SMR.1572 - 25

Workshop on
Novel States and Phase Transitions in Highly Correlated Matter

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Phase transitions and critical dimensions in quantum impurity models

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Phase Transitions and Critical Dimensions in Quantum Impurity Models

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1. **Impurity quantum phase transitions**

   Criticality in 0+1 dimensions

2. **Pseudogap Kondo model**

   Phase diagram: NRG
   RG around lower and upper critical dimensions
   Impurities in cuprate superconductors

3. **Spin-boson model**

   Phase diagram: Bosonic NRG
   Spin dynamics and coherence - decoherence crossover

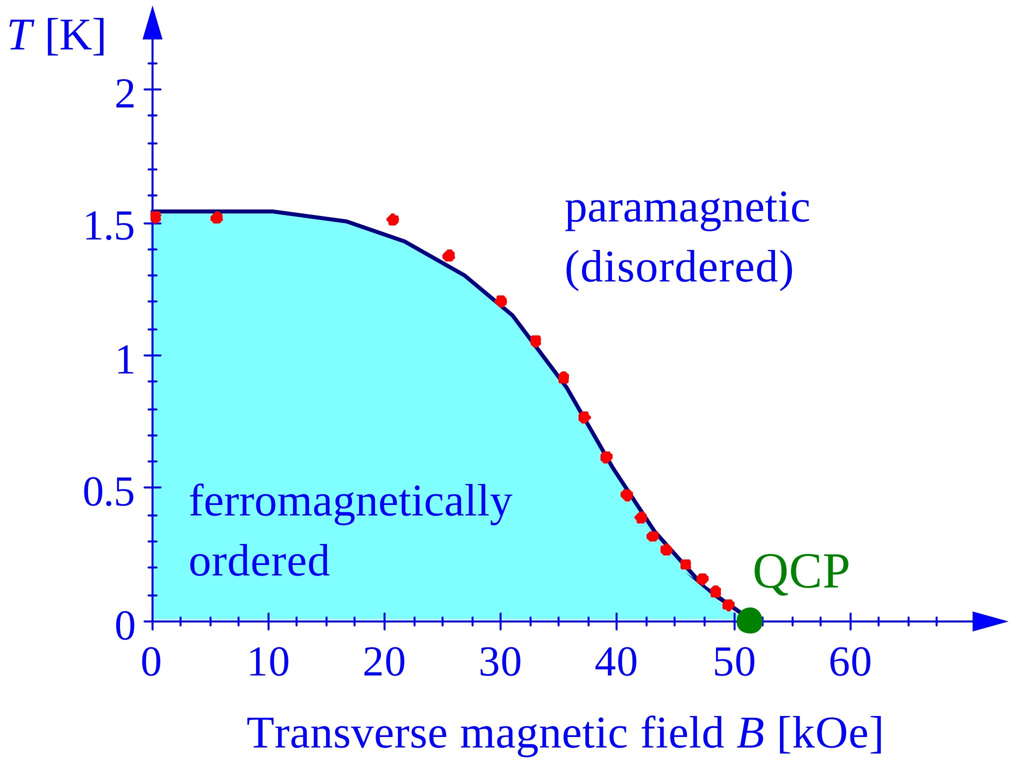
What is a quantum phase transition?

Phase transition at *T* = 0,
driven solely by quantum fluctuations,
occurs upon variation of a non-thermal control parameter *r*

More technically:
A quantum phase transition is a non-analyticity of the ground state properties as function of control parameter *r*

$LiHoF_4$ at 0 K and magnetic field ~ 50 kOe

Continuous transition ferromagnet - paramagnet;
described by Ising model in transverse field



(Bitko et al, PRL **77**, 940 (1996))

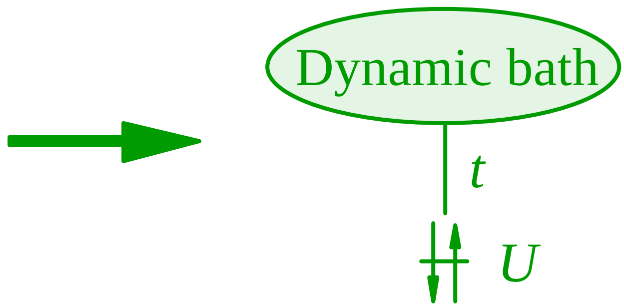
Dynamical mean-field theory

Models of interacting (itinerant) electrons
with a purely local (momentum-independent) self-energy
can be mapped to an effective single-impurity model.

