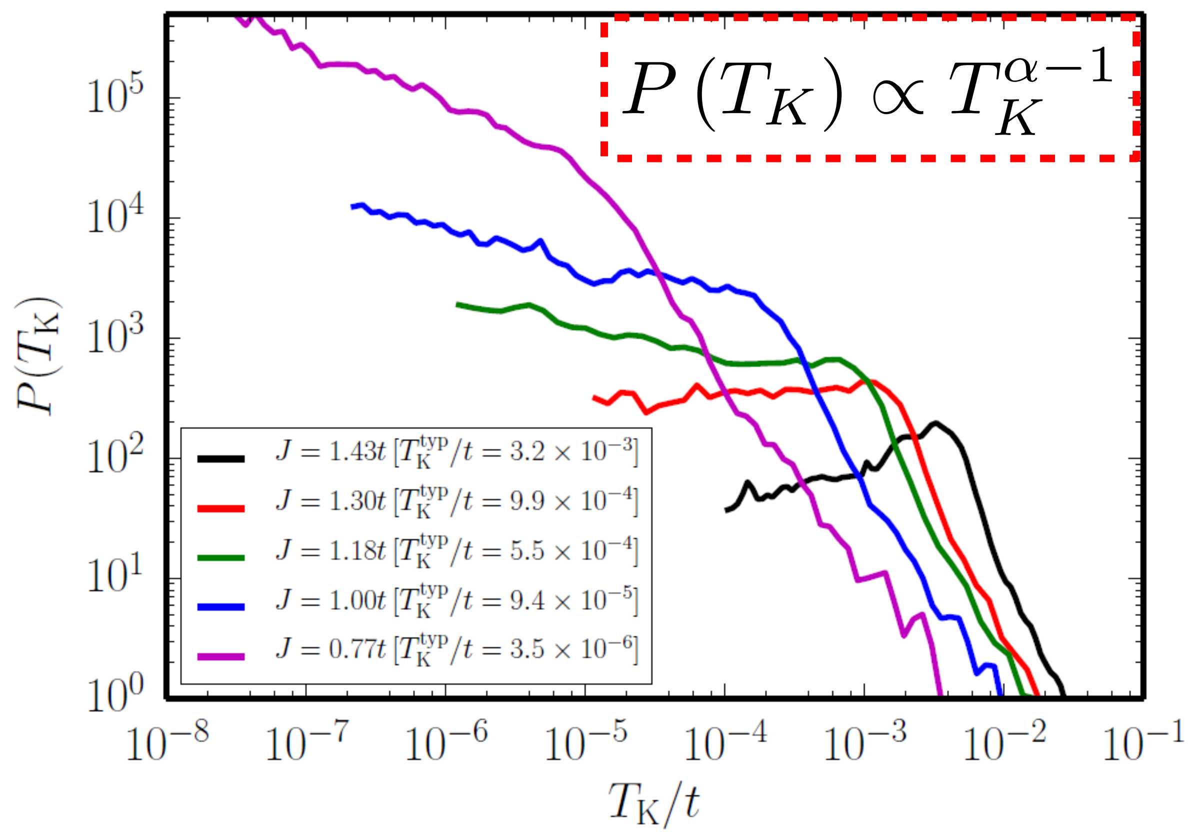


Power-law distribution of Kondo temperatures

- Quasicrystal → Different environments: $\Delta_{f\ell}(\omega) = V^2 G^c_{\ell\ell}(\omega)$
- One Kondo impurity at each site. N_a values of T_K: $P(T_K)$
- Remarkably, we get a power-law distribution at low-T_K



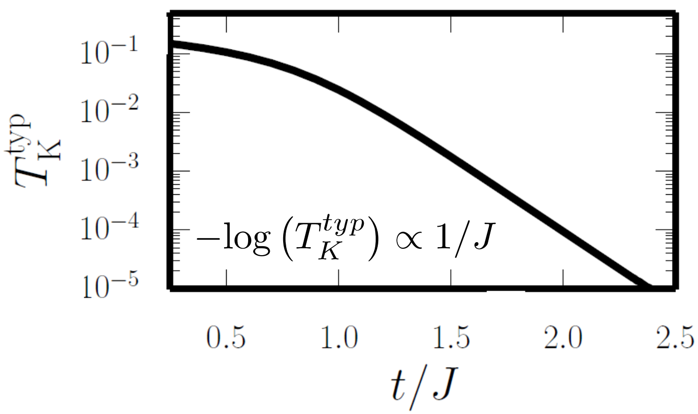
$$\mu = -2.2t$$
$$N_a = 1393$$
$$J = 2V^2/|E_f|$$



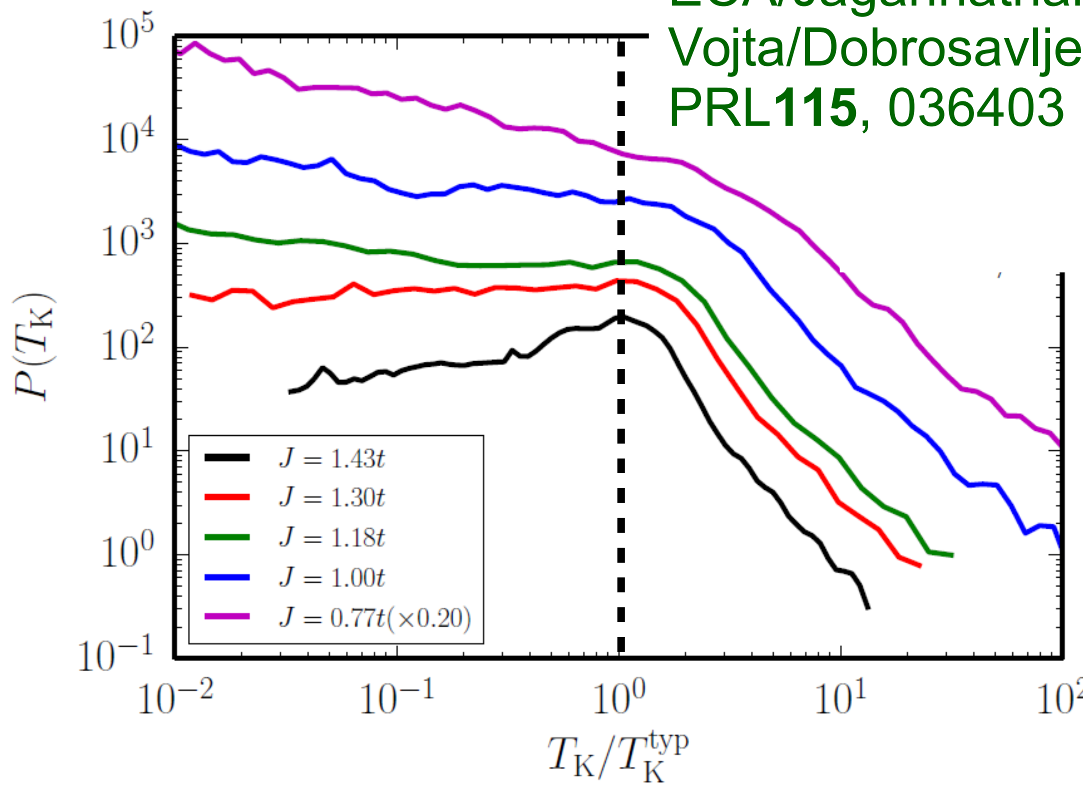
Power-law distribution of Kondo temperatures

