# Strong inhomogeneities and non-Fermi liquids in randomly depleted Kondo lattices

# Strong inhomogeneities and non-Fermi liquids in randomly depleted Kondo lattices

Matthias Vojta (Karlsruhe)
Ribhu K. Kaul (Duke)

1. **Depleted Kondo lattice systems**

   From a single Kondo impurity to the Kondo lattice

   Experiments

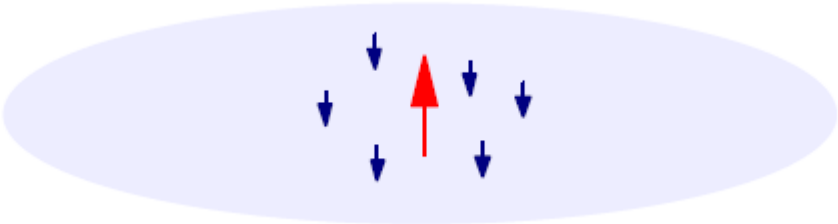
2. **Strong-coupling limit**

3. **Large-*N* formalism and results**

   Strong inhomogeneities and non-FL

   Kondo-disorder phenomenology

# Magnetic impurities in metals: Kondo effect



In the low-$T$ limit, the impurity moment will be **screened**.

$$\chi_{\text{imp}}(T \to 0) \to \text{const}$$

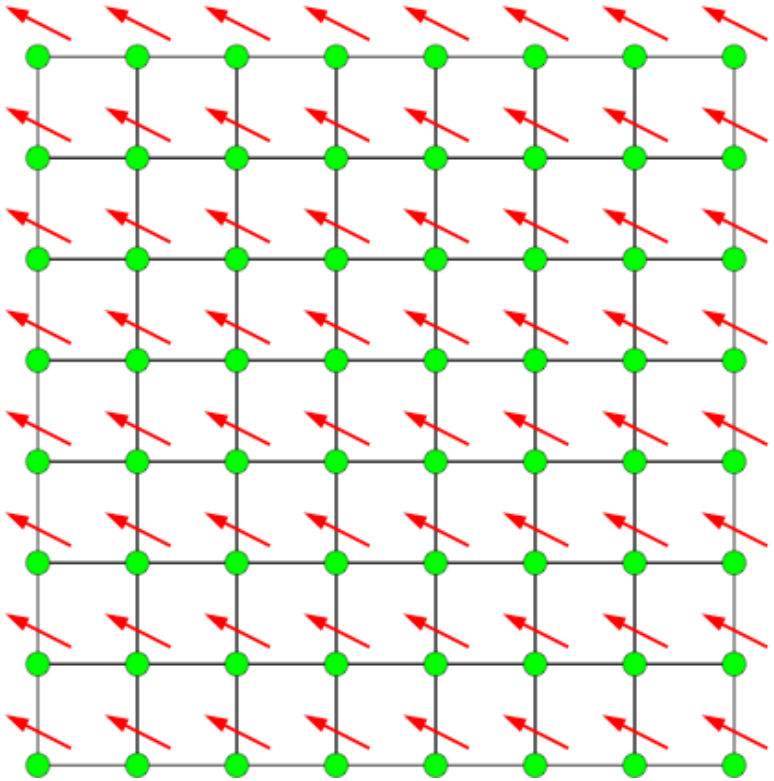
$$S_{\text{imp}}(T \to 0) \to 0$$

$$\boxed{H_{\text{imp},1} = J\,\vec{\boldsymbol{S}} \sum_{\boldsymbol{k}\boldsymbol{k}'} c_{\boldsymbol{k}\sigma}\,\vec{\boldsymbol{\sigma}}_{\sigma\sigma'}\,c_{\boldsymbol{k}'\sigma'} = J\,\vec{\boldsymbol{S}}\cdot\vec{\boldsymbol{s}}_0}$$

Low-energy physics of Kondo model is determined by single scale

$$\underline{T_K \sim D\exp(-D/J).}$$

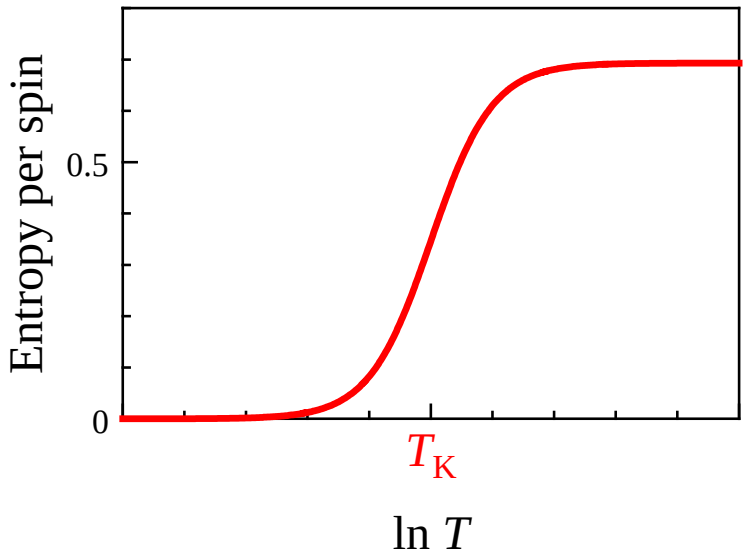
# Kondo lattice model



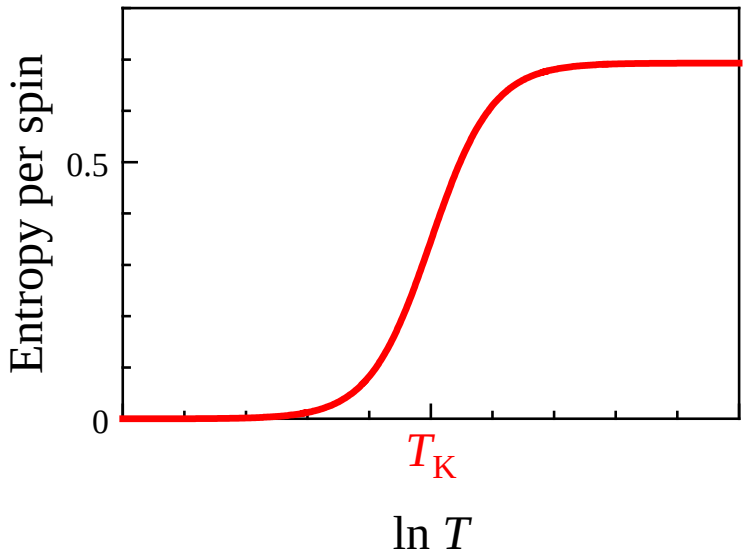
$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda} \mathcal{J} \mathcal{S}_i \cdot \mathbf{s}_i$$

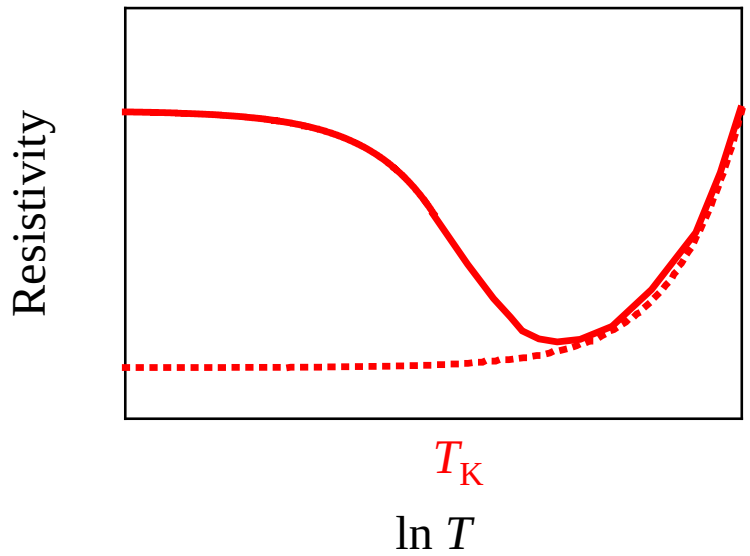
Kasuya (1956); Doniach (1977)

# Single impurity & Kondo lattice

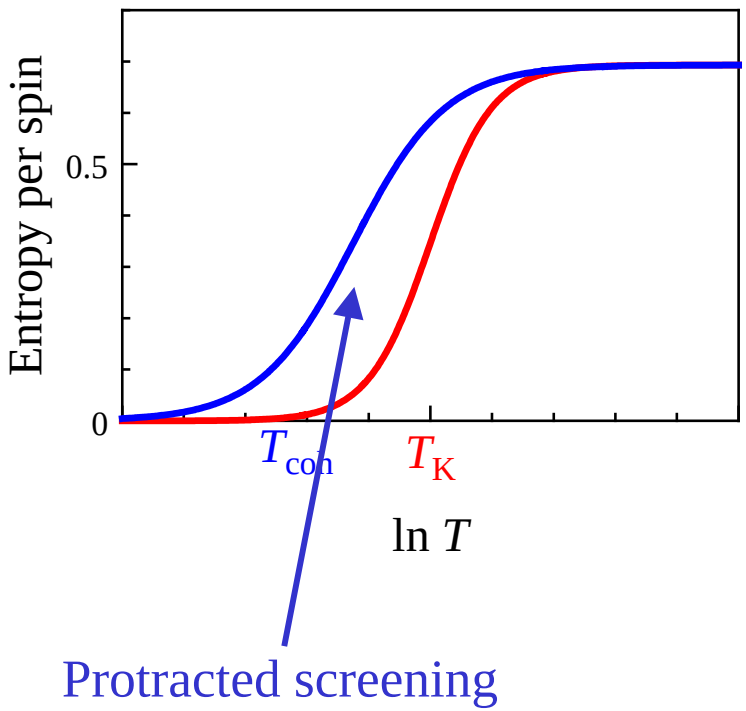


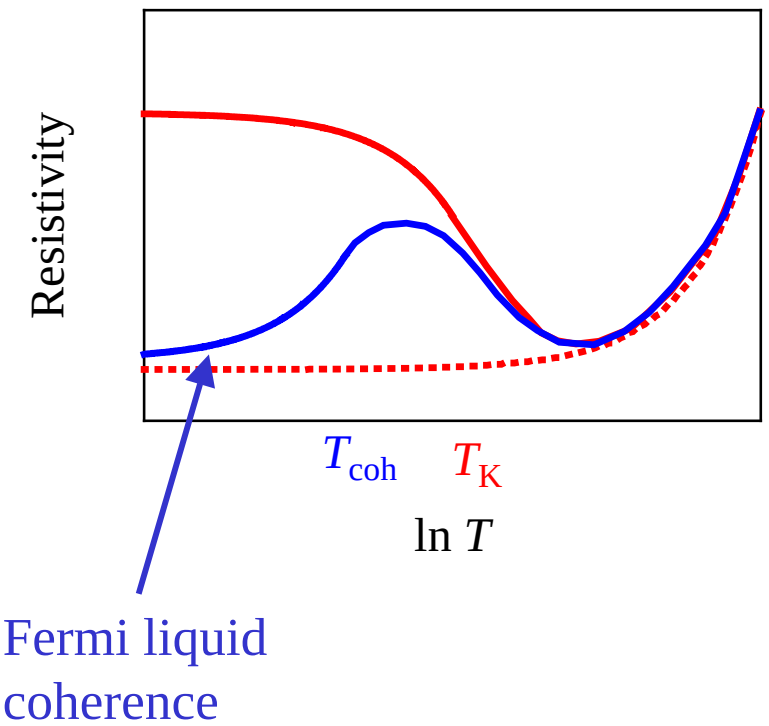
# Single impurity & Kondo lattice



# Single impurity & Kondo lattice



# Energy scales of Kondo lattice

Single-impurity Kondo temperature $T_K$

Fermi-liquid coherence temperature $T_{coh}$

Usually $T_{coh} << T_K$

Are $T_{coh}$ and $T_K$ two different scales?