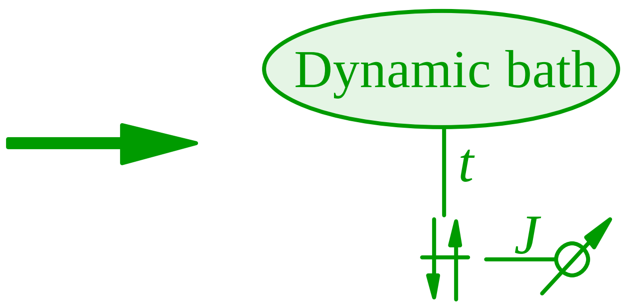
Mapping is exact in $d \to \infty$.

(Metzner / Vollhardt 1989)

Hubbard model



Kondo lattice model



Critical dimensions

Asymptotic critical behavior near a continuous (bulk) phase transition crucially depends on dimensionality

d_c^+: **upper critical dimension**

d_c^-: **lower critical dimension**

$d > d_c^+$

Transition shows mean-field behavior;
order parameter fluctuations are unimportant;
exponents do not depend on d

$d_c^- < d < d_c^+$

Fluctuations are important and strongly interacting;
exponents depend on d

$d < d_c^-$

No phase transition at all;
ordered phase does not exists due to strong fluctuations

Classical magnet: $d_c^+ = 4$, $d_c^- = 2$

Critical dimensions and renormalization group

d_c^+: upper critical dimension

d_c^-: lower critical dimension

How to calculate critical properties for $d_c^- < d < d_c^+$?

Near d_c^+:

Interactions between order parameter fluctuations are small.

Expand ϕ^4 theory in interactions.

$$S = \int d^d x \, [(\nabla_x \phi)^2 + m\phi^2 + u(\phi^2)^2]$$

Near d_c^-:

Transition temperature is small.

Expand non-linear sigma model around ordered state.

$$S = \frac{1}{T} \int d^d x \, (\nabla_x \boldsymbol{n})^2 \qquad \text{with } \boldsymbol{n}^2(x,\tau) = 1$$

$$\boldsymbol{n} = (\pi_1, \pi_2, \sqrt{1-\pi_1^2-\pi_2^2})$$

Both expansions describe same critical point!

