Universal crossovers and critical dynamics for quantum phase transitions in impurity models

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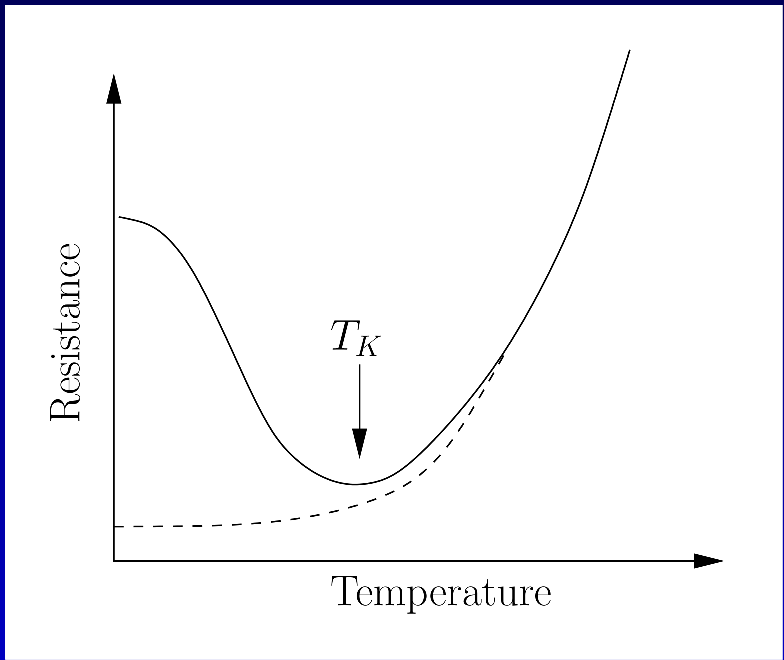
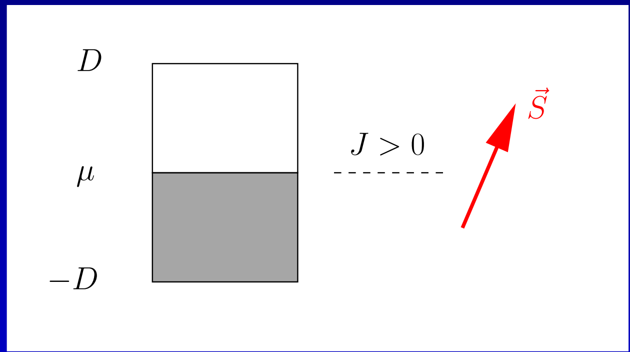
Summary

- The Kondo problem in a pseudogap
- RG strategy and CS equations
- Computation of universal crossovers
- Critical dynamics
- Influence of p-h asymmetry
- Spin $S = 1$ case: NFL and QPT

Where it started

Diluted magnetic impurities in a metal:





- Temperature dependent impurity scattering

Kondo model: basics

Model: Spin 1/2 with AF coupling to a Fermi sea

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J\vec{S} \cdot \sum_{\sigma\sigma'} c^\dagger_\sigma(0) \frac{\vec{\tau}_{\sigma\sigma'}}{2} c_{\sigma'}(0)$$

Physics: smooth crossover between two simple limits

Limit $J = 0$: local moment

- $S(T) = \log 2$ and $\chi_{imp}(T) = 1/(4T)$

Limit $J = \infty$: singlet state (screening)

- $S(T) = 0$ and $\chi_{imp}(T)$ finite

RG for Kondo problem

Perturbation theory ($j_0 = J/D$): badly convergent!

$$\chi_{imp}(T) = \frac{1}{4T}\left[1 - j_0 - j_0^2 \log\frac{D}{T} + \ldots\right]$$
$$= \frac{1}{4T}\left[1 \underbrace{- j_0 + j_0^2 \log\lambda}_{-j_0(\lambda)} - j_0^2 \log\frac{\lambda D}{T}\right]$$

Scaling form: $\chi_{imp}(T, j_0, D) = \chi_{imp}(T, j_0(\lambda), \lambda D)$

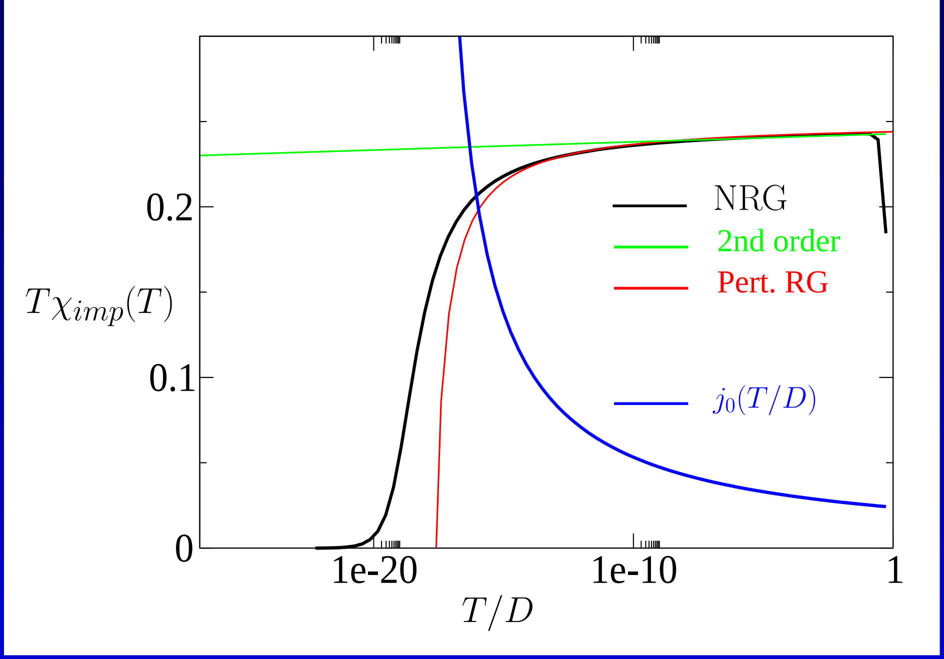
Iterate RG relation: $\beta(j_0) \equiv \frac{\partial j_0(\lambda)}{\partial \log\lambda} = -j_0^2(\lambda)$