(Do they have a different $J_K$ dependence?)

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Fermi-liquid coherence temperature $T_{coh}$

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VOLUME 85, NUMBER 5 PHYSICAL REVIEW LETTERS 31 JULY 2000

**Coherence Scale of the Kondo Lattice**

S. Burdin,[1,2] A. Georges,[3] and D. R. Grempel[1,4]

$$T_K = De^{-1/J_K\rho_0(\epsilon_F)}\sqrt{1-(\epsilon_F/D)^2}\,F_K(n_c), \quad (3)$$

$$F_K(n_c) = \exp\left(\int_{-(D+\epsilon_F)}^{D-\epsilon_F}\frac{d\omega}{|\omega|}\frac{\rho_0(\epsilon_F+\omega)-\rho_0(\epsilon_F)}{2\rho_0(\epsilon_F)}\right), \quad (4)$$

$$T^\star = De^{-1/J_K\rho_0(\epsilon_F)}(1+\epsilon_F/D)\frac{\Delta\epsilon_F}{D}F^\star(n_c), \quad (5)$$

$$F^\star(n_c) = \exp\left(\int_{-(D+\epsilon_F)}^{\Delta\epsilon_F}\frac{d\omega}{|\omega|}\frac{\rho_0(\epsilon_F+\omega)-\rho_0(\epsilon_F)}{\rho_0(\epsilon_F)}\right), \quad (6)$$

Slave-boson mean-field approximation:

$$\boldsymbol{T_{coh} = c\,T_K}$$

where $c$ depends on conduction band only

# Doniach's phase diagram for the Kondo lattice model

$$H = \sum_{i<j} t_{ij}\, c_{i\sigma}^{+} c_{j\sigma} + \sum_{i} J_{\mathrm{K}}\, \vec{S}_i\, c_{i\sigma}\, \vec{\sigma}_{\sigma\sigma'}\, c_{i\sigma'}$$

Two competing effects (at least):

* Kondo screening by conduction electrons ($T_K^{(1)} \sim D \exp(-D/J)$, $D$ = bandwidtl
* Magnetic ordering due to inter-impurity interaction ($I_{\mathrm{RKKY}} \sim J_{\mathrm{K}}^{2}/D$)

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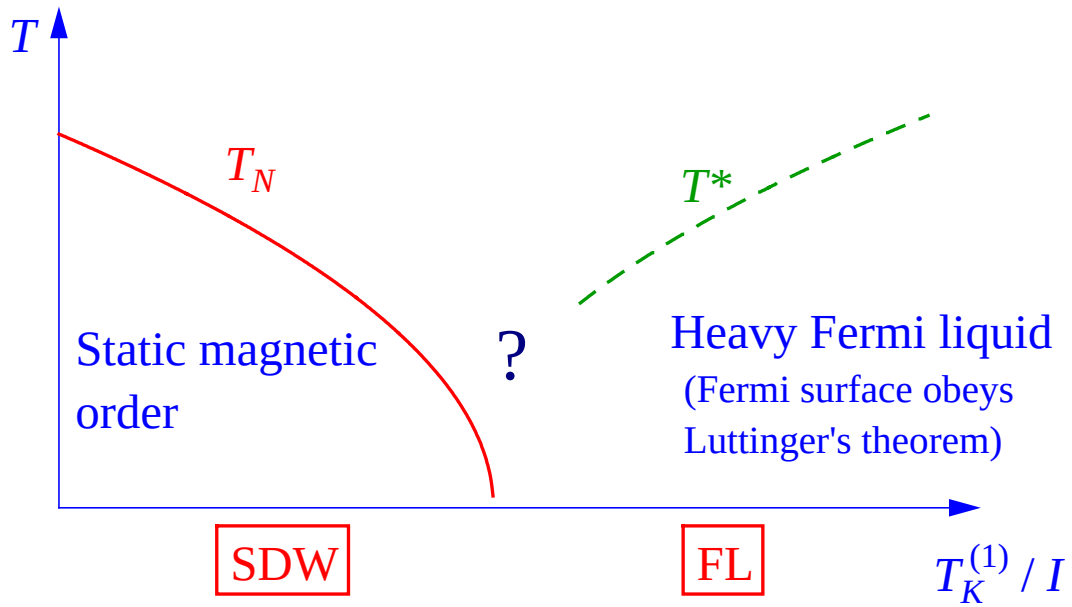
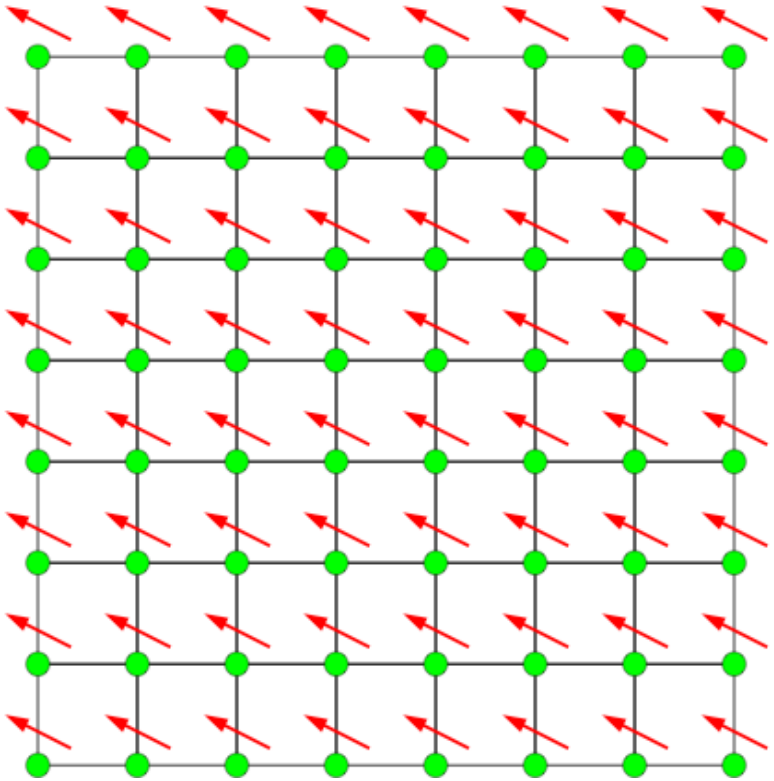


# Depleted Kondo lattices

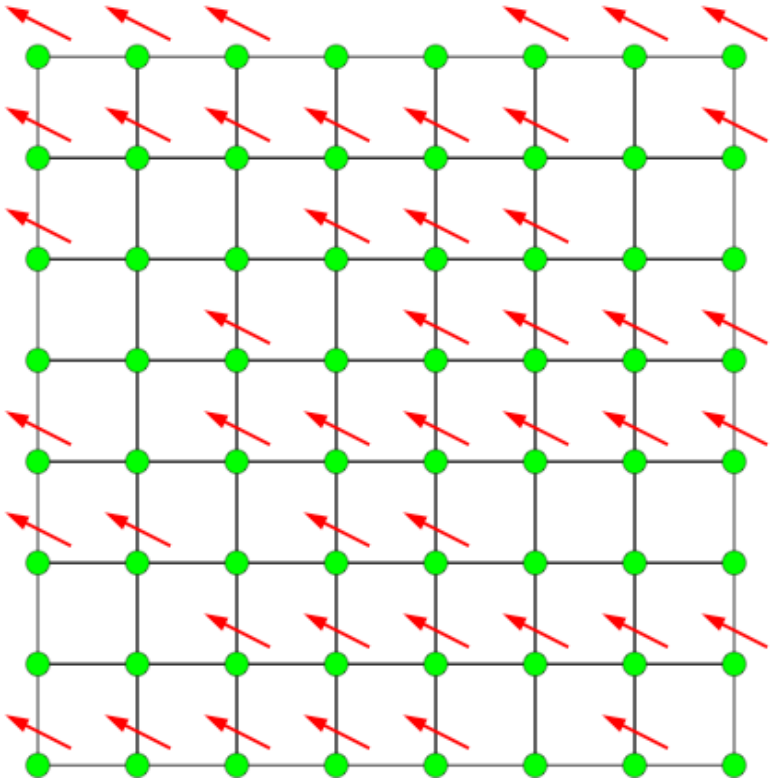
# Kondo lattice model



$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda} \mathcal{J} \mathcal{S}_i \cdot \mathbf{s}_i$$