- Quasicrystal → Different environments: $\Delta_{f\ell}(\omega) = V^2 G^c_{\ell\ell}(\omega)$
- One Kondo impurity at each site. N_a values of T_K: $P(T_K)$
- Remarkably, we get a power-law distribution below T_K^{typ}

$$T_K^{typ} \equiv \exp\left[\langle \ln (T_K) \rangle\right]$$



ECA/Jagannathan/Miranda/Vojta/Dobrosavljević PRL**115**, 036403 (2015)



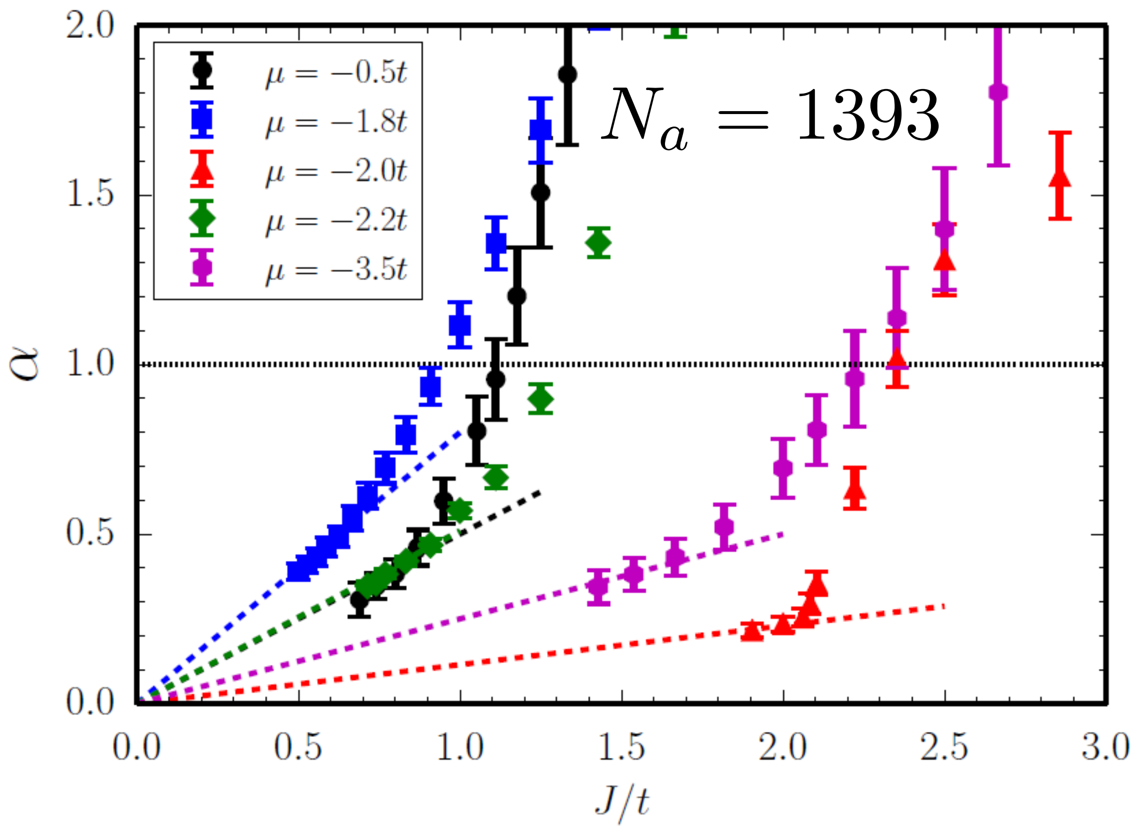
$$\mu = -2.2t$$

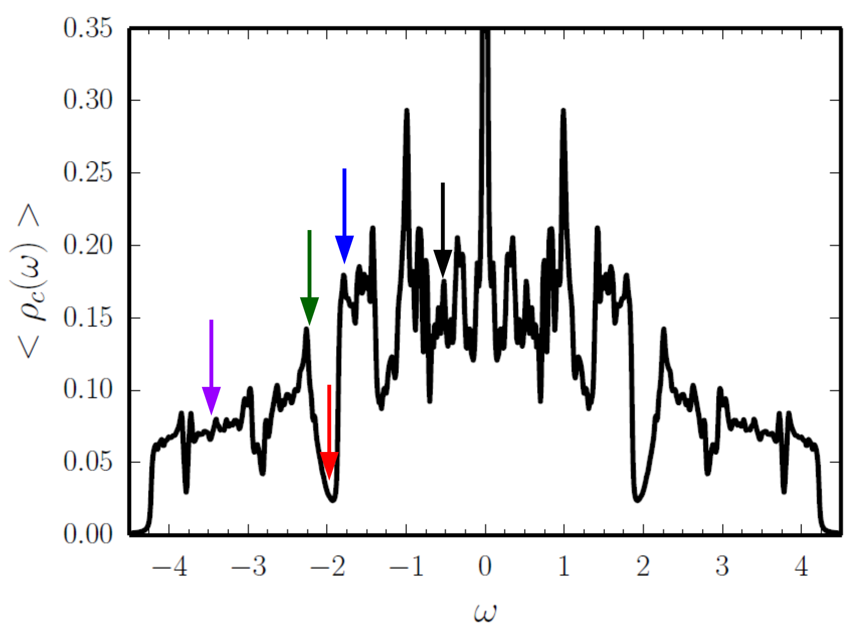
$$N_a = 1393$$

$$J = 2V^2/|E_f|$$

Non-universal power-law exponent α

- $P\left(T_K\right) \propto T_K^{\alpha-1}$ for all μ, with $\alpha \propto J\left\langle \rho_c\left(0\right)\right\rangle$ as $J \rightarrow 0$
- As the DOS, α has a huge energy dependence
- NFL liquid behavior for $\alpha < 1$. Unquenched spins: $T_K \rightarrow 0$