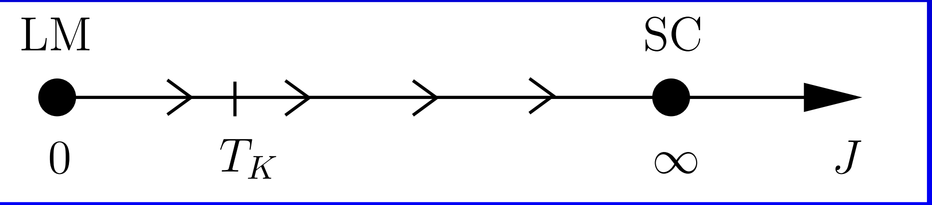
$\Rightarrow j_0(\lambda) = \frac{1}{\log(\lambda D/T_K)}$ with $T_K = D\exp(-1/j_0)$

RG flow

Trick: now we can choose $\lambda = T/D$

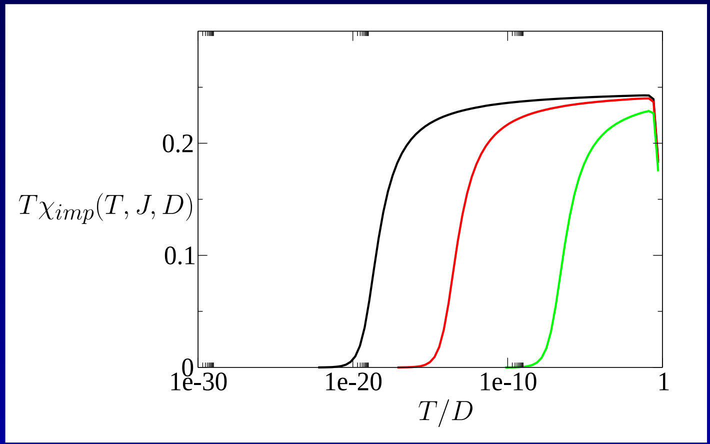
$$\chi_{imp}(T) = \frac{1}{4T}\left[1 - j_0(T/D)\right] = \frac{1}{4T}\left[1 - \frac{1}{\log(T/T_K)}\right]$$

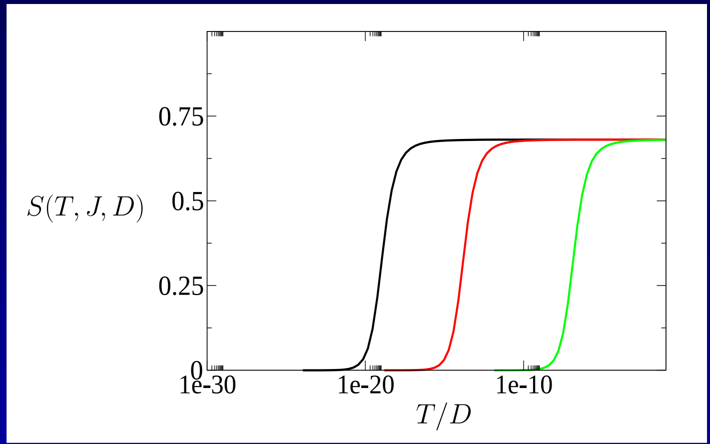


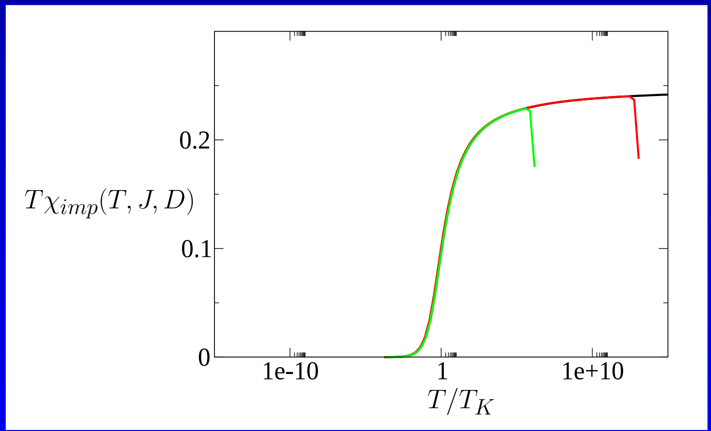


Universality

$$\text{RG} \Rightarrow T\chi_{imp}(T, j_0, D) = \Phi(T/T_K)$$







Collapse at $T \ll D$

Another view on RG

Universality $\Rightarrow$ take limit $D \to \infty$

Procedure: set $\chi_{imp}(T=\mu)$ finite at given scale μ

$$\chi_{imp}(T=\mu) \;=\; \frac{1}{4\mu}\left[1 - j_0 - j_0^2 \log\frac{D}{\mu}\right] \equiv \frac{1}{4\mu}\left[1 - j_R\right]$$

$$\Rightarrow \chi_{imp}(T) \;=\; \frac{1}{4T}\left[1 - j_R - j_R^2 \log\frac{\mu}{T}\right]$$