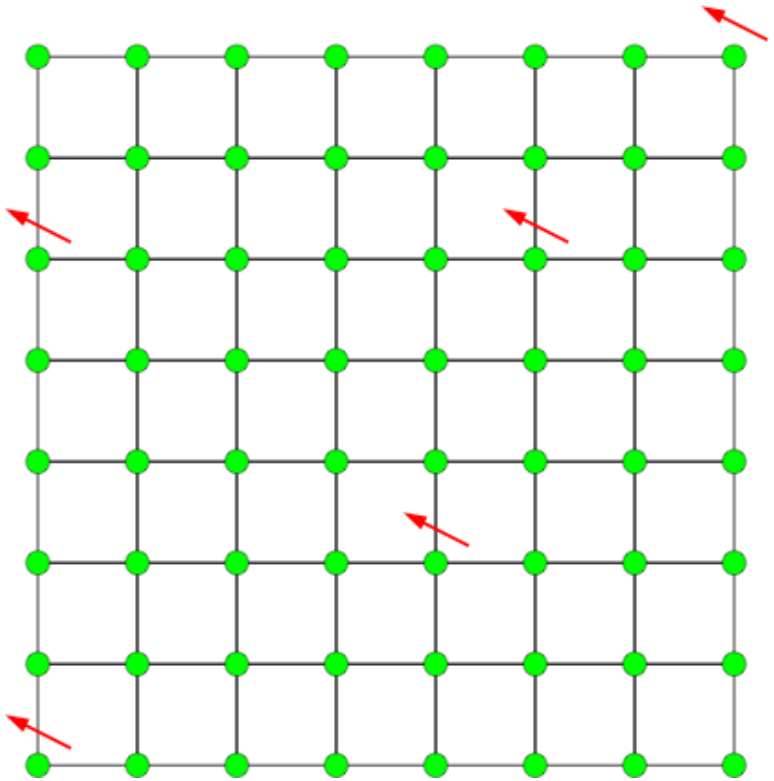
Kasuya (1956); Doniach (1977)

# Depleted Kondo lattice model



$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda_{dep}} \mathcal{J}\mathcal{S}_i \cdot \mathbf{s}_i$$

# Kondo impurity model



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# Experiments: Depleted Kondo lattices

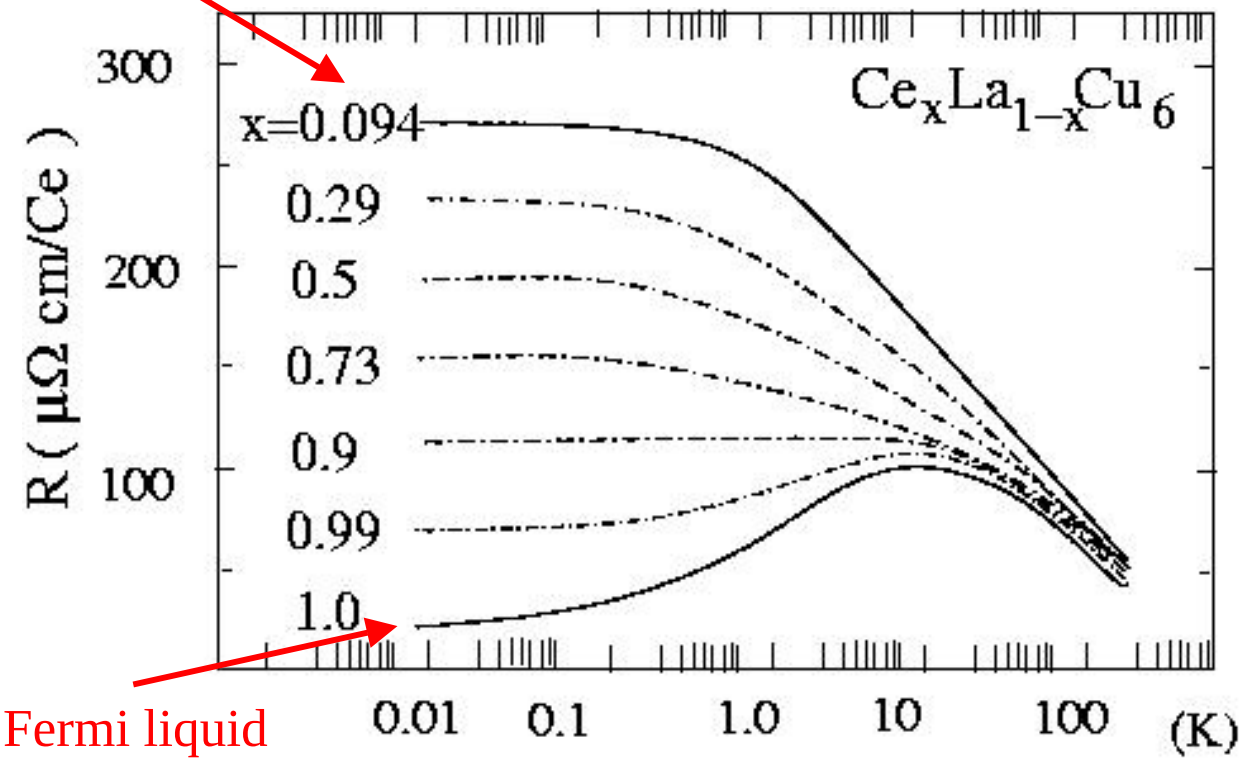
$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda_{dep}} \mathcal{J}\mathcal{S}_i \cdot \mathbf{s}_i$$

Substituational doping, e.g., Ce $\rightarrow$ La
in compounds like $CeCoIn_5$, $CePb_3$, $CeAl_2$ , ….

Local-moment concentration $n_f$ tunable between
$n_f$ =1 (dense lattice limit) and
$n_f$ =0 (single impurity limit)

# Experiment: $Ce_xLa_{1-x}Au_6$

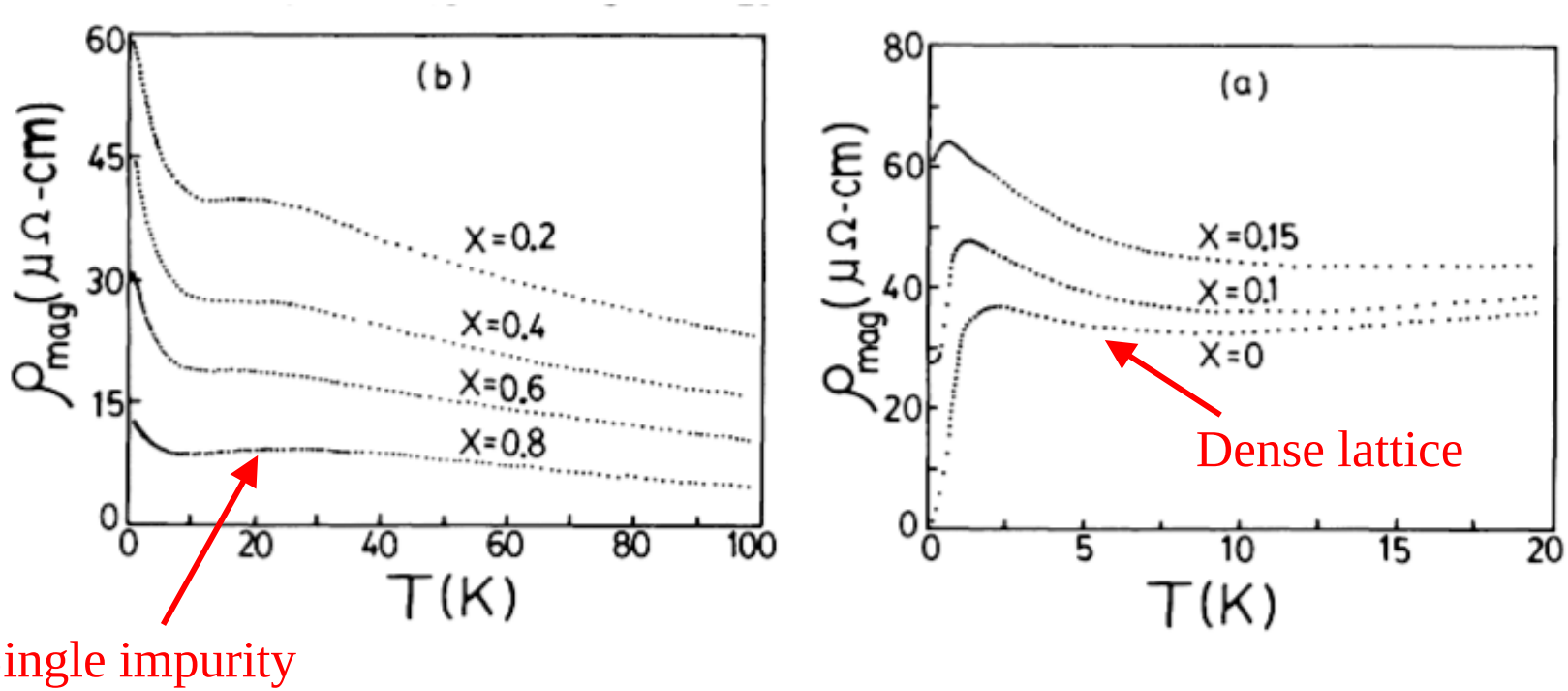
Single impurity




Coherent Fermi liquid
of dense lattice

Lin *et al.* (1987)