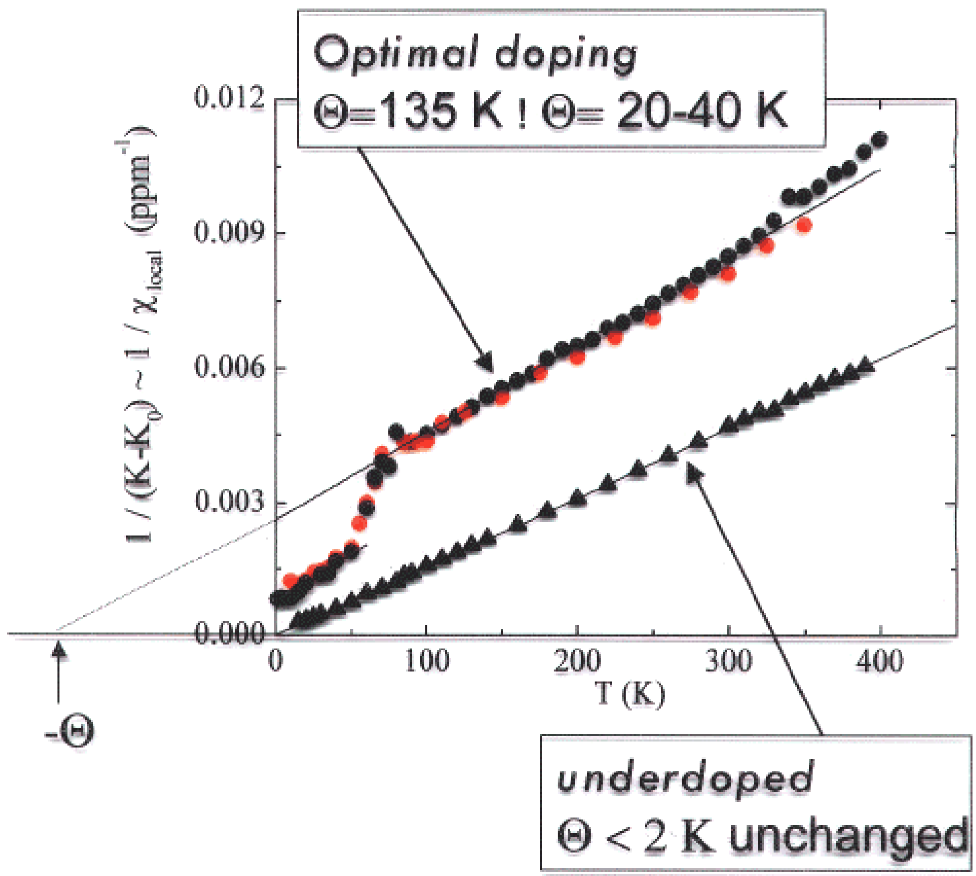
Pseudogap

Kondo model

NMR on Zn/Li impurities in YBCO

J. Bobroff, H. Alloul, W.A. MacFarlane, P. Mendels,
N. Blanchard, G. Collin, and J.-F. Marucco, PRL 86, 4116 (2001)

^{7}Li NMR below T_c



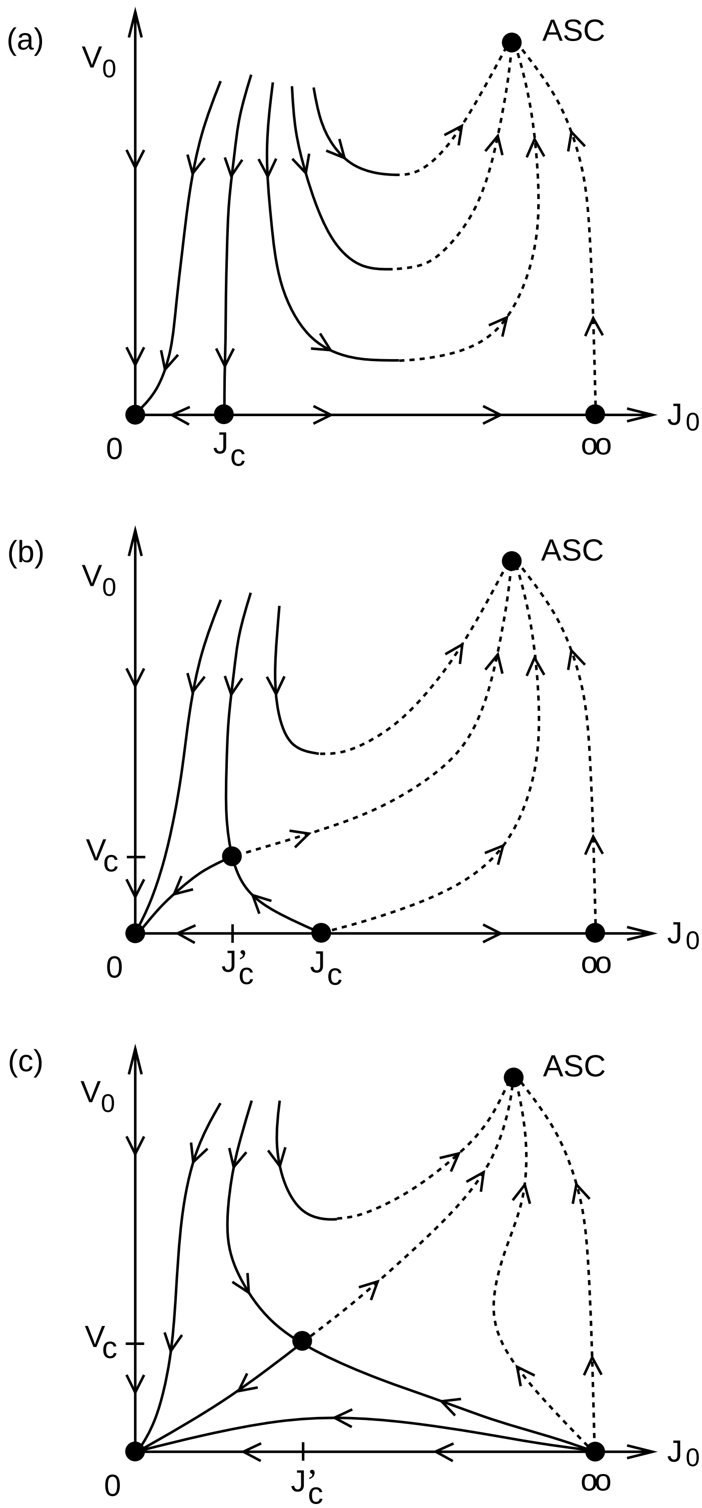
Inverse local susceptibility of isolated Li impurities in YBCO

Pseudogap Kondo model: RG flow

$0 < r < r^* = 0.3748$

$r^* < r < 0.5$

$r > 0.5$



Gonzalez-Buxton / Ingersent, PRB 57, 14254 (98)

Pseudogap Kondo model: Critical behavior

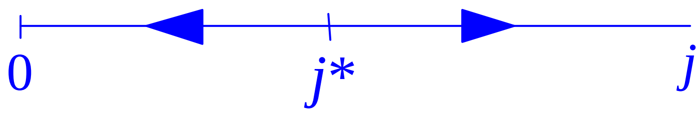
$\rho(\varepsilon) = \rho_0\, |\varepsilon/D|^r$ at small ε

Small r << 1

Critical coupling J_c small $\rightarrow$ Weak-coupling RG for $j = \rho\, J_K$

$$\beta(j) = j^2 - r\, j$$

Unstable fixed point at $j^* = r$.