ECA/Jagannathan/Miranda/
Vojta/Dobrosavljević
PRL**115**, 036403 (2015)

Free spins at low-T: route to NFL

- Number of free local moments at a given T

Spins with $T_K < T$: essentially free

$$n_{free}(T) = \int_0^T P(T_K)\, dT_K \sim \int_0^T T_K^{\alpha-1} dT_K \sim T^{\alpha}$$

- Susceptibility

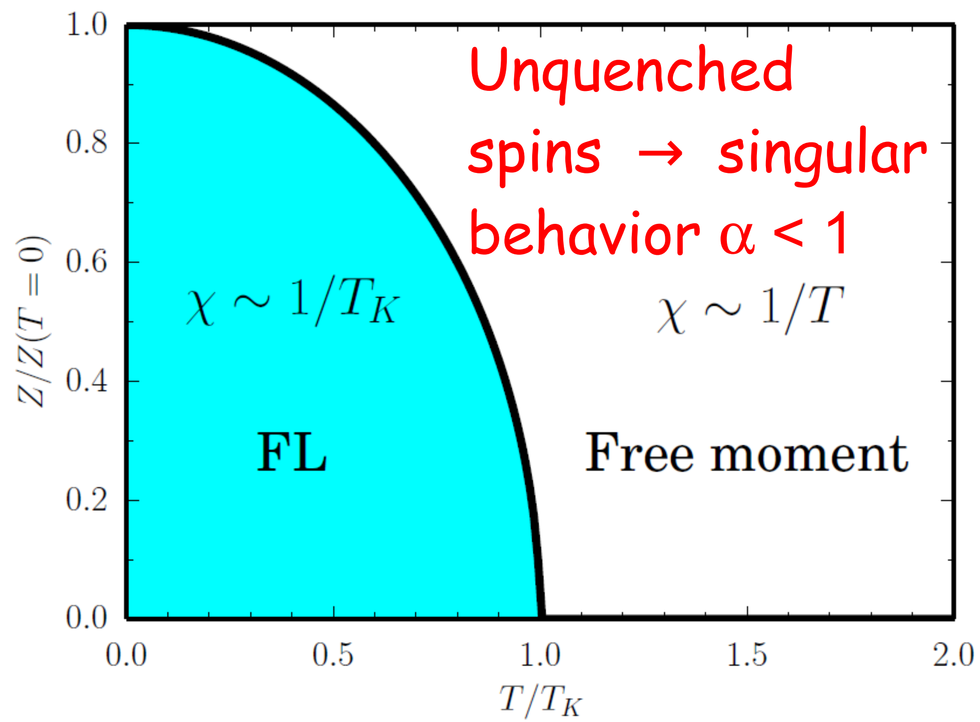
$$\chi(T) \sim n_{free}(T)/T \sim T^{\alpha-1}$$

- Entropy

$$S(T) \sim n_{free}(T)\, ln2 \sim T^{\alpha}$$

- Sommerfeld coefficient

$$\gamma(T) = \frac{C(T)}{T} = \frac{\partial S}{\partial T} \sim T^{\alpha-1}$$



NFL behavior – Free spins at T → 0

- Single energy scale: $\begin{cases} T \lesssim T_K, & \text{Fermi-liquid} \\ T \gtrsim T_K, & \text{Free spin} \end{cases}$ $\chi\left(T, T_K\right) = \frac{1}{T_K} f\left(\frac{T}{T_K}\right)$
- Averaged value of the single-impurity susceptibility

$$\langle \chi\left(T\right) \rangle = \int dT_K P\left(T_K\right) \chi\left(T, T_K\right) = \chi_r + \underbrace{\int_0^{\Lambda} dT_K T_K^{\alpha-1} \frac{1}{T_K} f\left(\frac{T}{T_K}\right)}_{\propto T^{\alpha-1}}$$

Regular + Singular

- Miranda/Dobrosavljević/Kotliar, J. Phys. Cond. Mat **8**, 9871 (1996)
- Rappoport/Boechat/Saguia/Continentino, EPL **61**, 831 (2003)
- Cornaglia/Grempel/Balseiro, PRL **96**, 117209 (2006)
- Kettemann/Mucciolo/Varga, PRL **103**, 126401 (2009)
- Miranda/Dias da Silva/Lewenkopf, PRB **90**, 201101 (2014)
- ...