# Experiment: $Ce_{1-x}La_xPb_3$

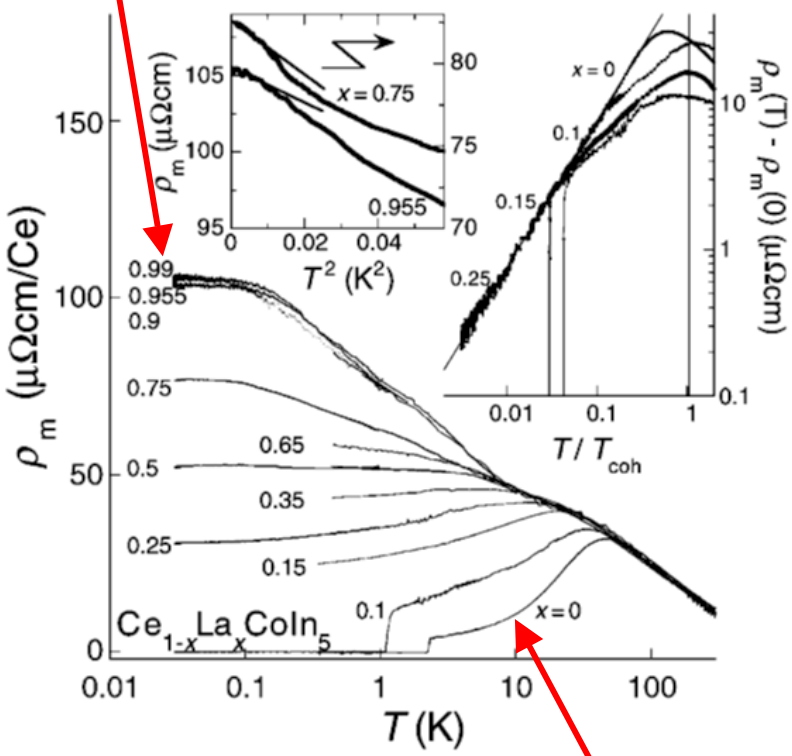


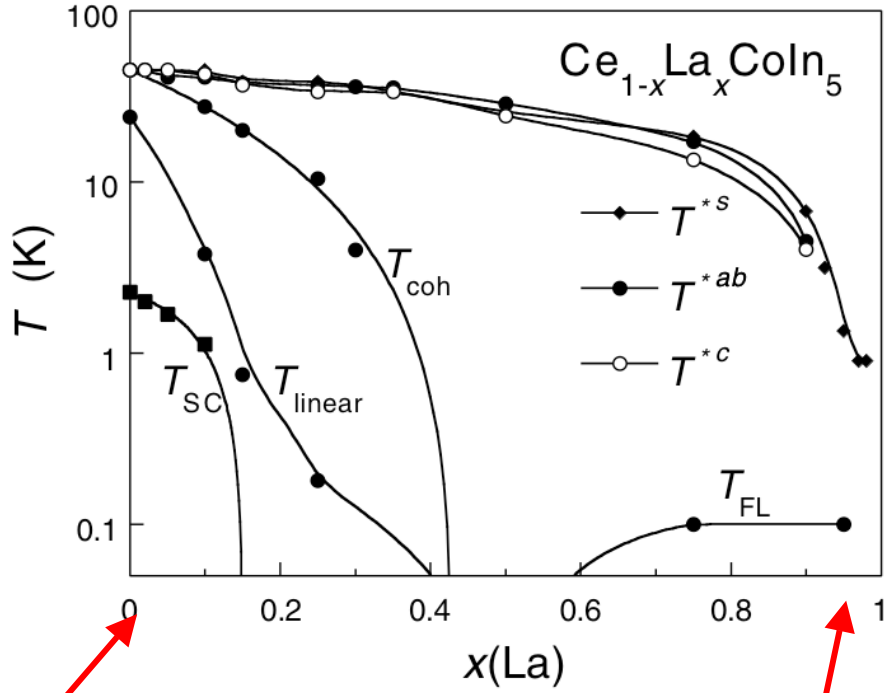

**Single-impurity behavior between $n_f$ =0 and $n_f$ =0.8 (!)**

Lin *et al.*, PRL **58**, 1232 (1987)

# Experiment: $Ce_{1-x}La_xCoIn_5$

Single impurity




Single impurity

Dense lattice

Nakatsuji *et al.*, PRL **89**, 106402 (2002)

# Theory: Depleted Kondo lattices

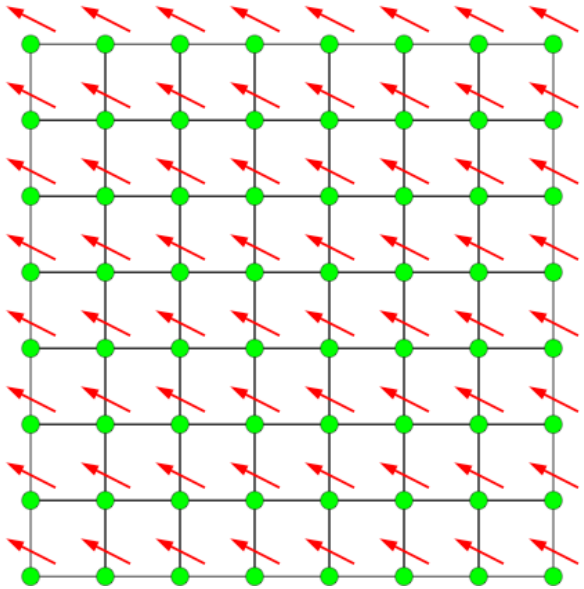
$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda_{dep}} \mathcal{J}\mathcal{S}_i \cdot \mathbf{s}_i$$

**How are single-impurity Fermi liquid and heavy lattice Fermi liquid connected?**

# Strong-coupling limit

# Strong coupling limit: $J/t \to \infty$

$$n_c \lesssim 1$$



$n_f = 1$: Kondo lattice, Fermi liquid of $(1-n_c)$ holes

# Strong coupling limit: $J/t \to \infty$

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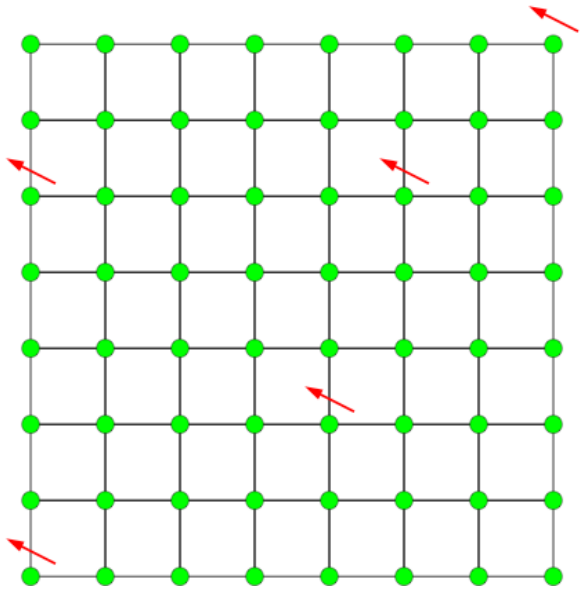

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$n_f \to 0$: Single impurity, Fermi liquid of $(n_c - n_f)$ particles

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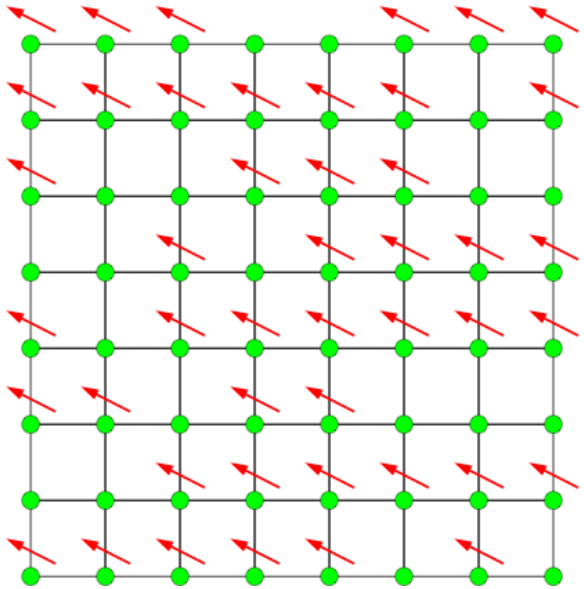

$n_f = 1$: Kondo lattice, Fermi liquid of $(1-n_c)$ holes

$n_f \to 0$: Single impurity, Fermi liquid of $(n_c - n_f)$ particles

$n_c = n_f$: **Gapped insulator!**

# Large-$N$ formalism and results

# Mean-field theory

$$H_{\mathrm{KLM}} = \sum_{i,j\in\Lambda} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i\in\Lambda_{dep}} \mathcal{J}\mathcal{S}_i \cdot \mathbf{s}_i$$

$$\mathcal{S}_i = f^\dagger_{i\sigma} \overrightarrow{\sigma}_{\sigma\sigma'} f_{i\sigma'}, \quad f^\dagger_{i\sigma} f_{i\sigma} = Q = N/2$$

$$H_{\mathrm{MF}} = H_{\mathrm{cond}} + b_i (c^\dagger_{i\sigma} f_{i\sigma} + \mathrm{h.c.}) + \mu_i f^\dagger_i f_i$$

$$b_i = \mathcal{J}\langle c^\dagger_i f_i \rangle \quad \langle f^\dagger_i f_i \rangle = 1/2$$

Read/Newns (1984); Millis/Lee (1987)
Coleman (1987); Auerbach/Levin (1986)

# Mean-field theory

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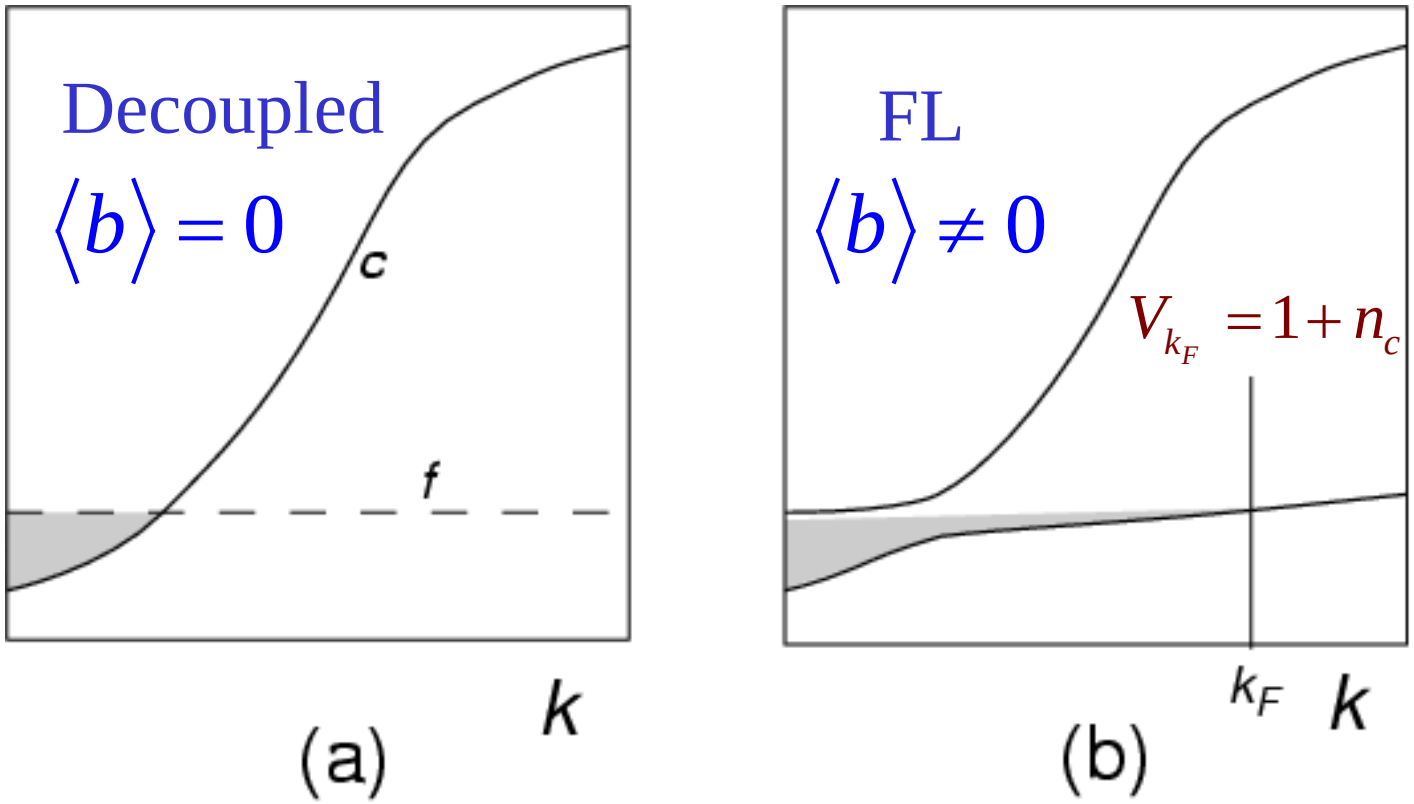
Read/Newns (1984); Millis/Lee (1987)
Coleman (1987); Auerbach/Levin (1986)