Larger r » 1

No apparent small parameter ...

? ? ?

Pseudogap Kondo model: Critical behavior

Numerics: Hyperscaling is obeyed for $r < 1$, but not for $r > 1$

$r = 1$ is upper-critical "dimension"

$r = 0$ is lower-critical "dimension"

Q: What is the "gaussian" theory for $r > 1$?

A: Simple level crossing !

Level crossing between spin-1/2 doublet and screened singlet, weakly coupled to low-energy conduction electrons

Represent impurity levels by $|\sigma\rangle$, $|s\rangle$.

$$H_{imp} = s\,|\sigma\rangle\langle\sigma| + g\,(\,|\sigma\rangle\langle s|\,c_\sigma(0) + \text{h.c.})$$

Coupling g to conduction electrons (c) is marginal at $r = 1$!
dim[g] = $(1-r)\,/\,2$

Vojta / Fritz, cond-mat/0309262

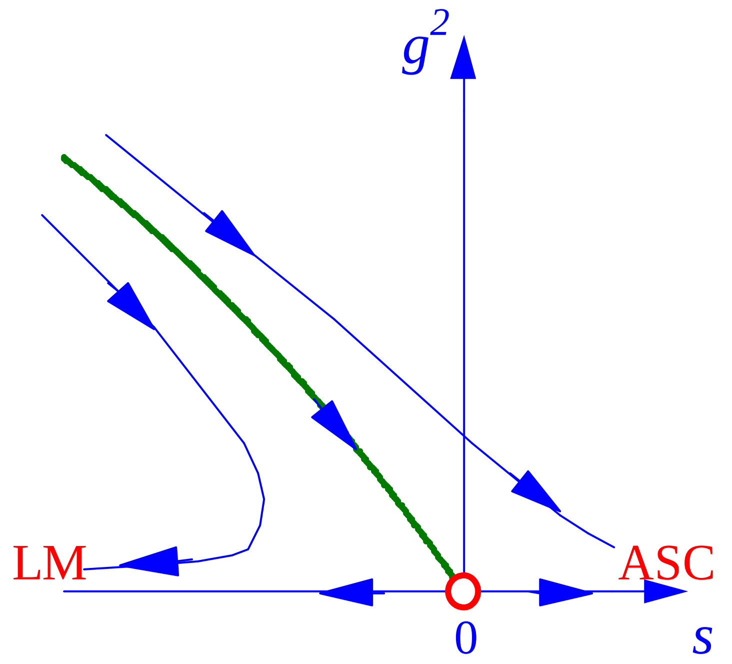
Pseudogap Kondo model: RG around $r = 1$

$$H_{imp} = (s + \lambda) f_\sigma^+ f_\sigma + \lambda\, b_s^+ b_s + g\,(f_\sigma^+ b_s\, c_\sigma(0) + \text{h.c.})$$

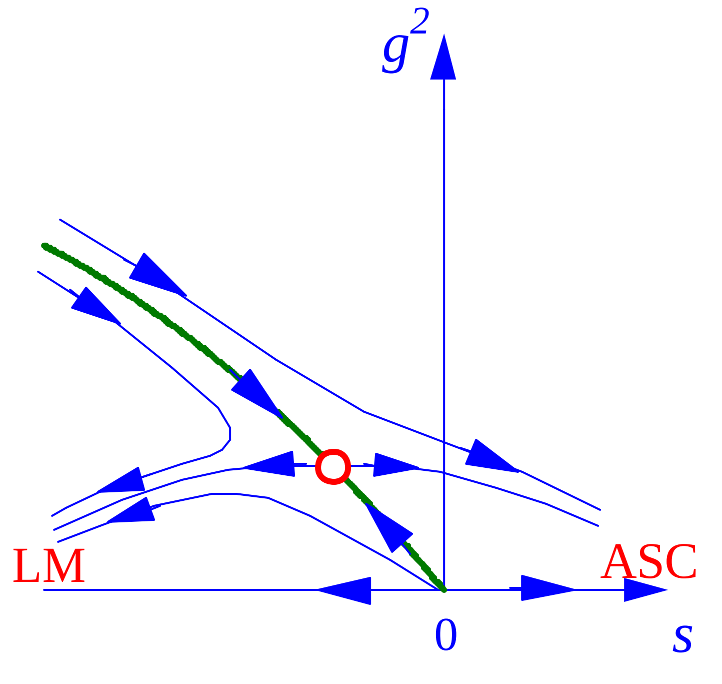
dim[g] = $(1-r)/2$ $\rightarrow$ g relevant below $r < 1$