$$\chi\left(T\right) \sim N(T)/T \propto T^{\alpha-1}$$

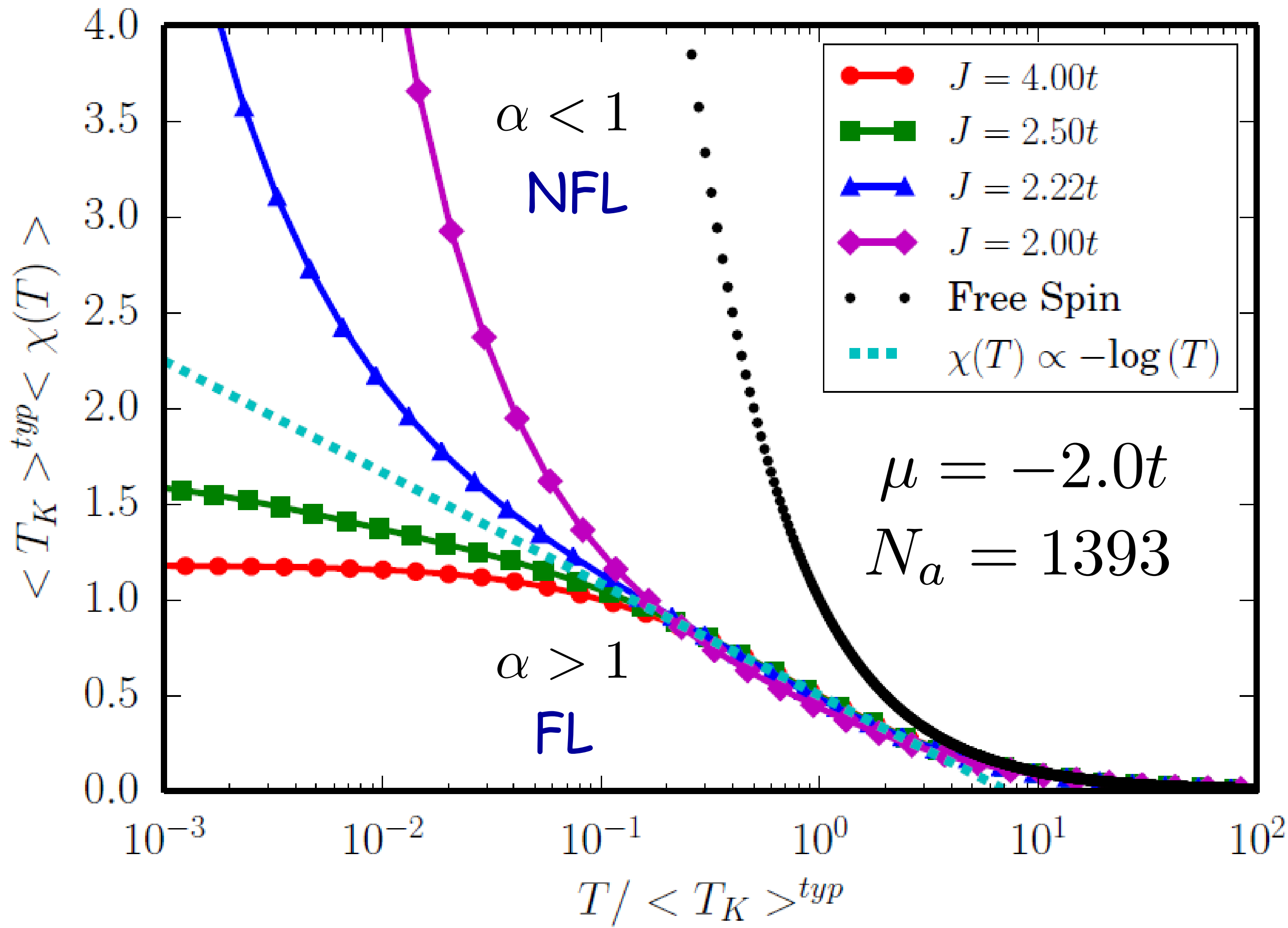
$$C/T = \gamma\left(T\right) \propto T^{\alpha-1}$$

$$\chi/\gamma \sim cte$$

$$1/T_1 T \propto T^{\alpha-2}$$

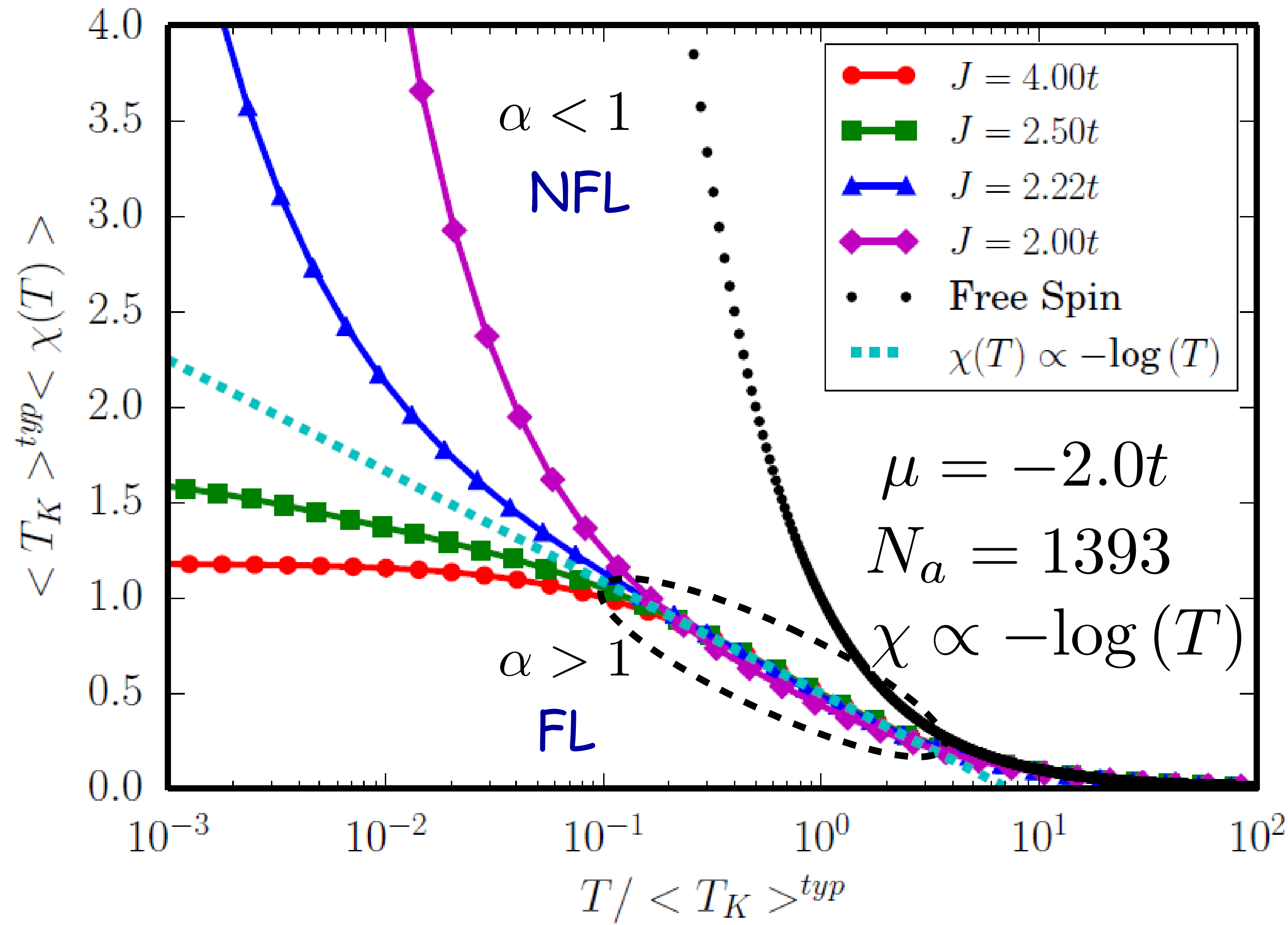
NFL behavior – Octagonal tiling

A power-law distribution of Kondo temperatures, leads to a power-law susceptibility