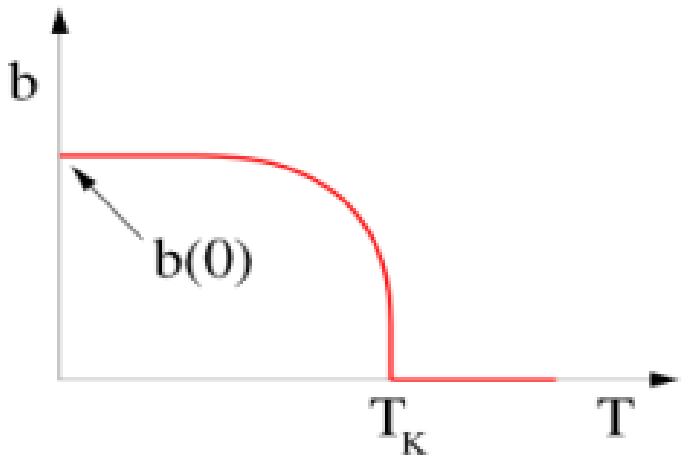
# Mean-field theory: Dense Kondo lattice

$$H_{\mathrm{MF}} = H_{\mathrm{cond}} + b_i(c_{i\sigma}^\dagger f_{i\sigma} + \mathrm{h.c.}) + \mu_i f_i^\dagger f_i$$

$$b_i = \mathcal{J}\langle c_i^\dagger f_i\rangle \qquad \langle f_i^\dagger f_i\rangle = 1/2$$



# Mean-field theory: Condensation at $T_K$

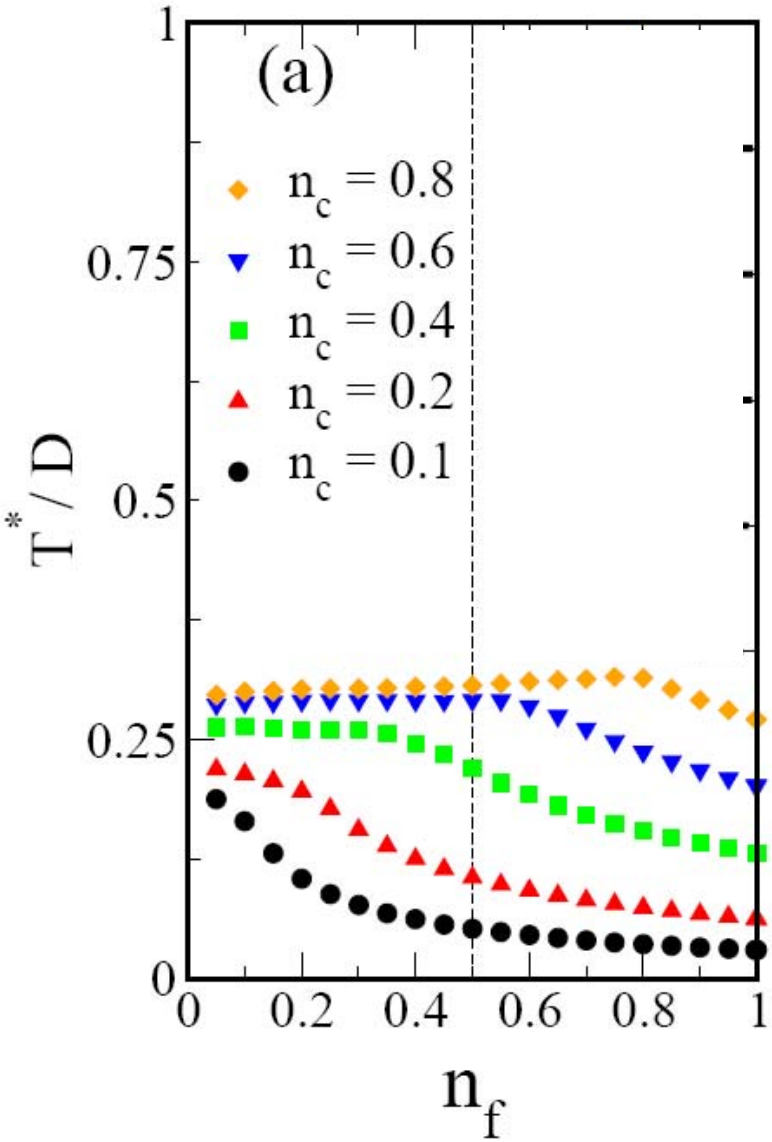



Define energy scale: $T^* = \langle |b_r(T=0)|^2 \rangle / D$

$$T^* = T_K \text{ for SI}$$
$$T^* = T_{\text{coh}} \text{ for KLM}$$

Burdin/Georges/Grempel, Phys. Rev. Lett. **85**, 1048 (2000)