RG in analogy to ε expansion in ϕ^4 theory

a) $r > 1$



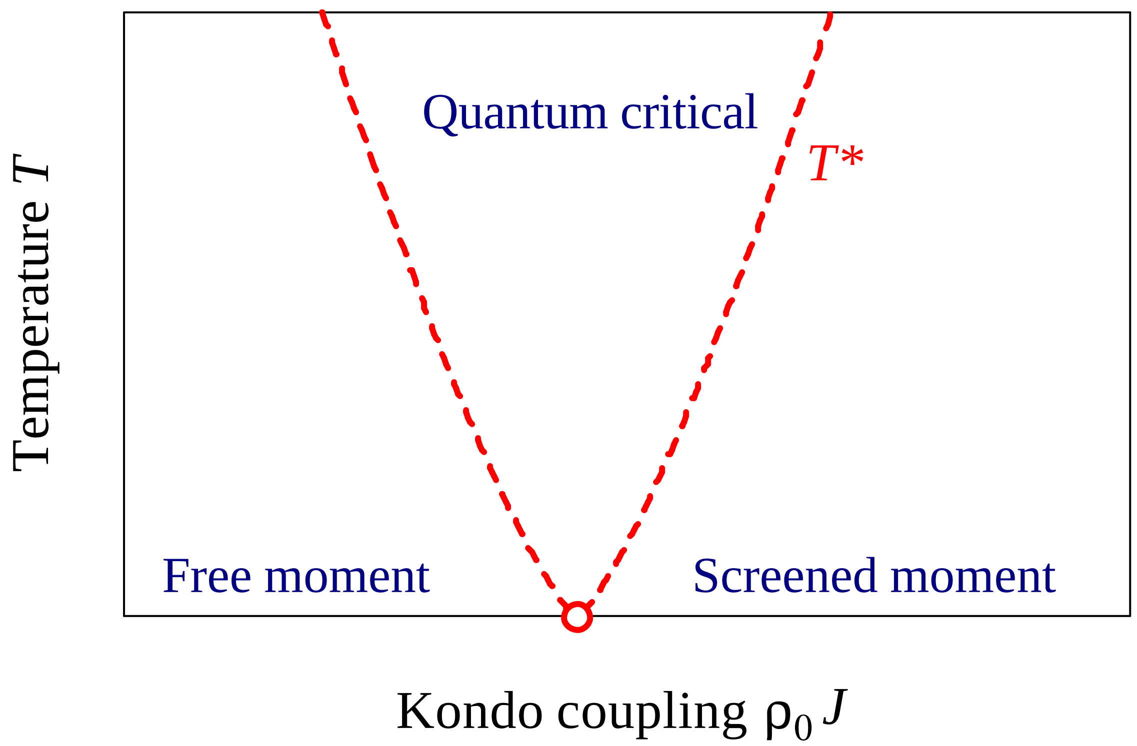
b) $r < 1$



Vojta / Fritz, cond-mat/0309262

Pseudogap Kondo model: Phase diagram

$\rho(\varepsilon) = \rho_0 \, |\varepsilon/D|^r$ at small ε



Quantum critical regime characterized by

- non-trivial value of effective moment
  $T\chi_{imp} = S(S+1)/3$ with **fractional** effective spin S