Scaling form: $\chi_{imp}(T, j_R, \mu) = \chi_{imp}(T, j_R(\lambda), \lambda\mu)$

RG: $j_R(\lambda) = \log^{-1}(\lambda\mu/T_K)$ and $T_K = \mu \exp(-1/j_R)$

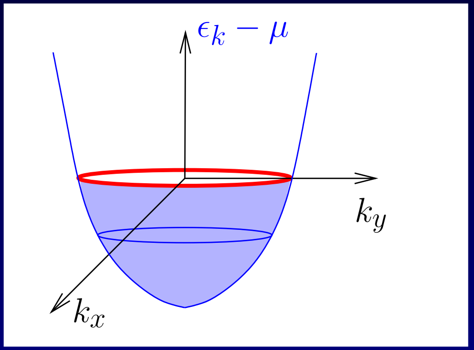
Origin: Choice of μ arbitrary $\Rightarrow \mathrm{d}\chi_{imp}/\mathrm{d}\mu = 0$

$$\Rightarrow \boxed{\left[\mu\frac{\partial}{\partial\mu} + \beta(j_R)\frac{\partial}{\partial j_R}\right]\chi_{imp}(T, j_R, \mu) = 0} \text{ (CS eq.)}$$

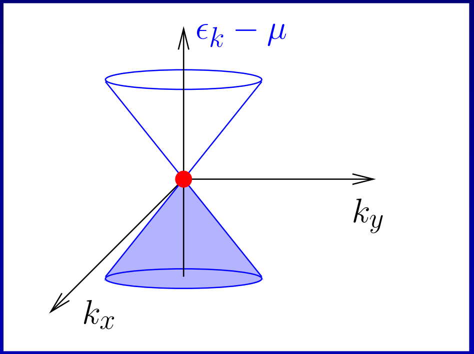
Pseudogap Kondo model

Gapless host DOS: $\rho(\epsilon) \propto |\epsilon|^r$

- Metals: $r = 0$

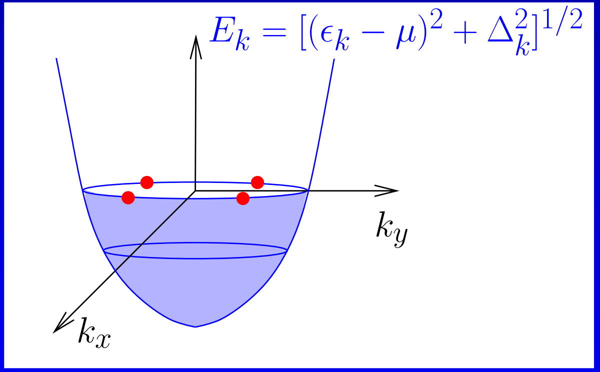


- Semiconductors: $r = 1$



- HTc SC: $r = 1$

  $\Delta_k = \Delta(\cos k_x - \cos k_y)$



RG for pseudogap Kondo

Weak coupling RG: easy guess as $[J] = -r$

$$\beta(j_R) = \frac{\partial j_R(\lambda)}{\partial \log \lambda} = r j_R(\lambda) - j_R^2(\lambda)$$

Proper method:

- Set $j_0 = (D/\mu)^r Z_j j_R$
- Consider interaction vertex
  $\Gamma^R(\omega) = Z_j j_R \left[1 - |\omega/\mu|^r j_R/r + \ldots\right]$
- Impose $\Gamma^R(\omega = \mu) \equiv j_R = Z_j j_R \left[1 - j_R/r\right]$
- Absorb poles with $Z_j = 1 + j_R/r$
- But one has $\mathrm{d}j_0/\mathrm{d}\mu = 0$
  $\Rightarrow \beta(j_R) = r j_R - j_R\, \beta(j_R)\, \mathrm{dlog}\, Z_j/\mathrm{d}j_R$

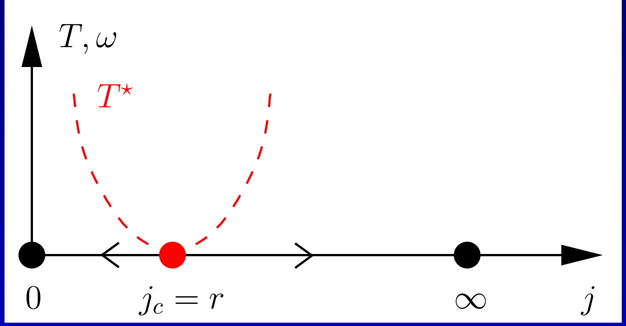
Quantum Phase Transition

Analyze flow equation: vary $\mu \longrightarrow \lambda\mu$

Solve $\frac{\partial j_R(\lambda)}{\partial \log \lambda} = r j_R(\lambda) - j_R^2(\lambda)$ with $j_R(1) = j_R$

$$j_R(\lambda) = \frac{r j_R \, \lambda^r}{r - j_R + j_R \, \lambda^r} = \frac{r}{1 + \mathrm{Sgn}(r - j_R) \, |\lambda\mu/T^\star|^{-r}}$$

with $T^\star \equiv \mu \left| \frac{r - j_R}{j_R} \right|^{1/r}$



- $j_R < r \Rightarrow j_R(\lambda) \propto \lambda^r$ for $\lambda\mu < T^\star$ (flow to LM)
- $j_R = r \Rightarrow j_R(\lambda) = r$ for all λ (fixed point)
- $j_R > r \Rightarrow j_R(\lambda)$ diverges at $T^\star$ (flow to SC)