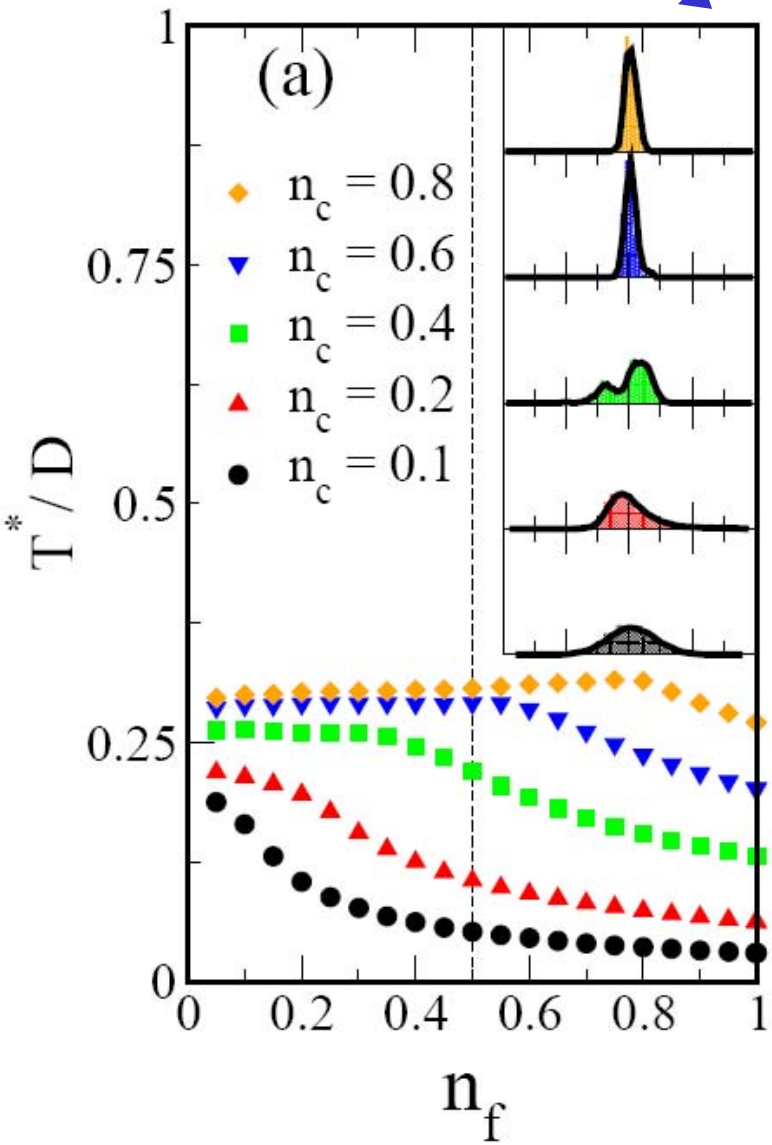
# Summary of mean-field results




Kaul/Vojta, cond-mat/0603002

# Summary of mean-field results

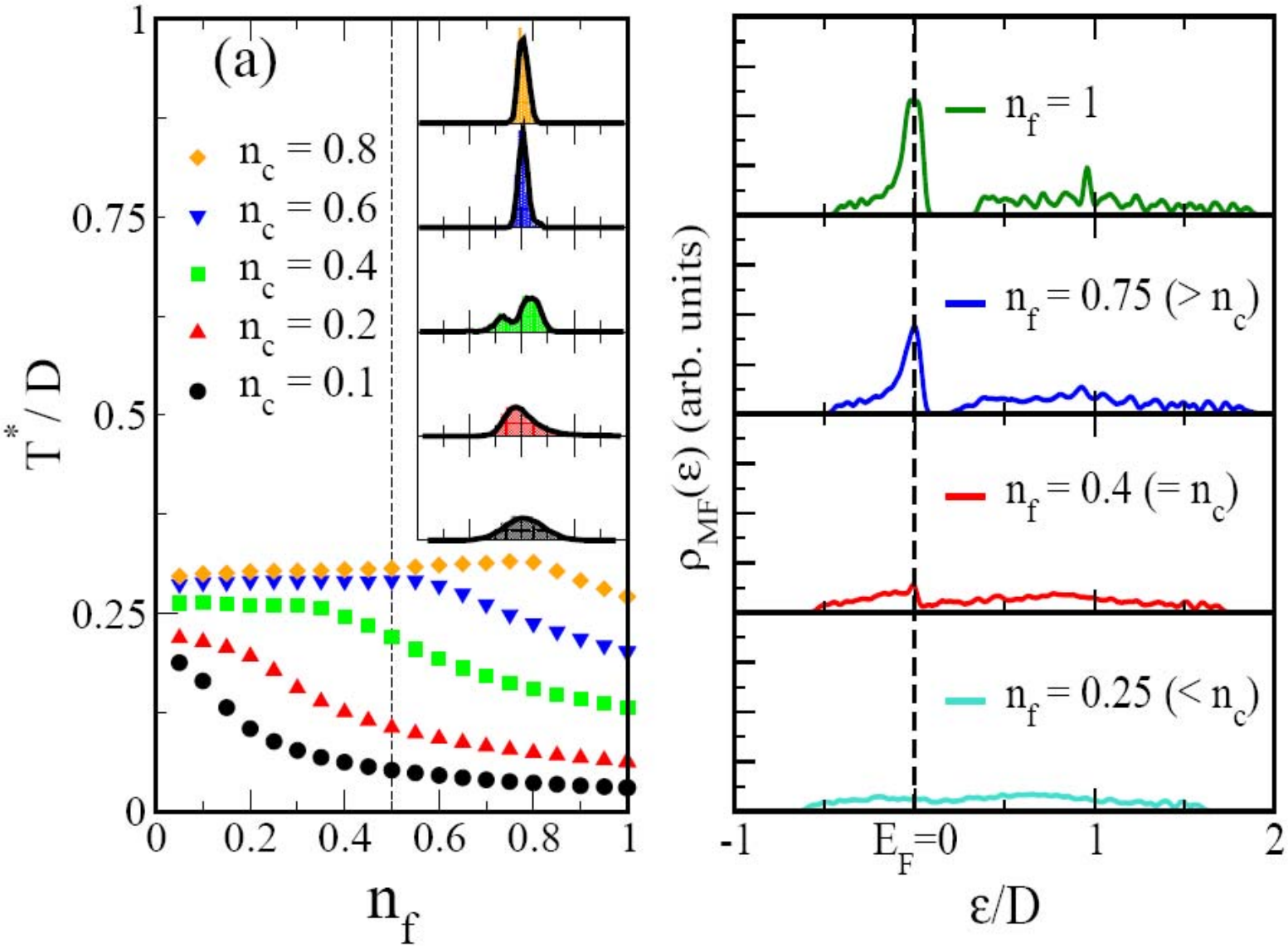
Distribution of $b^2$ at $n_f = 0.5$




**Sharp crossover around $n_f = n_c$**

Kaul/Vojta, cond-mat/0603002

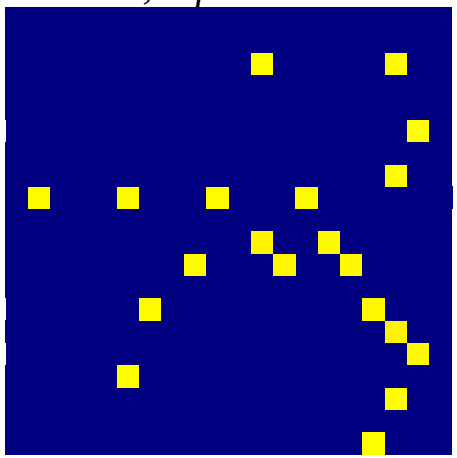
# Summary of mean-field results



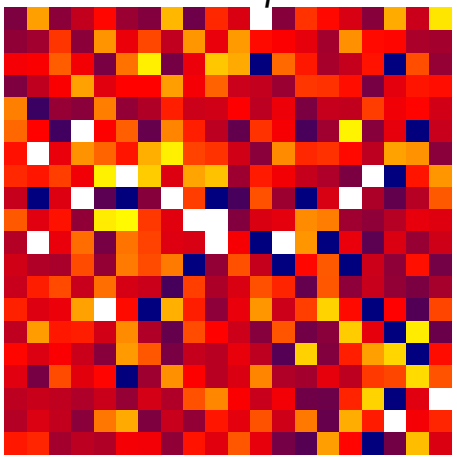

Kaul/Vojta, cond-mat/0603002

# Local observables at fixed $n_c$ = 0.8 and varying $n_f$

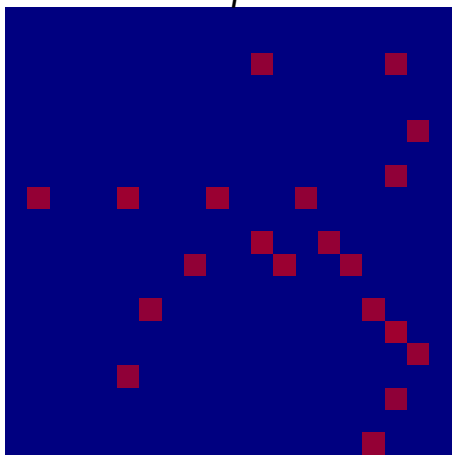