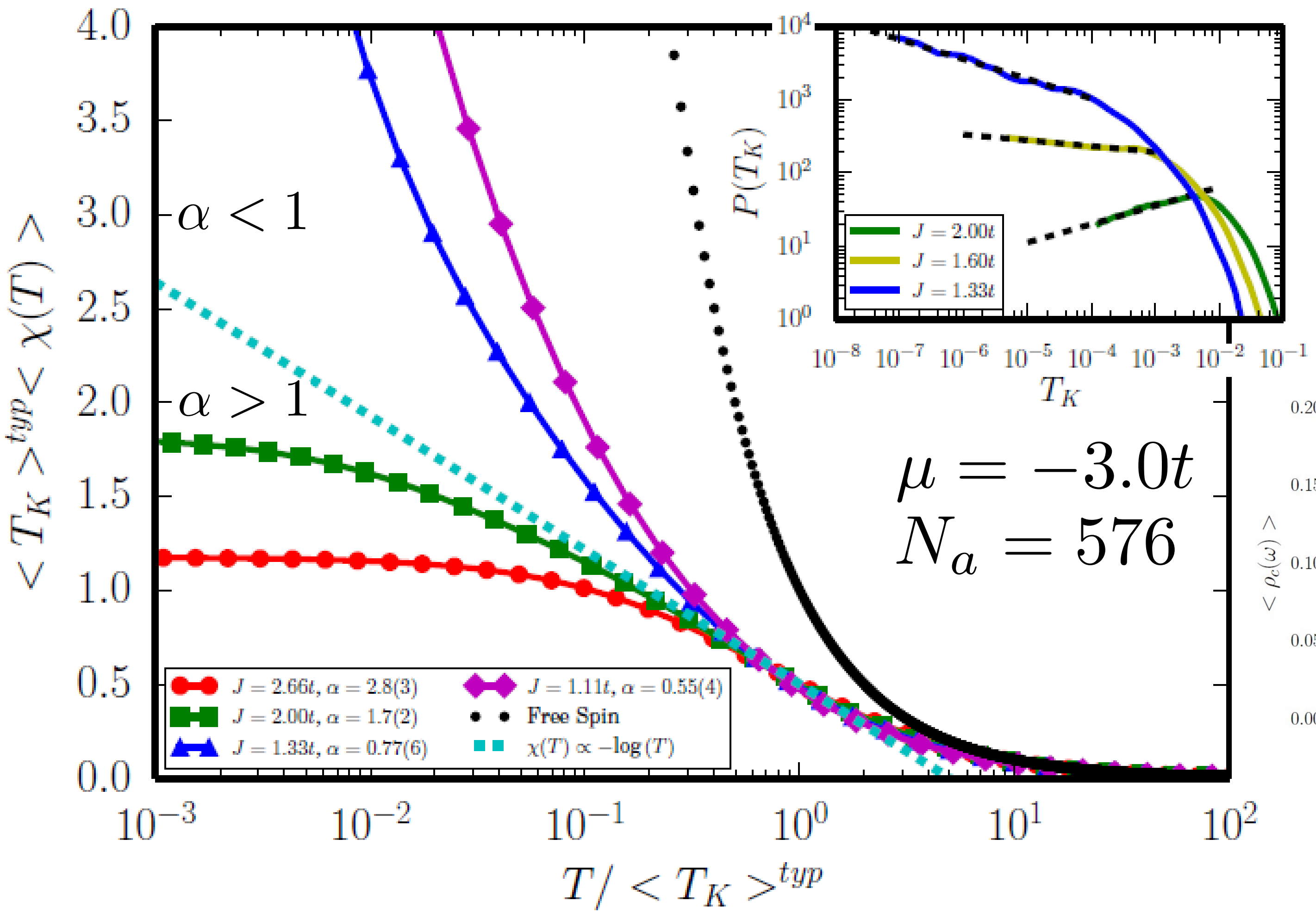
NFL behavior – Octagonal tiling

Crossover regime: *log* divergence for all *J*

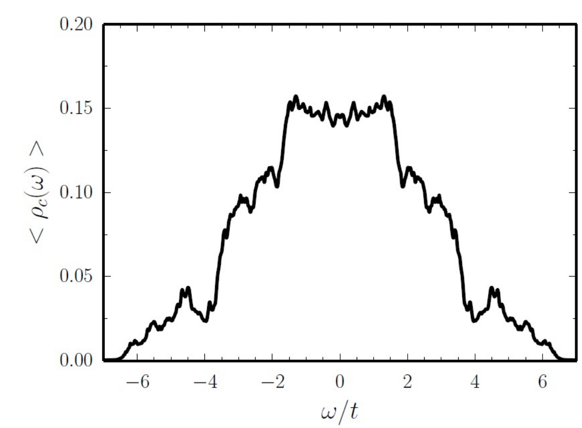


NFL behavior – Three dimensions

- Similar behavior in 3D: rhombohedra (Ammann-Kramer) tiling
- There seems to be little dimensionality dependence (*D* = *2,3*)