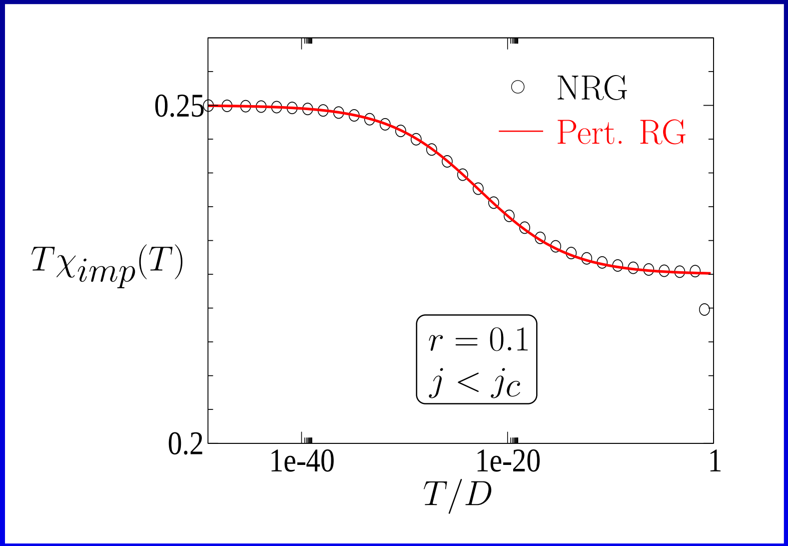
Impurity susceptibility

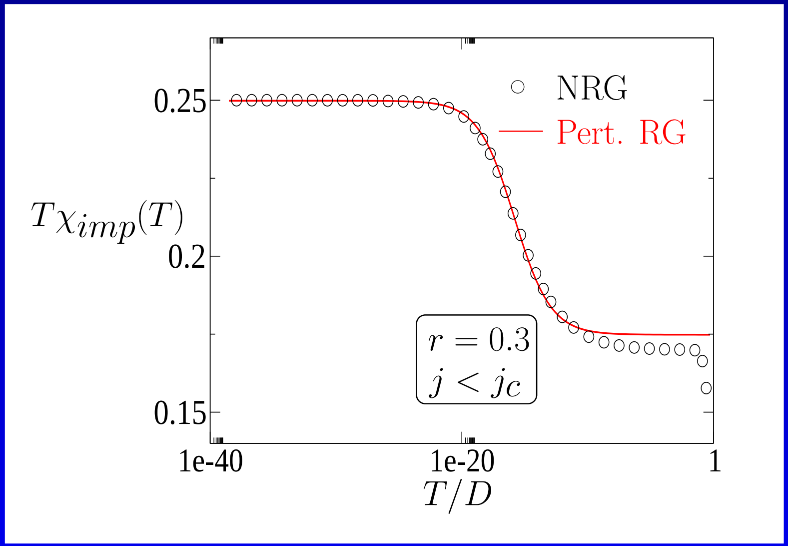
At lowest order: $\chi_{imp} = 1/(4T)[1 - j_R(T/\mu)]$

Quantum critical point: fractional spin

$$\chi_{imp}(T, j_R = j_c) \simeq \frac{1}{4T}(1-r) \neq \frac{S(S+1)}{3T}$$

Universal crossover: from CR to LM ($j < j_c$)





Local susceptibility

The direct computation is still divergent:

$$T\chi^0_{loc}(T) = 1 - j_R^2|T/\mu|^{2r}(1/2r + \mathrm{Cst.})$$

Needs extra renormalization factor:

$$\chi^R_{loc}(T) = Z_\chi \chi^0_{loc}(T) \text{ with } Z_\chi = 1 + j_R^2/2r$$

$$T\chi^R_{loc}(T) \simeq 1 - j_R^2 \log(T/\mu)$$

Scaling analysis: $\chi^0_{loc}(T)$ is independent of μ

$$\Rightarrow \boxed{\left[\mu\frac{\partial}{\partial\mu} + \beta(j_R)\frac{\partial}{\partial j_R} + \eta_\chi(j_R)\right]\chi^R_{loc}(T, j_R, \mu) = 0}$$

with $\eta_\chi(j_R) = \beta(j_R)\frac{\partial \log Z_\chi}{\partial j_R} = j_R^2$

Solution:

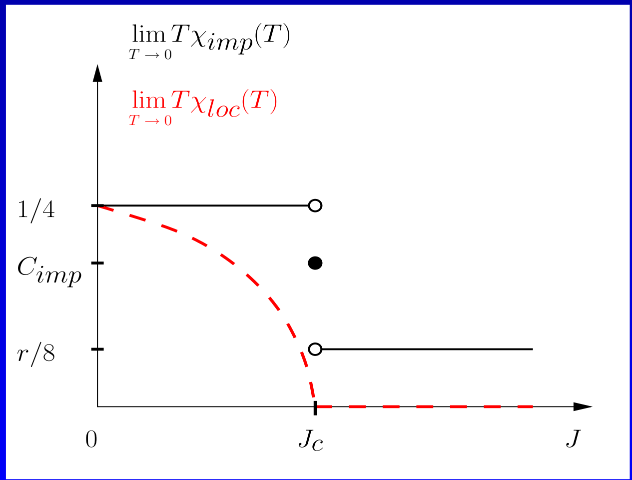
$$\chi^R_{loc}(T, j_R, \mu) = \exp\left(\int_{j_R}^{j_R(\lambda)} \frac{\eta_\chi}{\beta}\right) \chi^R_{loc}(T, j_R(\lambda), \lambda\mu)$$

Choose $\lambda = T/\mu$:

$$T\chi^R_{loc}(T, j_R, \mu) \propto \left[r - j_R + \left|\frac{T}{\mu}\right|^r\right]^r$$