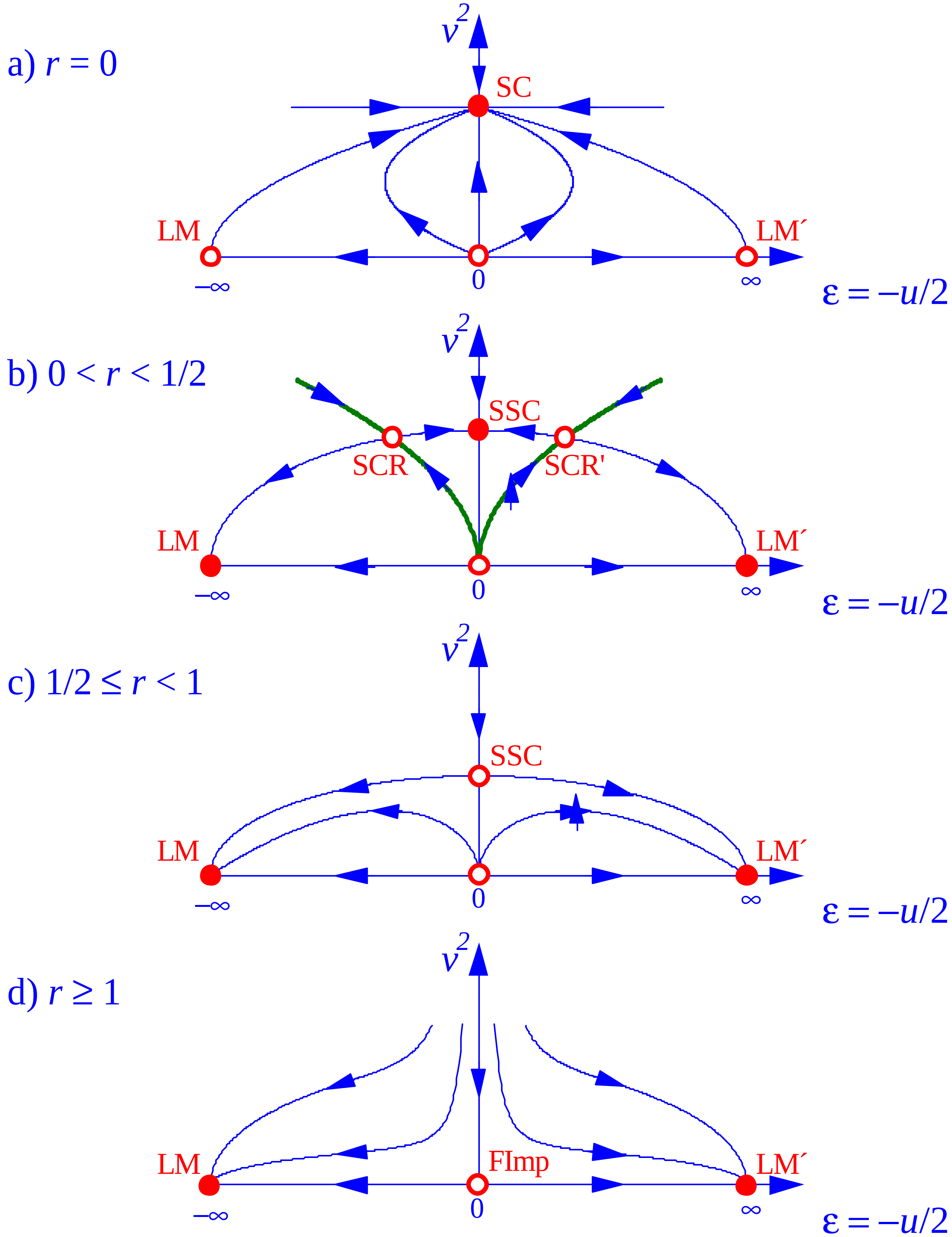
- anomalous power laws in local susceptibility,
  impurity Green's function etc.

Vojta, Phys. Rev. Lett. **87**, 097202 (2001)
Vojta / Bulla, Phys. Rev. B **65**, 014511 (2002)
Vojta / Fritz, cond-mat/0309262

Pseudogap Kondo model: RG around $r = 1/2$

$$S_{imp} = \sum f_\sigma \, \mathrm{sgn}(\omega_n)\, |i\omega_n|^r f_\sigma + \int d\tau\, u\, f_\uparrow f_\uparrow f_\downarrow f_\downarrow$$

$\dim[u] = (2r-1) \to u$ relevant for $r > 1/2$



Spin-boson model

Spin-boson model

$$H = \Delta\,\sigma_x/2 \; + \; \sigma_z/2 \sum_i \lambda_i (a_i^+ + a_i)$$

Bath spectral function

$$J(\omega) = 2\pi\,\alpha\,\omega^s K^{1-s}, \quad 0 < \omega < \omega_c$$

Ohmic bath *s* = 1

Kosterlitz-Thouless transition between

$\alpha < \alpha_c$: weak damping (delocalized)

$\alpha > \alpha_c$: strong damping (localized)