$b_i$, $n_f$ = 0.05



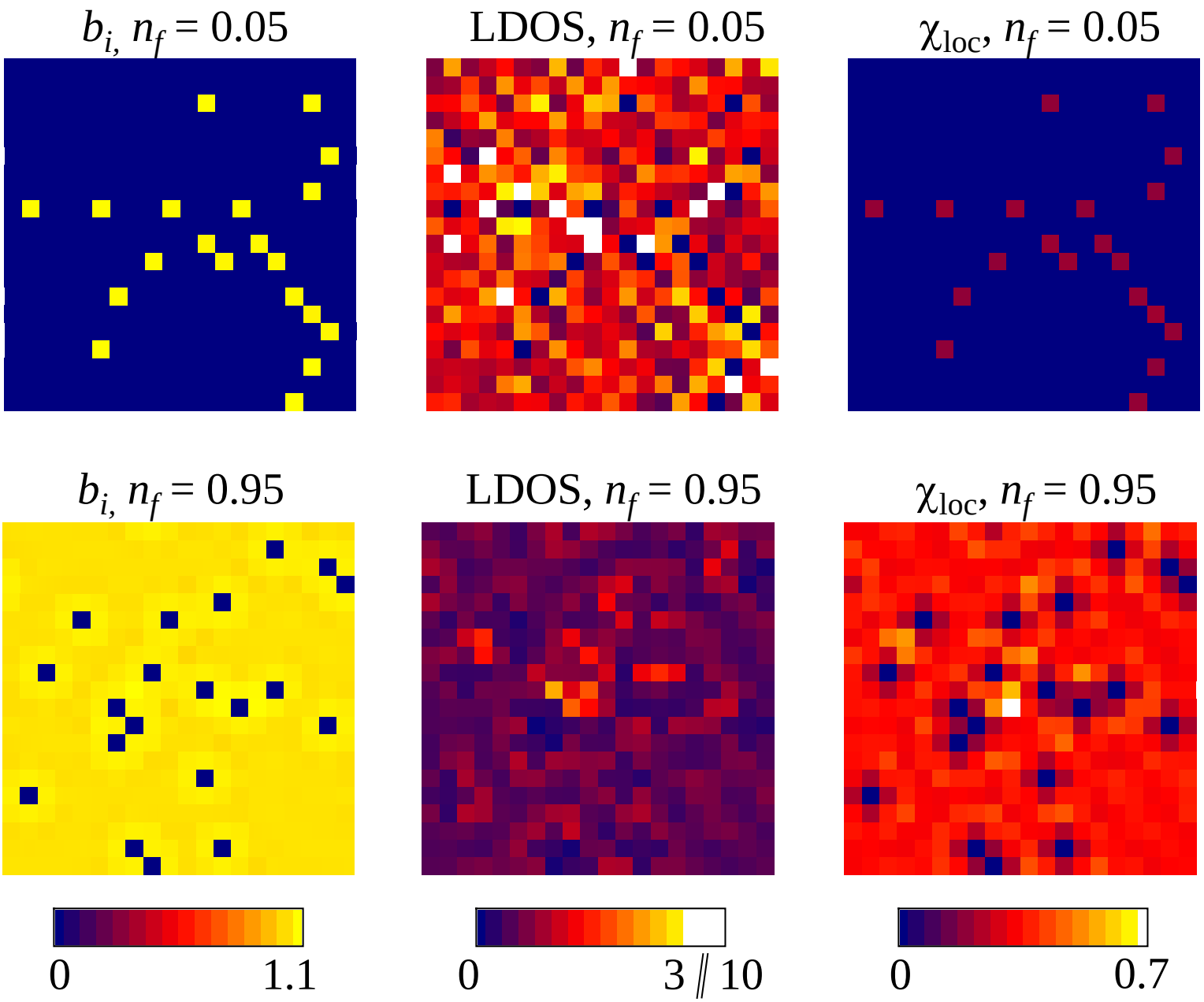
LDOS, $n_f$ = 0.05

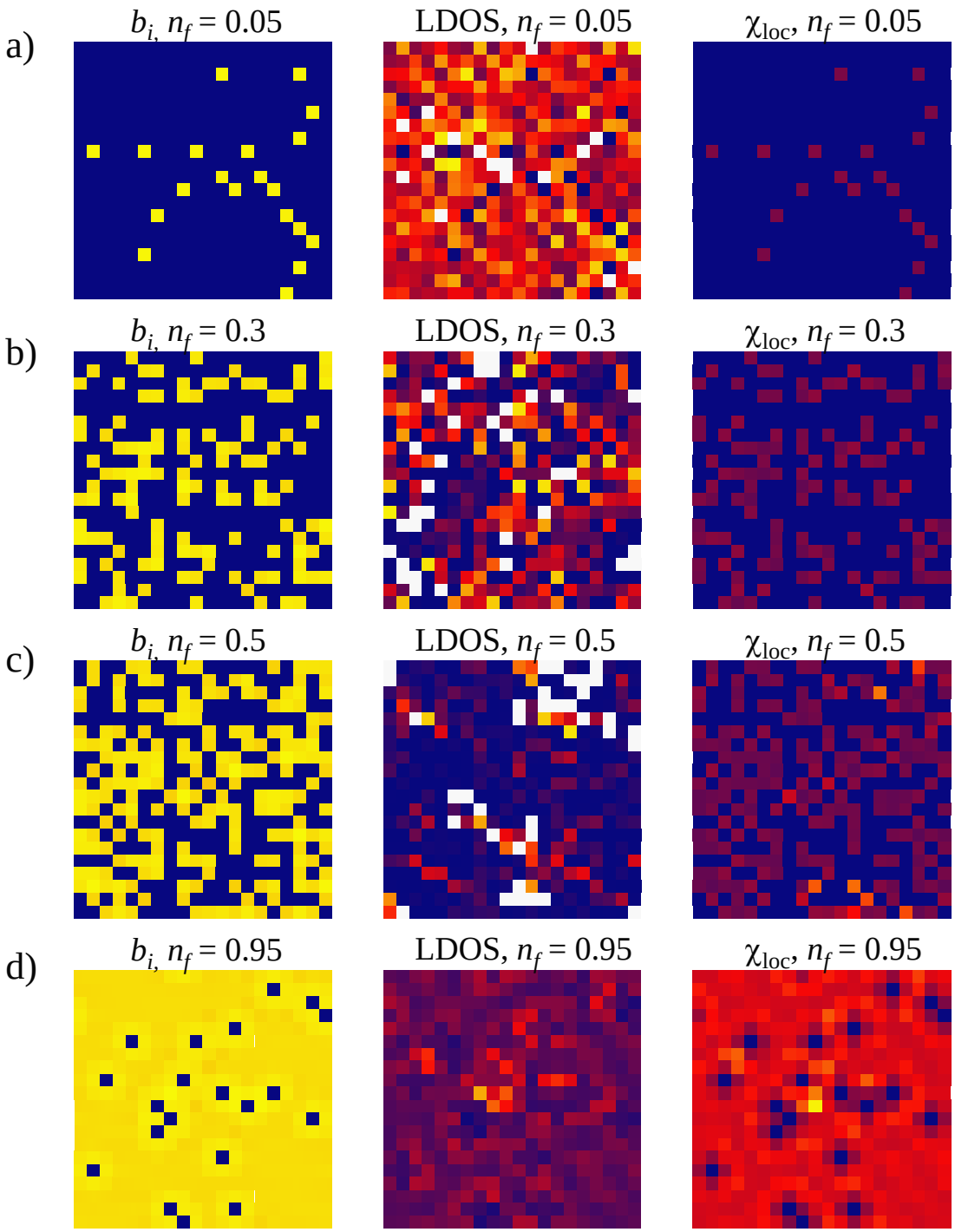


$\chi_{loc}$, $n_f$ = 0.05



# Local observables at fixed $n_c$ = 0.8 and varying $n_f$

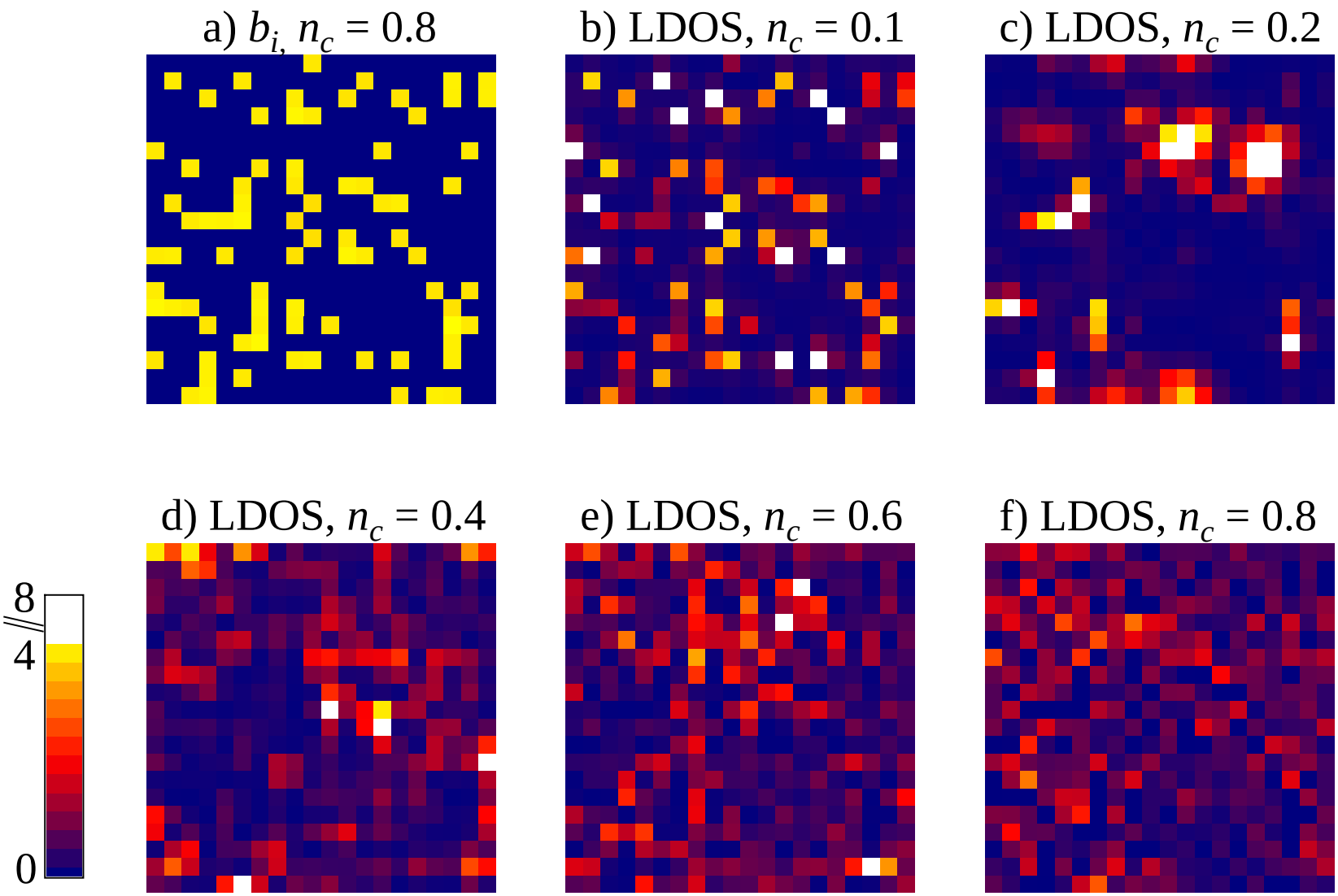





Isolated impurities

Isolated vacancies

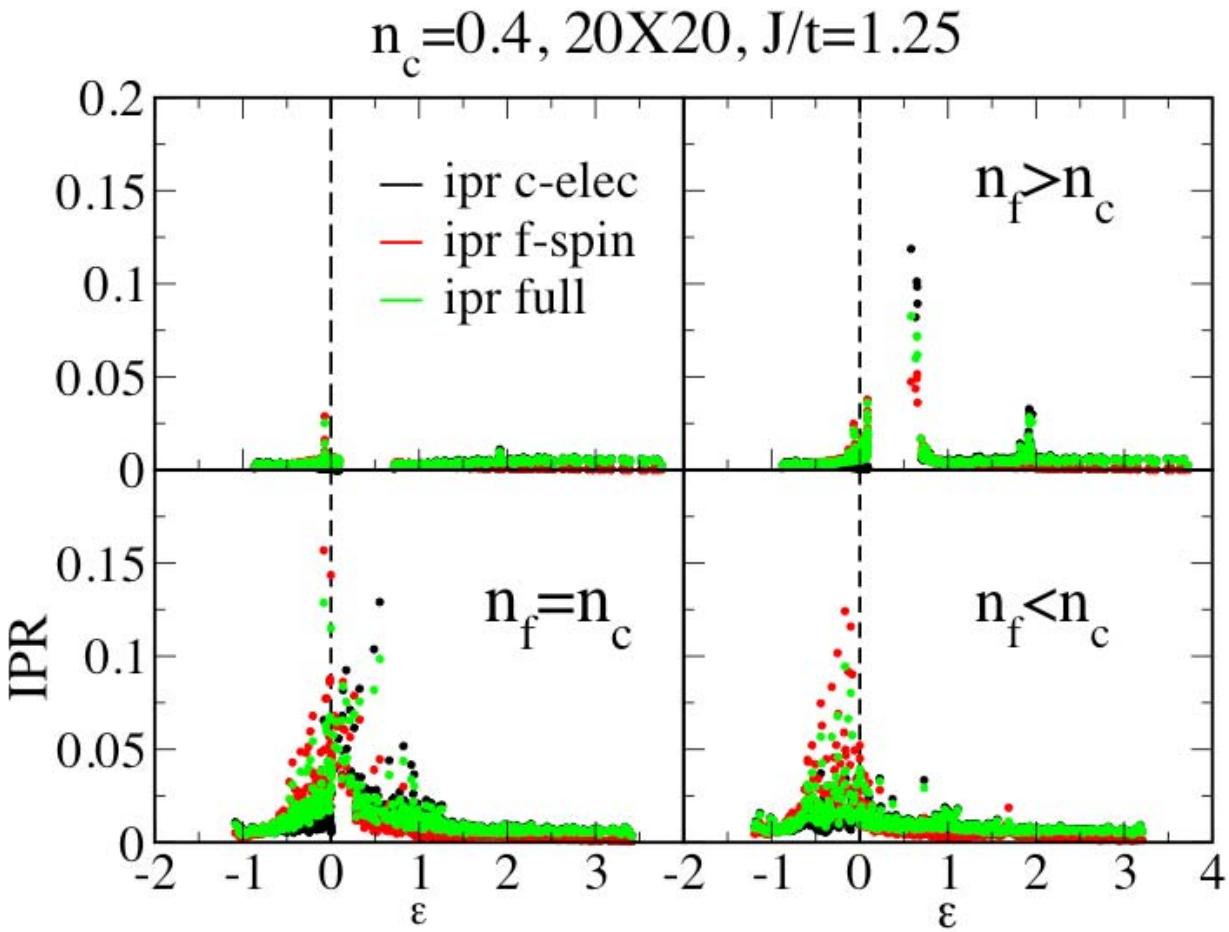
# Local DOS at fixed $n_f$ = 0.2 and varying $n_c$



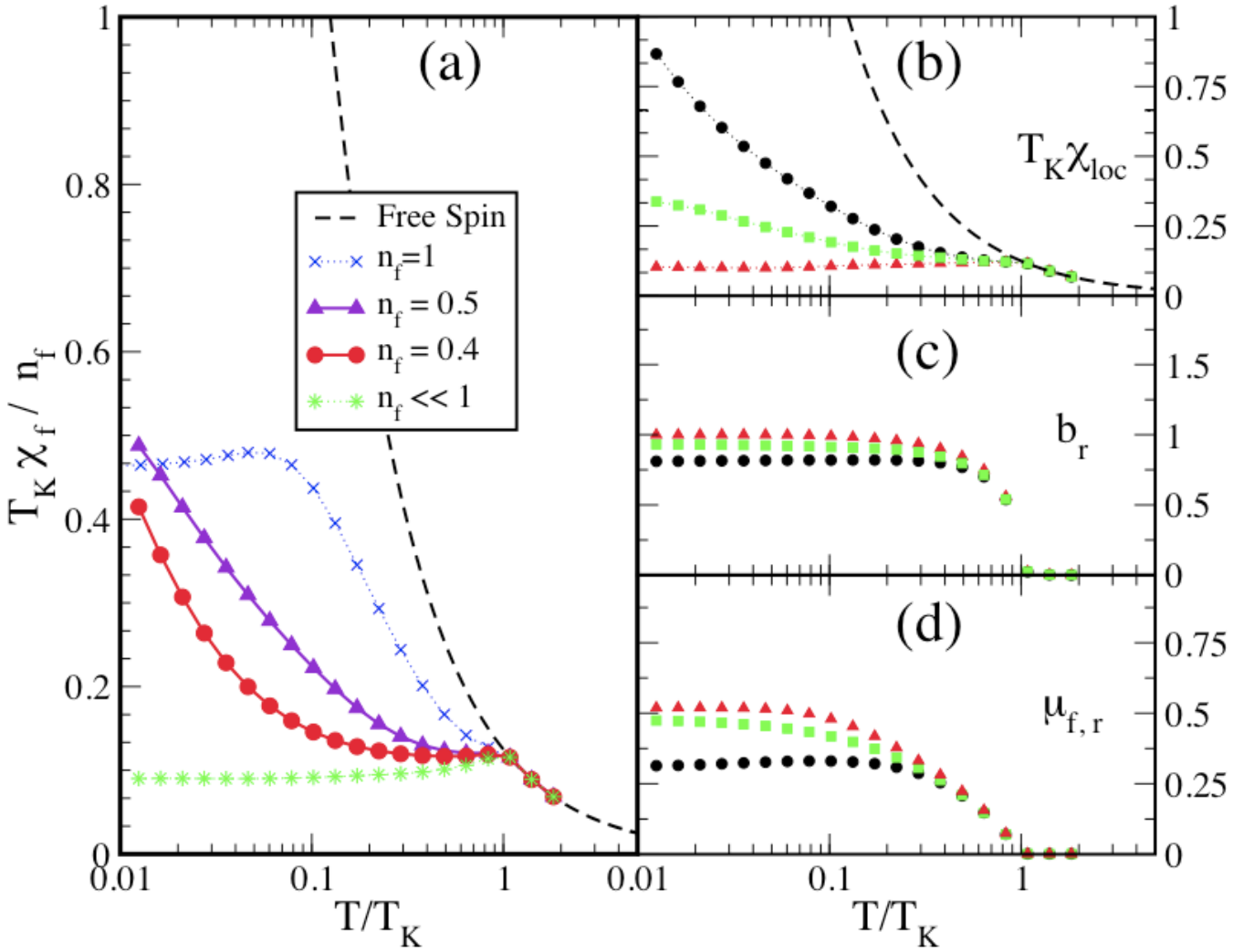
# Mean-field wavefunctions: Localization near $n_f = n_c$