Interpretation:

- $j_R < r$: $T\chi^R_{loc} \propto (r - j_R)^r$ (order parameter)
- $j_R = r$: $\chi^R_{loc}(T) \propto 1/T^{1-r^2}$ (anomalous behavior)



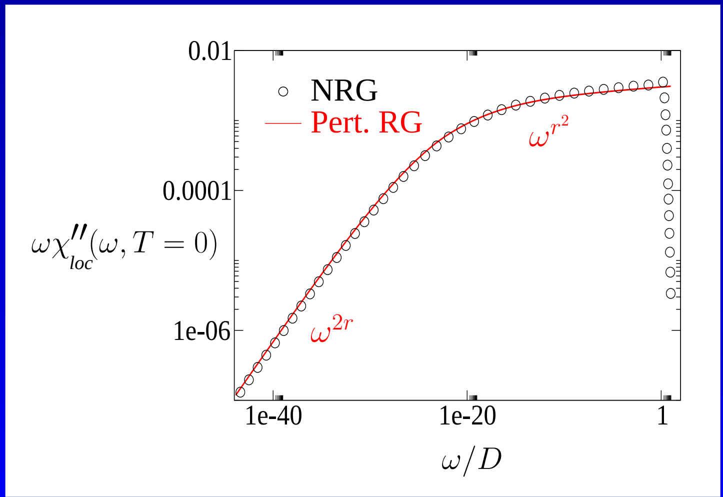
Two vastly different susceptibilities

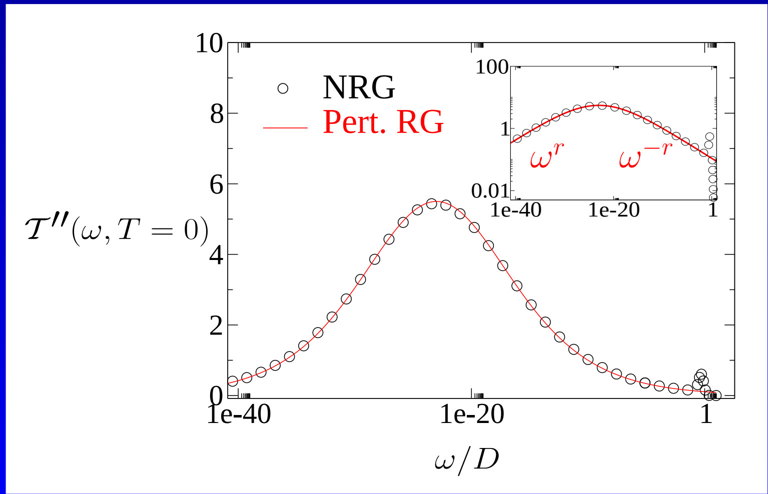
Zero temperature dynamics

Strategy:

- Compute in renormalized perturbation theory
- Choose RG scale λ to control the expansion
- Apply CS equation

Example: for $r = 0.1$ and $j < j_c$





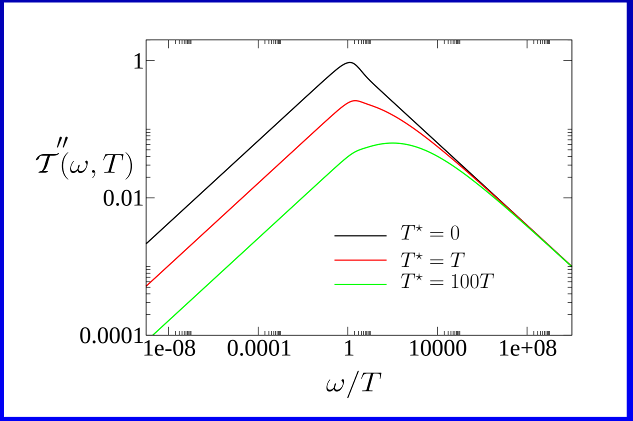
Finite temperature dynamics

Problem: "The ϵ-expansion and the analytic continuation do NOT commute for $\omega \ll T$" (Sachdev)

Let's try: we apply CS in this regime to the T-matrix

$$T''(\omega) \simeq \frac{\omega^r}{[(T^\star)^r \pm (T + |\omega|)^r]^2} \quad \text{(not too bad)}$$

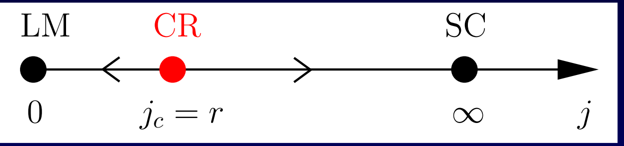
$$T''(\omega) \simeq_{r\to 0} \frac{1}{[\log((T + |\omega|)/T_K)]^2} \quad \text{(BAD!)}$$



Still a challenge for the NRG at $\omega \sim T$

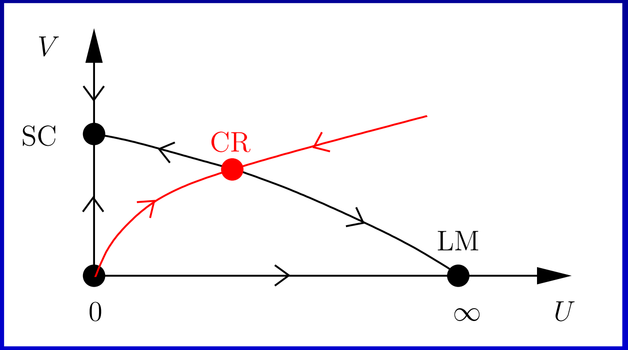
On the other side of the street

Question: Can we capture the crossover to SC?