$\alpha_c \to 1$ as $\Delta \to 0$

Subohmic bath *s* < 1

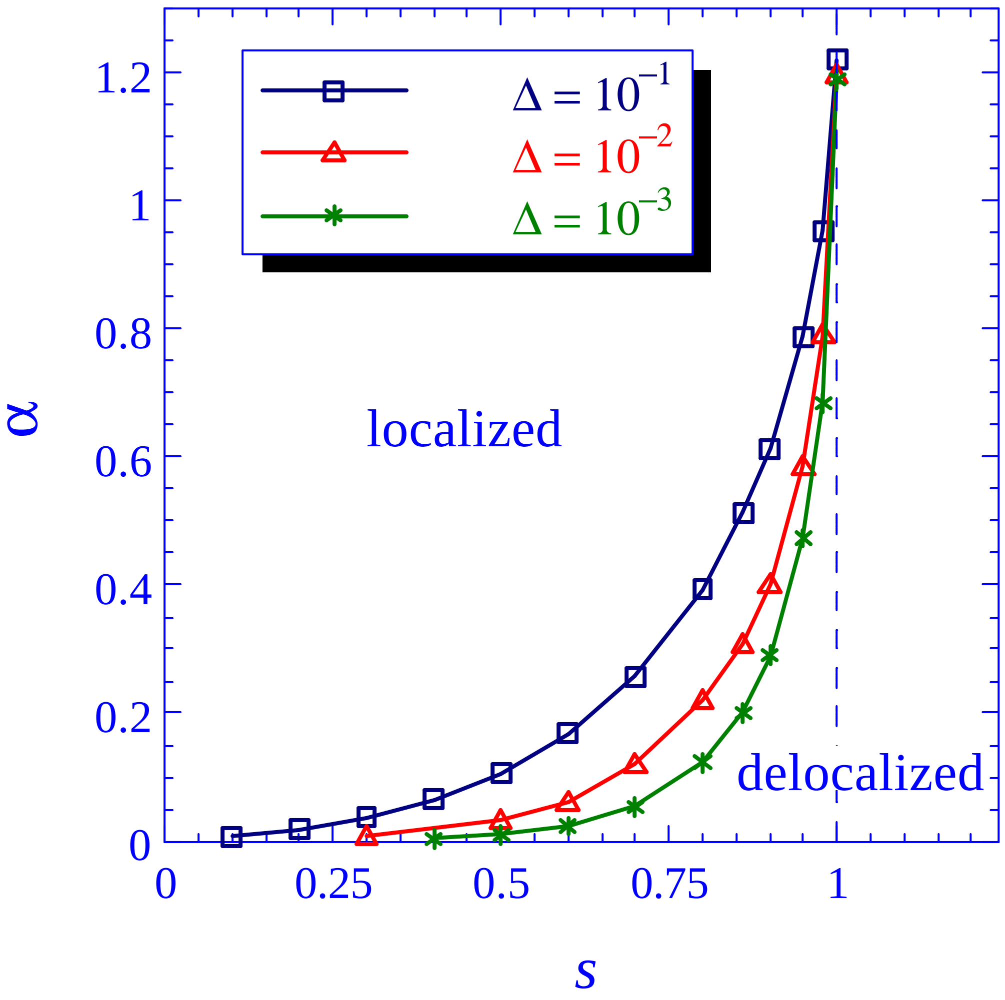
System localized in the limit $\Delta \to 0$ for any α;

behavior at finite Δ not studied systematically

Subohmic spin-boson model: Phase diagram

Method:
Numerical Renormalization group (Wilson), generalized to bosonic systems, can access arbitrarily low energies/temperatures

Result:
Continuous quantum phase transition for all $0 < s < 1$ between localized and delocalized phase;
exponents vary with s



Bulla / Tong / Vojta, cond-mat/0306708

Spin-boson model: Kink gas mapping

Spin-boson model with ω^s bath spectrum is equivalent to Ising model with long-range interaction falling off as $|r|^{-1-s}$.

Ising model can be analyzed in "kink gas" representation.
(kink = Ising domain wall / tunnel event)

Perturbative RG (Kosterlitz PRL 1976)

Tunnel splitting:	$\beta(\Delta) = \Delta\,(1-\alpha)$
Dissipation strength	$\beta(\alpha) = -\alpha\,(\Delta^2 + s - 1)$