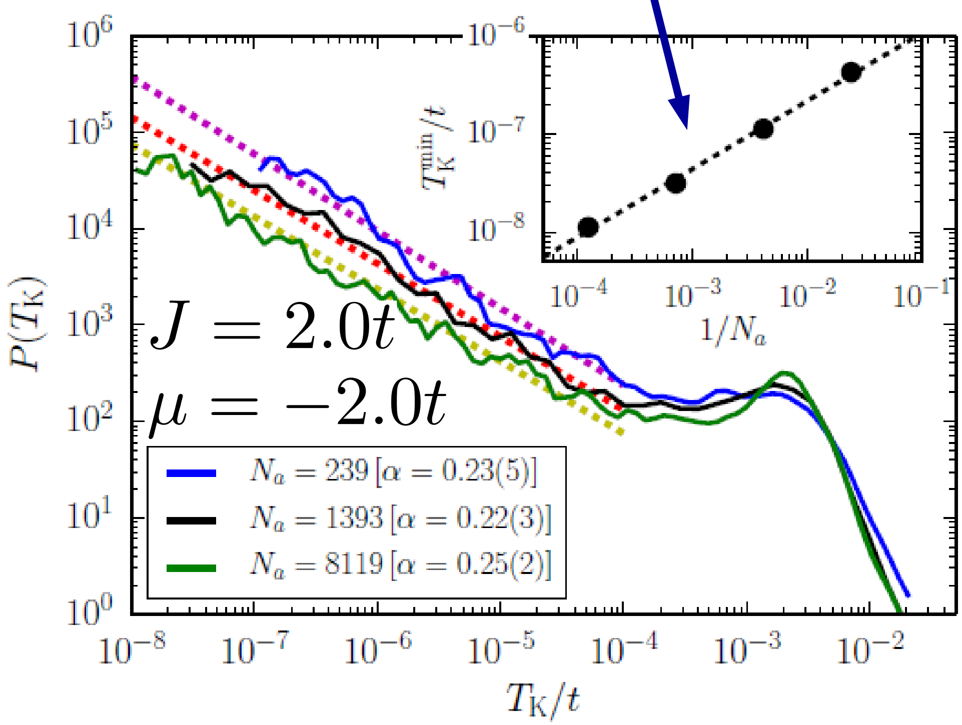
Provided by M. Mihalkovic

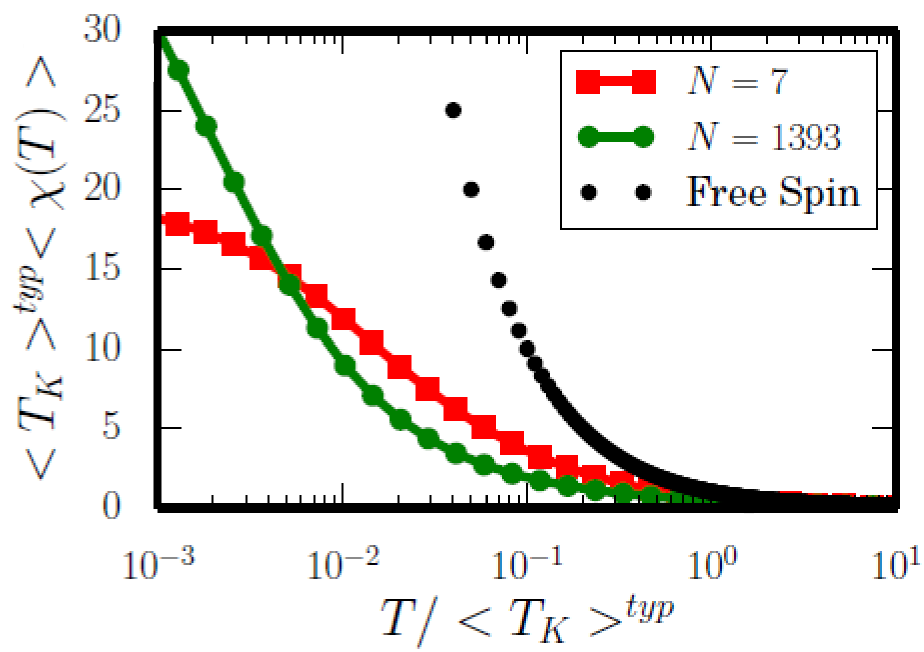


FL behavior in small approximants

- For any approximant, there is a finite number of T_K's, and therefore a minimum one.
- Below this T_K^{min} , FL behavior is recovered.
- Only in an infinite quasicrystal there is true NFL behavior.