$1/\mathrm{IPR}_n = \sum_i |\psi_n(r_i)|^4$

Mean-field results for $n_f = 1, 0.9, 0.4, 0.25$.



# Temperature dependence




**Disorder is „self-generated“ below $T_K$ !**

# Relation to Kondo-disorder models

VOLUME 78, NUMBER 2 PHYSICAL REVIEW LETTERS 13 JANUARY 1997

**Disorder-Driven Non-Fermi-Liquid Behavior in Kondo Alloys**

E. Miranda and V. Dobrosavljević
*National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Drive, Tallahassee, Florida 32306*

G. Kotliar

Random $J_K$ or random conduction band DOS $\rho$

$\rightarrow$ distribution of $(\rho J_K)$

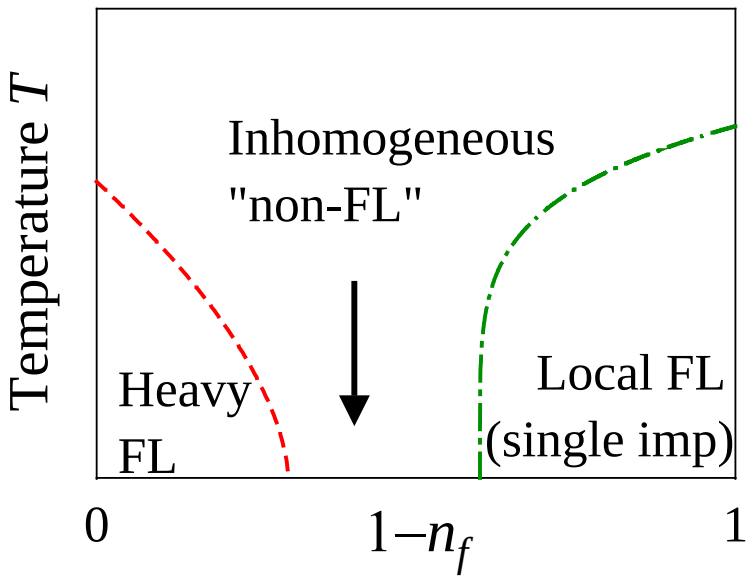
$\rightarrow$ broad distribution of local $T_K$

$\rightarrow$ apparent non-Fermi-liquid behavior

Kondo disorder: Dobrosavljevic/Kirkpatrick/Kotliar (1993)
Miranda et al (1997); Castro-Neto/Castilla/Jones (1998)

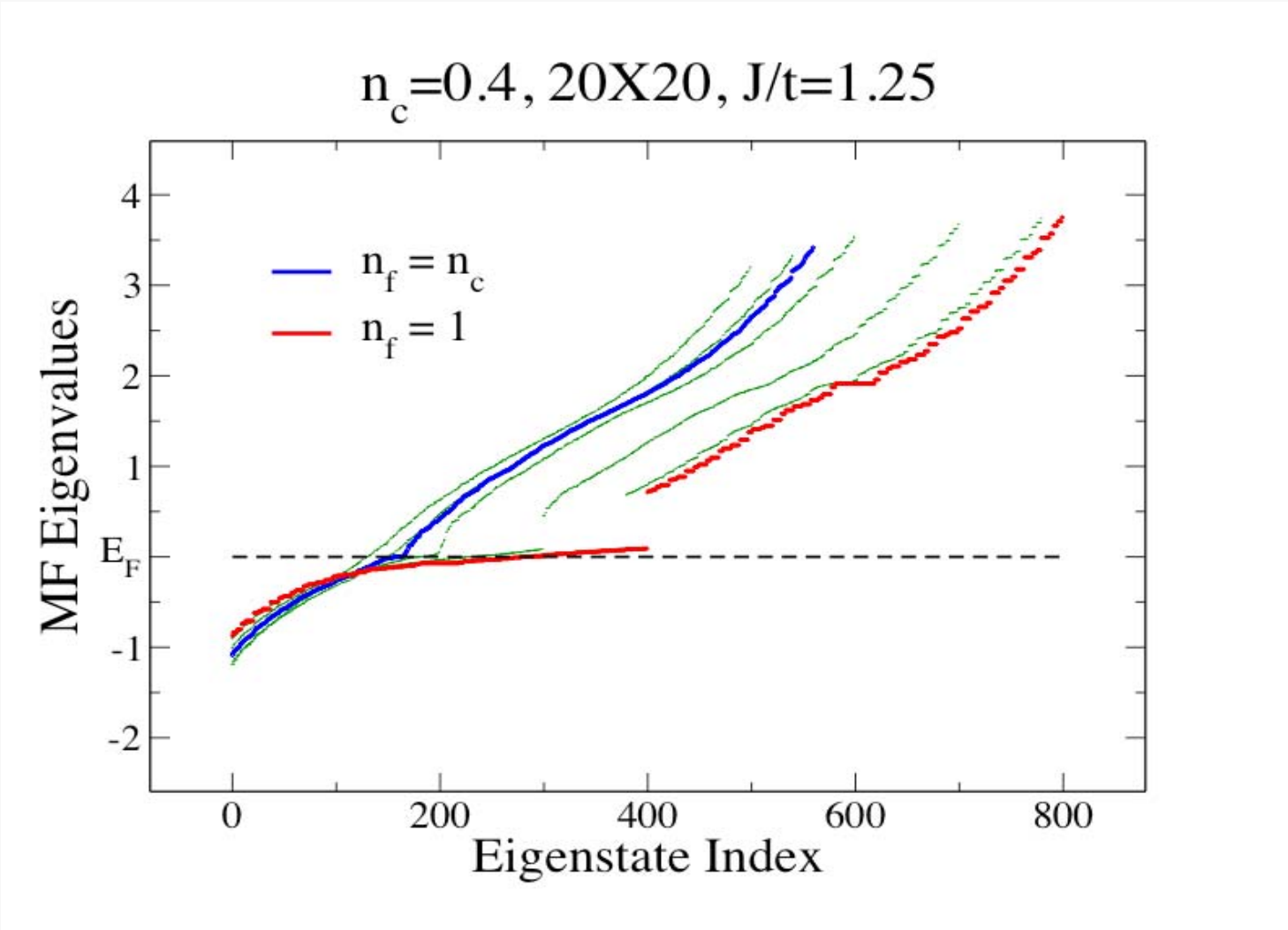
## Summary

1. Depleted Kondo lattice: From Kondo Impurity to Heavy FL
2. Strongly inhomogeneous low-$T$ phases around $n_f = n_c$
3. NFL behavior (similar to Kondo disorder scenario)
4. Experiments on $Ce_{1-x}La_xCoIn_5$ & $Ce_{1-x}La_xPb_3$



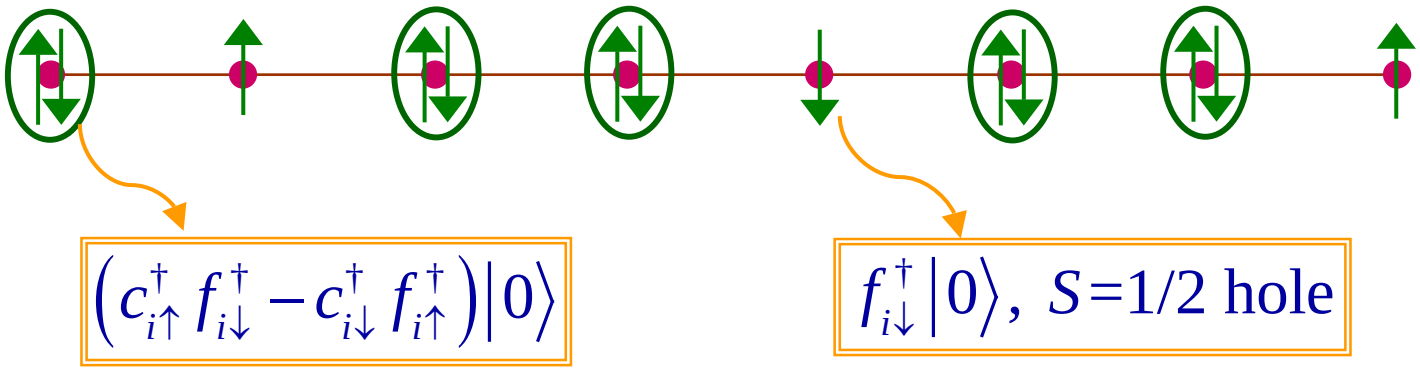

Kaul/Vojta, cond-mat/0603002

# Mean-field theory: Spectrum



# Argument for the Fermi surface volume of the FL phase

Single ion Kondo effect implies $J_K \to \infty$ at low energies




Fermi liquid of $S$=1/2 holes with hard-core repulsion

$$\text{Fermi surface volume } = -\left(\text{density of holes}\right) \bmod 2$$
$$= -\left(1-n_c\right) = \left(1+n_c\right) \bmod 2$$