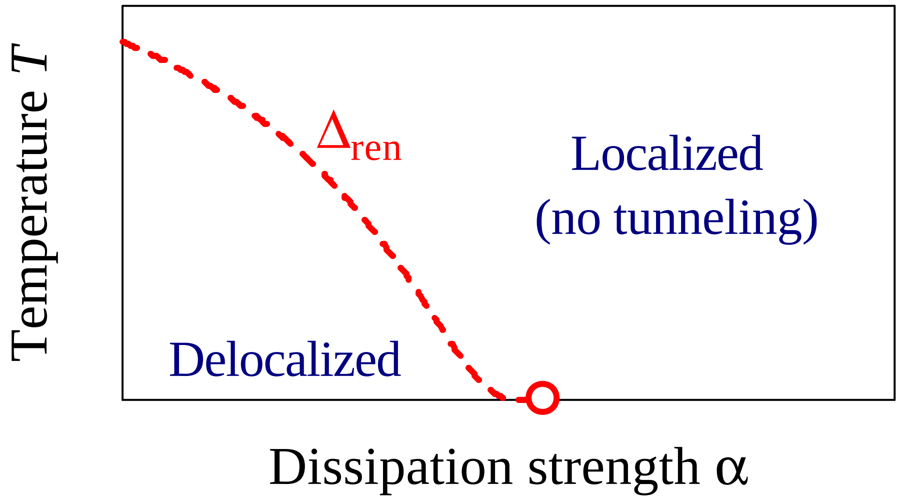
$s = 1$: Line of stable FP at $\Delta = 0$, $\alpha \geq 1$

$s < 1$: Critical FP at $\alpha* = 1$, $\Delta*^2 = 1 - s$

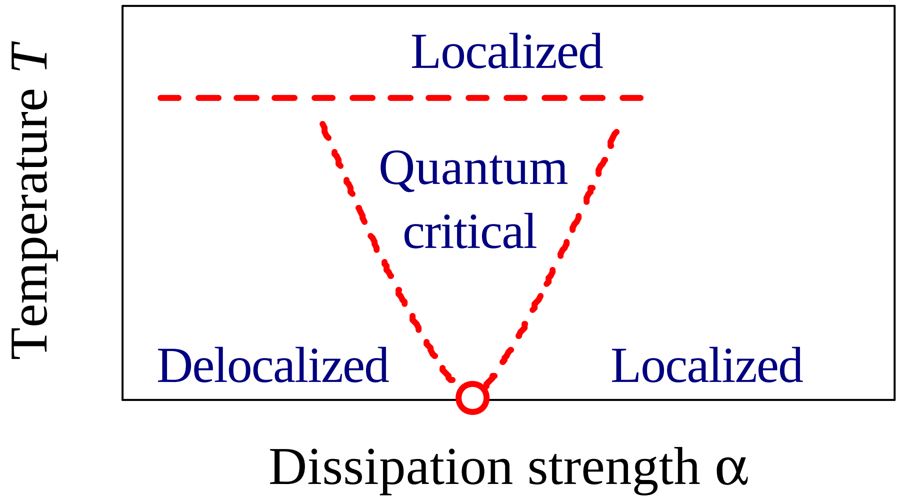
(Valid for $1 - s << 1$)

Spin boson model: Phase diagrams

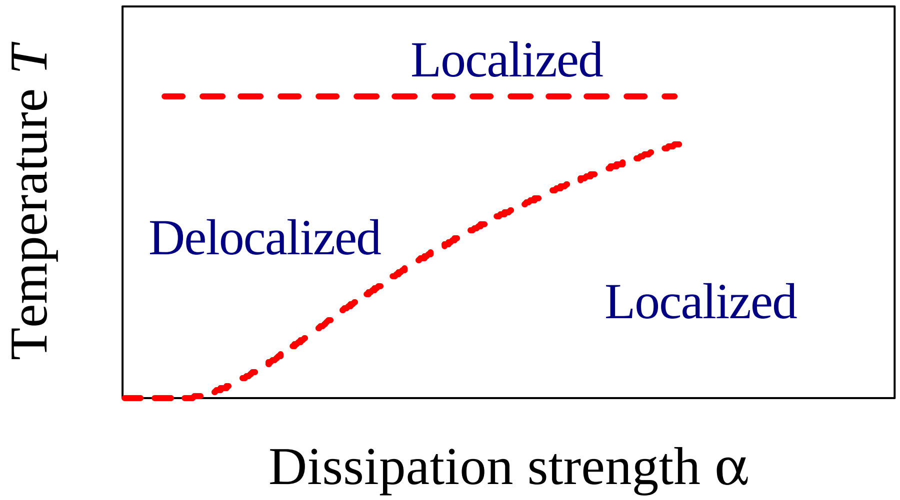
***s* = 1**



0 < *s* < 1



***s* = 0**



Conclusions

- Zero-temperature phase transitions in impurity systems can influence finite-temperature properties of system over a wide range of the phase diagram

- Pseudogap Kondo model allows for RG expansion around lower and upper-critical dimensions

- Subohmic spin-boson model shows continuous transition for $0 < s < 1$ with hyperscaling properties

- Applications in:
  Impurities in *d*-wave superconductors (NMR, STM)
  Multilevel or coupled quantum dots (transport)
  Noisy qubits
  Local criticality in bulk systems (cuprates, heavy fermions)