Minimum value of Kondo temperature: T_K^{min}



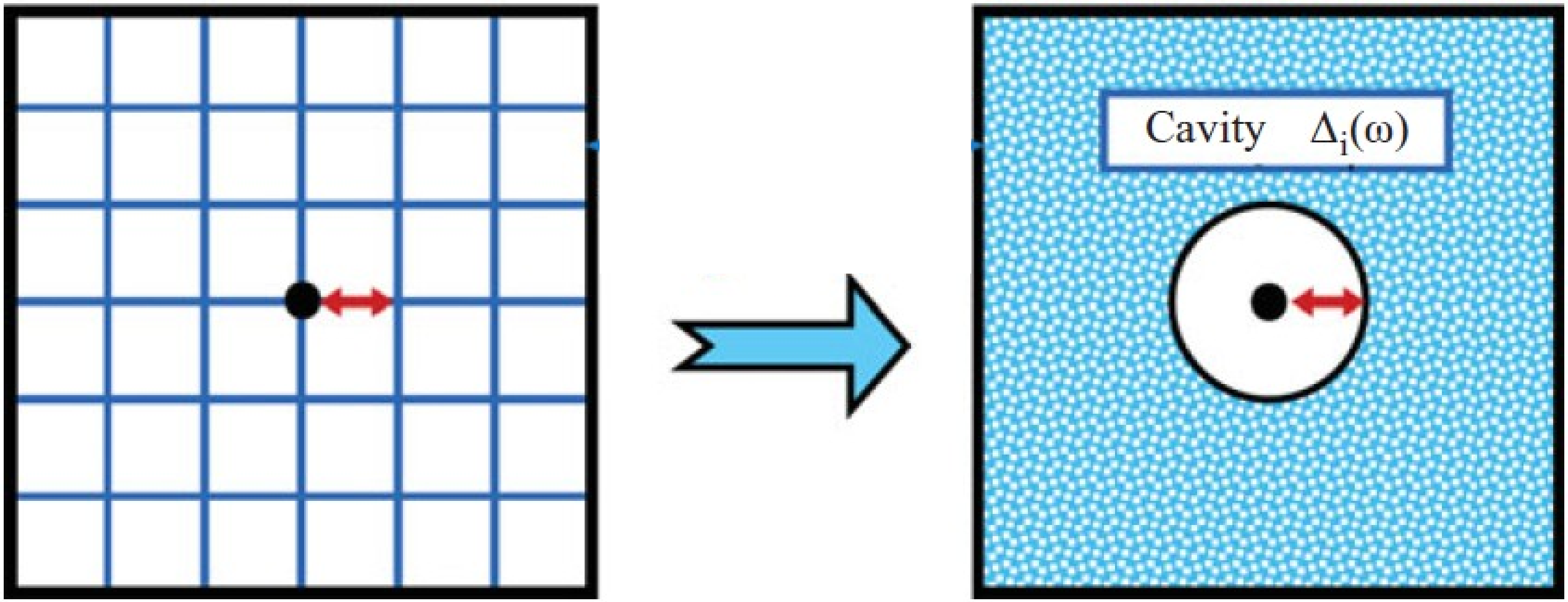


Why power-law? Disordered metals

- Hints from the disordered problem

$$G^c_{\ell\ell}(\omega) = 1/\left(\omega - \varepsilon_\ell - \Delta_{c\ell}(\omega)\right) \qquad \tilde{\varepsilon}_\ell = \varepsilon_\ell + \Delta'_{c\ell}(0)$$

Cavity function: How a given electron hybridizes?



Tanasković/Miranda/Dobrosavljević, PRB **70**, 205108 (2004)

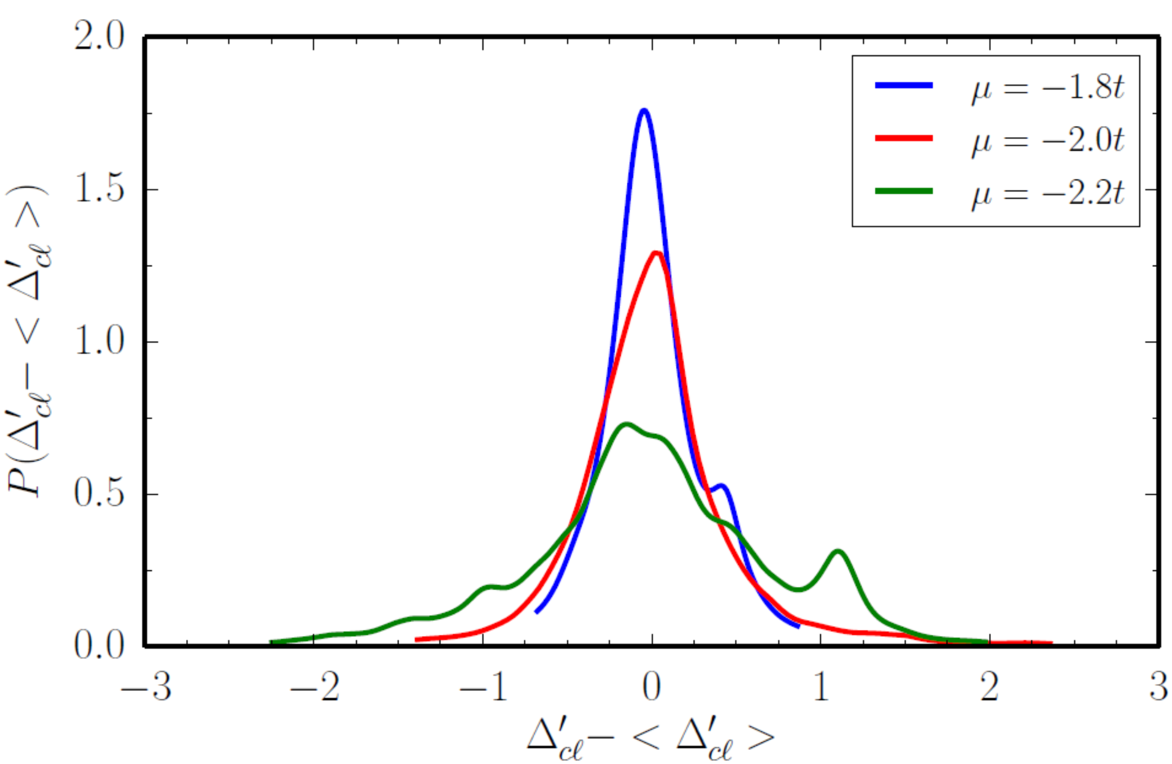
Why power-law? Metallic quasicrystal

- Define an "effective site energy": $\tilde{\varepsilon}_\ell = \Delta'_{c\ell}(0)$

$$G^c_{\ell\ell}(\omega) = 1/\left(\omega - \Delta_{c\ell}(\omega)\right)$$

$$T^\ell_K = T^0_K e^{-\tilde{\varepsilon}^2_\ell / J\langle\rho_c(0)\rangle t^2} \quad P(\tilde{\varepsilon}) \sim e^{-\tilde{\varepsilon}^2/2\sigma^2} \quad P(T_K) \propto T_K^{\alpha-1}$$

$$\alpha = J\langle\rho_c(0)\rangle t^2/2\sigma^2$$



Gaussian-like tails in $P(\Delta'(0))$ immediately leads to singular behavior in $P(T_K)$

Akin to disordered metals

Tanasković/Miranda/Dobrosavljević PRB **70**, 205108 (2004)

From Kondo impurities to the Kondo lattice

- Disordered systems: Power-law distribution of T_K

  Miranda/Dobrosavljević, Rep. Prog. Phys. **68**, 2337 (2005)

- NFL region is associated to an "Electronic Griffiths phase"