Answer: not with Kondo, but Anderson is good!

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_\sigma V [d^\dagger_\sigma c_\sigma(0) + H.c.]$$



Scaling analysis: $[U] = 2r - 1 \equiv -\epsilon$

$\Rightarrow$ Perform ϵ-expansion near $r = 1/2$!!

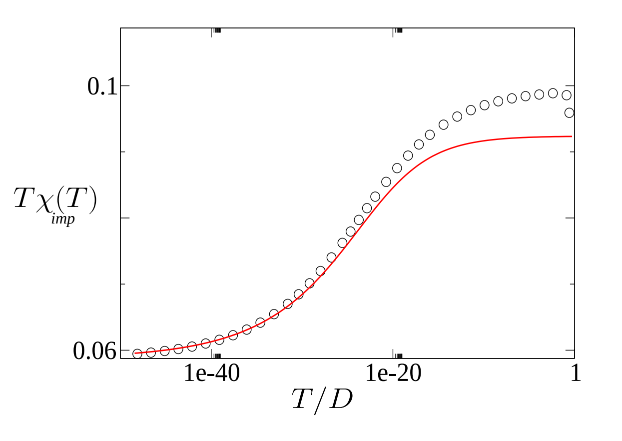
RG for pseudogap Anderson

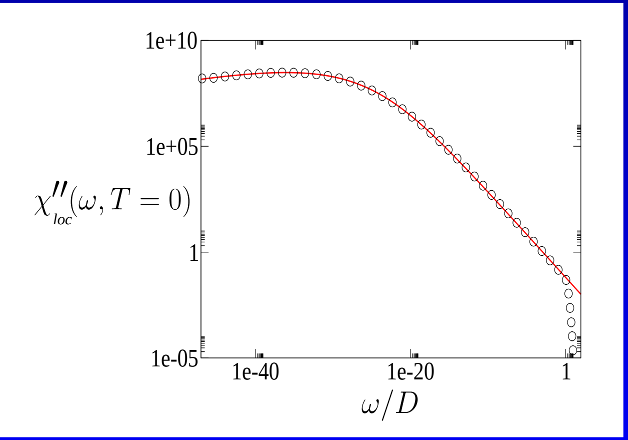
Flow equation:

$$\beta(u) = \epsilon u - \frac{3(\pi - 2\ln 4)}{\pi^2} u^3$$

Critical point at $u_c \propto \sqrt{\epsilon} \Rightarrow$ Poor convergence

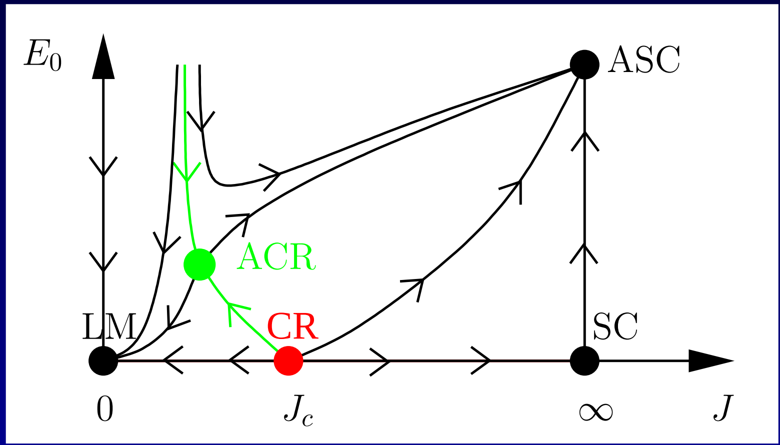
Example: for $r = 0.47$ and $j > j_c$





With particle-hole asymmetry

NRG result: for $0.375 < r < 1$



Effective theory: $U = \infty$ Anderson model

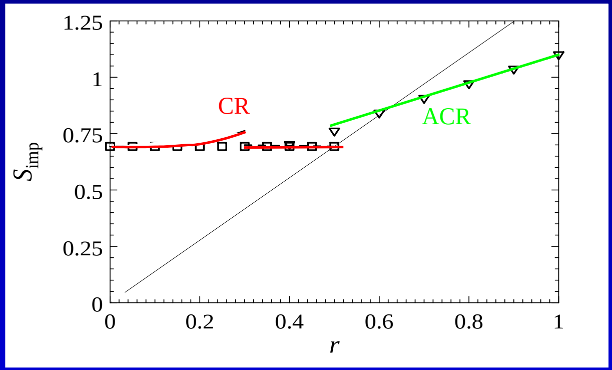
$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_f \sum_\sigma f_\sigma^\dagger f_\sigma + V \sum_{k\sigma} \left[f_\sigma^\dagger b \; c_{k\sigma} + \text{h.c.} \right]$$

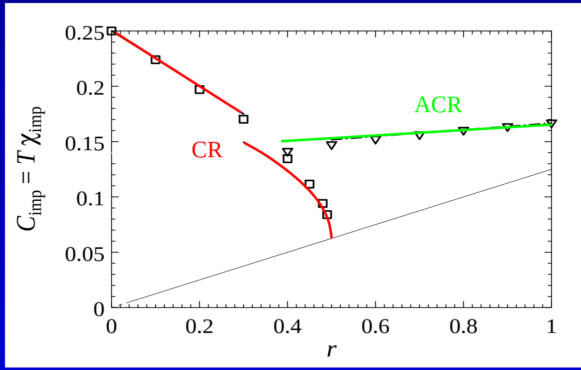
RG: V marginal at $r = 1 \Rightarrow$ expansion in $\epsilon' = 1 - r$