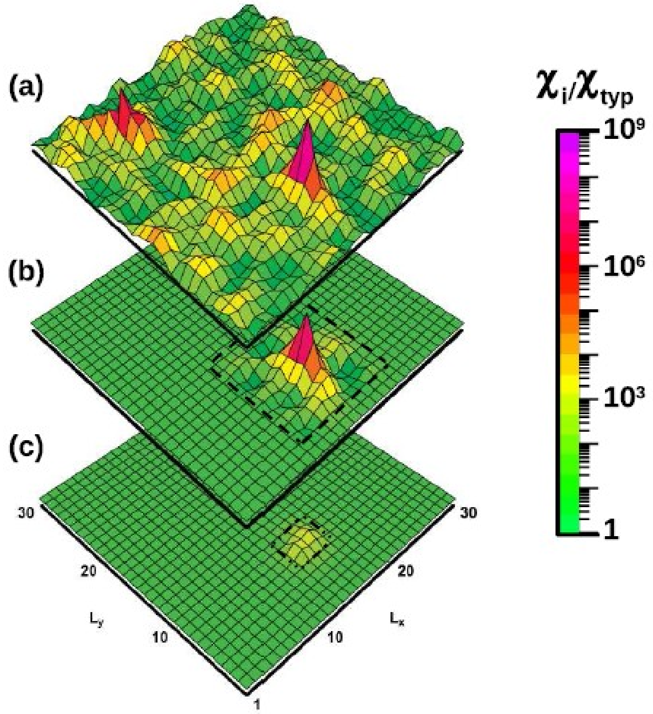
  ECA/Miranda/Dobrosavljević, PRL **102**, 206403 (2009)

- *Assume* the same link holds for QC's

$$\chi(T) \propto T^{\alpha-1} \quad C/T = \gamma(T) \propto T^{\alpha-1}$$

- Transport?
- Inter-site magnetic correlations?

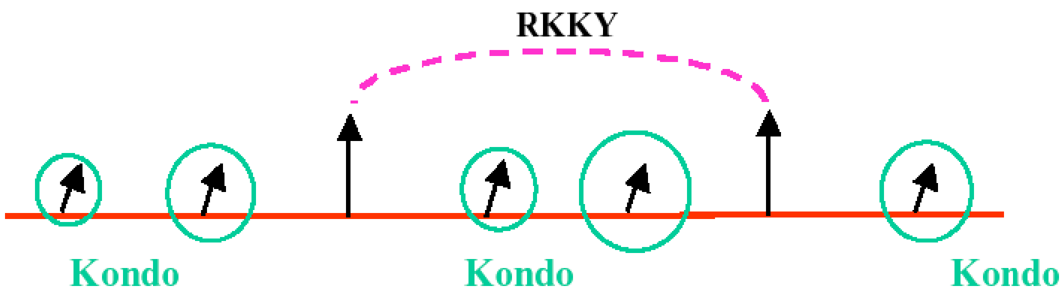
  Hartman/Chiu/Scalettar arXiv:1601.07214v1

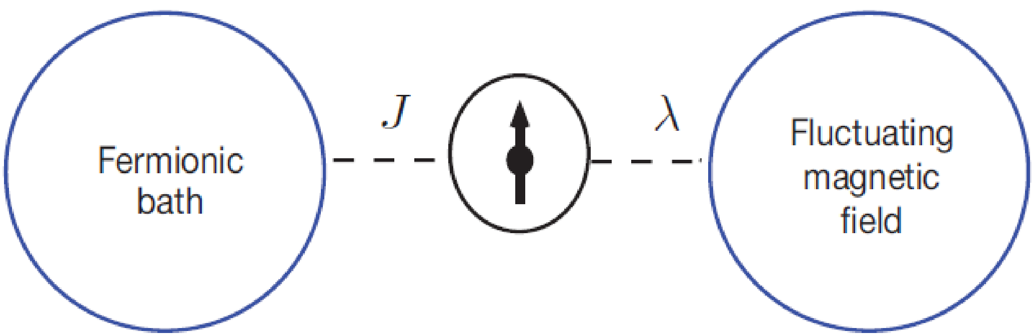


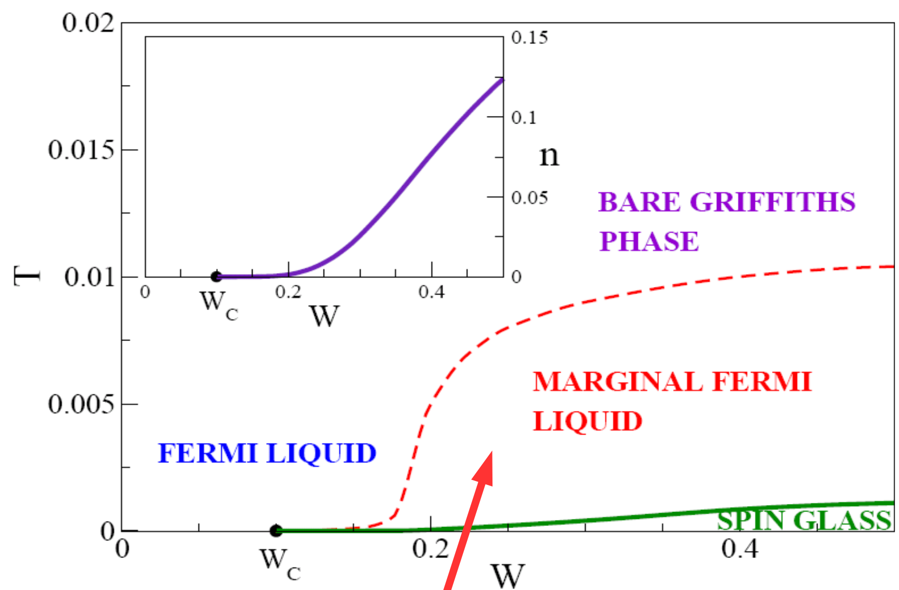
From Kondo impurities to the Kondo lattice

RKKY interaction couples the free spins at low-T!

Crossover from Griffiths to Marginal Fermi Liquid







$$\delta\rho\left(T\right) \sim T \quad \chi \sim \ln\left(T_o/T\right)$$

Tanasković/Miranda/Dobrosavljević, PRL **95**, 167204 (2005)

Weaker than power-law and universal!

Conclusions

- NFL behavior in the $Au_{51}Al_{34}Yb_{15}$ quasicrystal
  - No tunning of external parameters
  - Approximant and quasicrystal different
- Diluted Kondo impurities in metallic quasicrystals: Power-law distribution of T_K and NFL. Akin to *weakly* disordered systems
  - Strong energy dependence
  - NFL behavior changes/disappears in small approximants
- Lattice problem: Diluted impurity scenario survives? Inter-site spin correlations?