Interpretation:

- Kondo and Anderson: same universality class
- Origin of the asymmetric QCP: competition doublet (spinon) vs. singlet (holon) states

$$\begin{cases} S_{\mathrm{imp}}^{\mathrm{ACR}} = \ln 3 - \frac{8\ln 2}{9}(1-r) \\ T\chi_{\mathrm{imp}}^{\mathrm{ACR}} = \frac{1}{6} - \frac{3-2\ln 2}{18}(1-r) \end{cases}$$





Open problem: transition between CR and SCR

Interesting generalization

- Spin S=1 Kondo model
- ACR persists with $S_{imp} = \ln 5$ at $r = 1$

Effective theory: crossing triplet-doublet

$$
\begin{aligned}
H &= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \epsilon_f \sum_m f^\dagger_m f_m \\
&\quad + V \sum_k \left[f^\dagger_0 b_\downarrow c_{k\uparrow} + f^\dagger_0 b_\uparrow c_{k\downarrow} \right] + \text{h.c.} \\
&\quad + \sqrt{2} V \left[f^\dagger_1 b_\uparrow c_{k\uparrow} + f^\dagger_{-1} b_\downarrow c_{k\downarrow} \right] + \text{h.c.}
\end{aligned}
$$

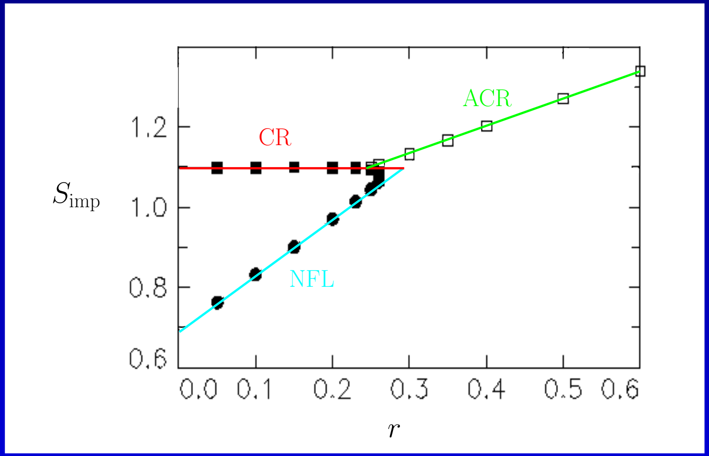
Reproduces Kondo for $\epsilon_f \to -\infty$

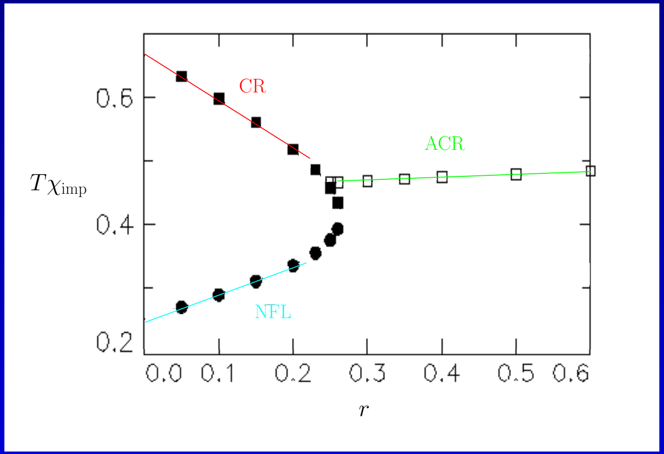
Crucial to introduce the good degrees of freedom!!

Check

Results: properties of the ACR critical point

$$\begin{cases} S_{\text{imp}}^{\text{ACR}} = \ln 5 - \frac{24 \ln 2}{25}(1-r) \\ T\chi_{\text{imp}}^{\text{ACR}} = \frac{1}{2} - \frac{3-2\ln 2}{10}(1-r) \end{cases}$$

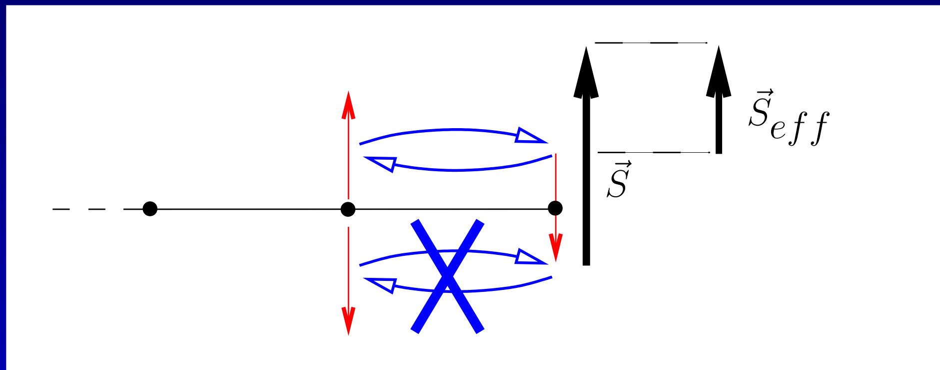




$S = 1$ PG Kondo at p-h sym

Strong coupling limit:

- effective spin $S_{\text{eff}} = 1/2$
- effective FERRO coupling $j_{\text{eff}} = -1/j < 0$



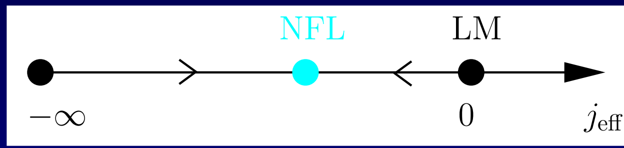
- effective bath exponent $r_{\text{eff}} = -r < 0$

$$\langle c_\sigma^\dagger(\mathbf{0}, i\omega) c_\sigma(\mathbf{0}, \omega) \rangle^{-1} = i\omega - t_{01}^2 \langle c_\sigma^\dagger(\mathbf{1}, i\omega) c_\sigma(\mathbf{1}, \omega) \rangle$$

Extra NFL fixed point

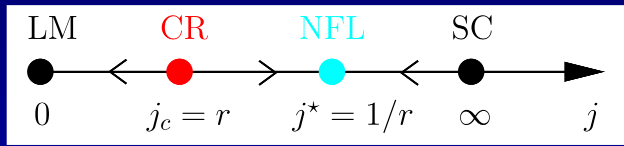
RG: usual Kondo scaling equation

$$\frac{\partial j_{\mathrm{eff}}}{\partial \ln \Lambda} = r_{\mathrm{eff}} j_{\mathrm{eff}} - j_{\mathrm{eff}}^2$$

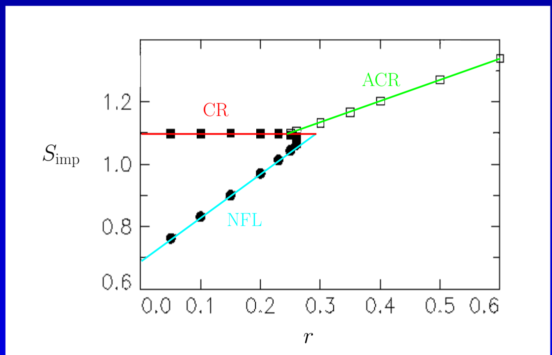


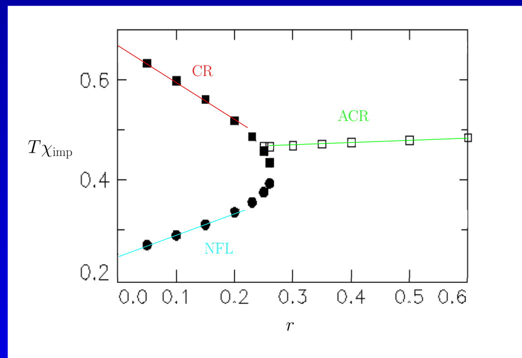
$$\Rightarrow j^\star_{\mathrm{eff}} = r_{\mathrm{eff}} = -r$$

$$\Rightarrow j^\star = 1/r$$



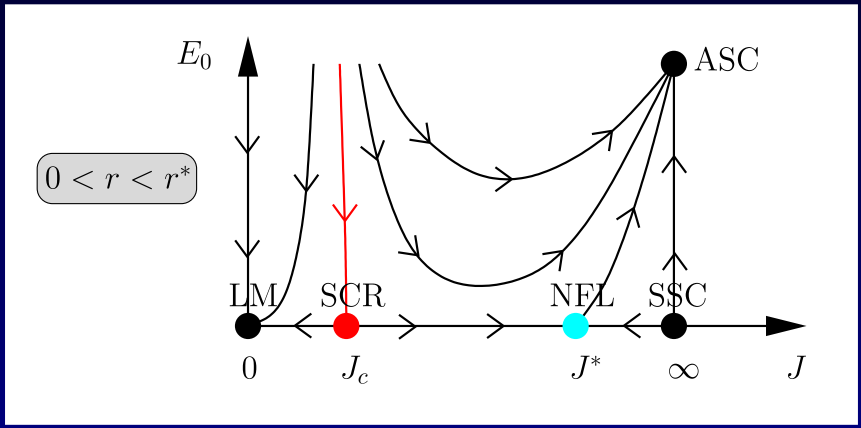
Critical properties:

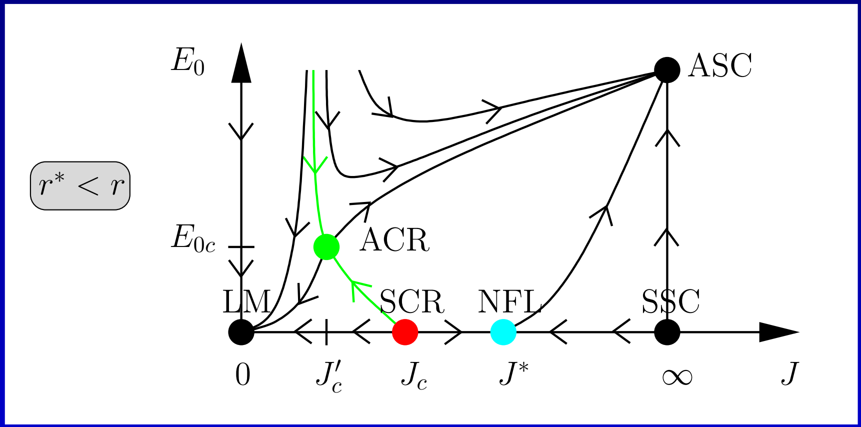




$$S_{\mathrm{imp}}^{\mathrm{NFL}} = \ln 2 + 2r \ln 2 \qquad T\chi_{\mathrm{imp}}^{\mathrm{NFL}} = 1/4 + 3r/8$$

Summary $S = 1$ PG Kondo





Conclusion

- Quantum phase transition in pseudogap Kondo: well under control!
- Computation of universal crossover possible
- Quantitative comparison between NRG and perturbative RG
- Low ω dynamics not fully controlled
  $\Rightarrow$ apply functional RG?
- Transition between critical points not understood