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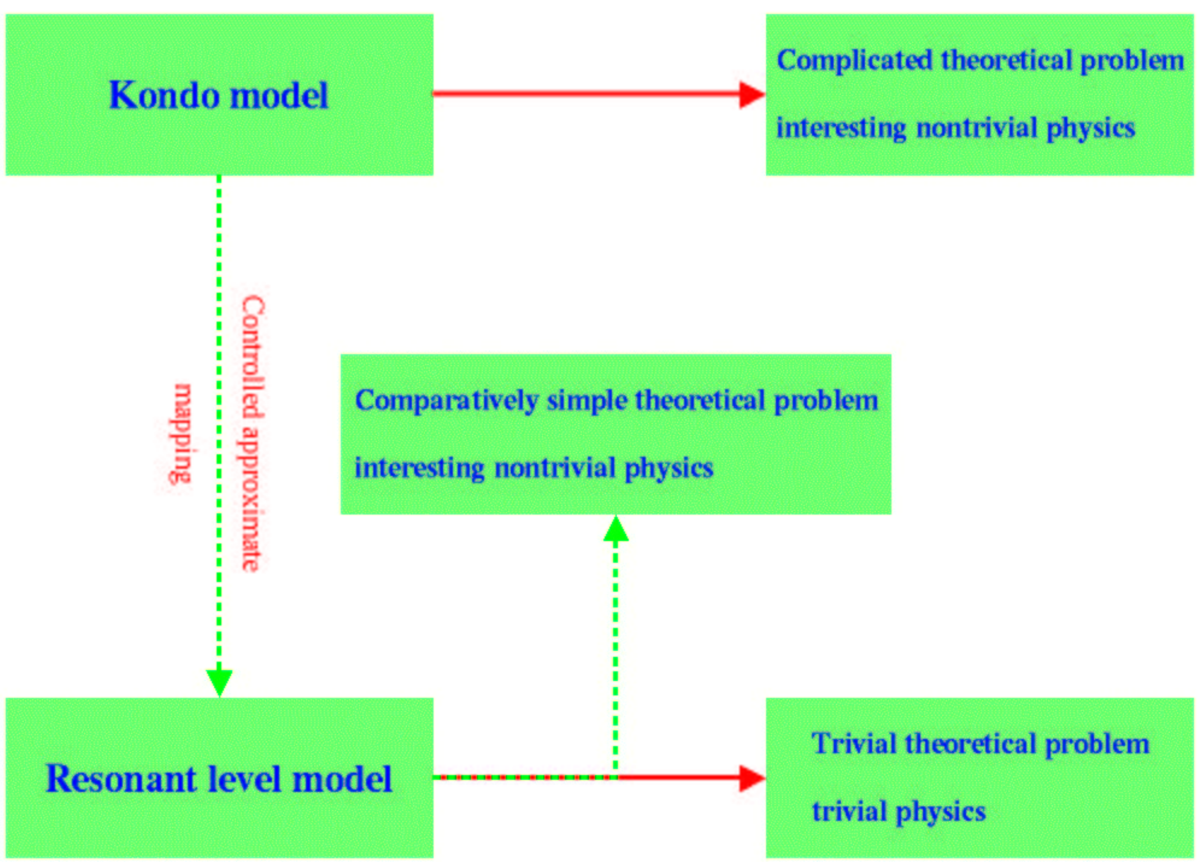
SFB 484

Semi-analytical Solution of the Kondo Model in a Magnetic Field

Thomas Pruschke

Co-workers:
C. Slezak, S. Kehrein, M. Jarrell



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- Yet another 'impurity solver'
- Introduction to flow-equations
- The Toulouse limit
- From Toulouse to Kondo
- Results
- Summary & perspectives

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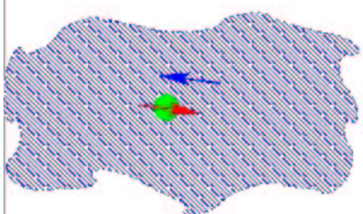
Ancient problem:

- Calculation of physical properties of Kondo Model

J. Kondo, Theor. Phys 32, 27 ('64)

Protagonists:



The localized impurity spin

The free spin in the Fermi see

The exchange coupling

The dynamics:

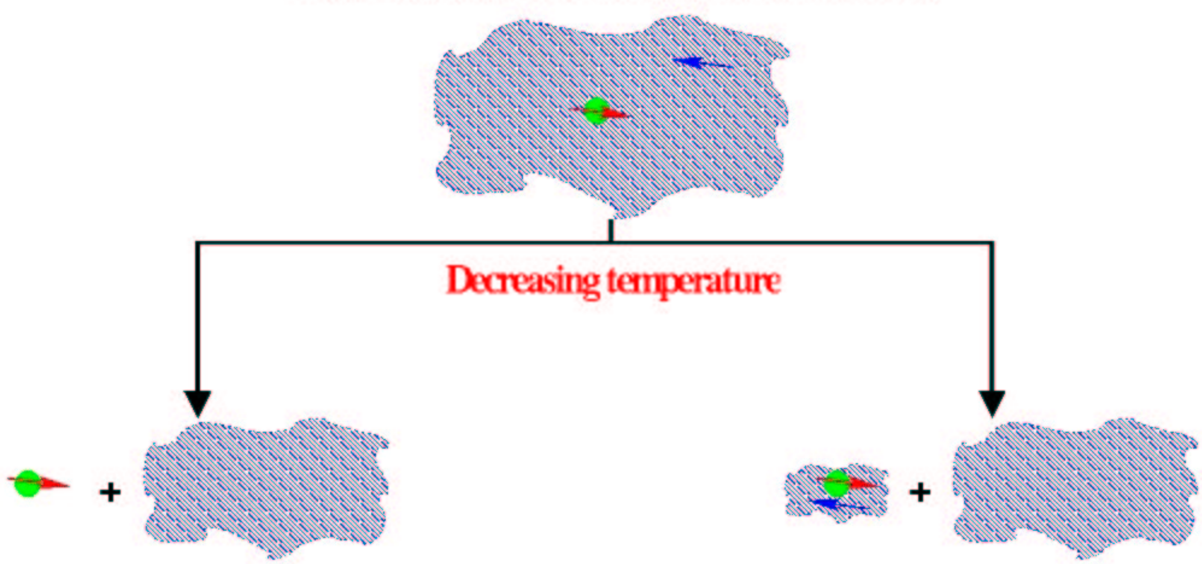
$$H=\sum_{k\sigma}\epsilon_{k\sigma}c_{k\sigma}^{dagger}c_{k\sigma}+J_{parallel}S_z s_z(0)+\frac{J_{bot}}{2}\left(S_+ s_-(0)+h.c.\right)$$

Possible outcome?

Kondo model well studied and physics well understood

see e.g.: A.C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge Univ. Press '93

High temperatures: Free moment in Fermi sea



Free moment + Fermi sea

- Ferromagnetic $J_{\|}<0$
- Pseudo- gap and $J_{\|}<J_c$

Quenched moment + Fermi sea

- $J_{\|}>J_c$: Kondo effect, strong coupling
- Strongly renormalized Fermi sea

Then why bother?

Can we really solve the Kondo model?

Well, not really ...

Bethe ansatz:	Quantum Monte- Carlo:	Wilson's NRG:
Andrei, Furuya, Lowenstein, RMP 55, 331('85)	Hirsch & Fye, PRL 56, 2521('86)	Wilson, RMP 47, 773('75)
✔ Exact, arbitrary J & T	✔ Exact	✔ Arbitrary J
✔ Thermodynamic limit	✔ Thermodynamic limit	✔ Thermodynamics
✔ Thermodynamics	✔ Thermodynamics	✔ Dynamics (low energy)
✗ Dynamics	✗ Low T & small J	✗ Dynamics (medium, high energy)
✗ Realistic band dispersion	✗ Purely numerical	✗ Purely numerical

New methods still interesting & necessary

E.g.: Local Moment Ansatz

Logan, Eastwood, Tusch, JPCM 10, 2673('98)

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Ultimate goal:

Diagonalize Hamiltonian

Many roads to get there:

Exact diagonalization of small systems, variational ansatz, iterative diagonalization (NRG, DMRG), ...

Here:

Successive infinitesimal unitary transformations:

flow-equation procedure

Basic idea:

Glatzek & Wilson, PRD 48, 5863('93)
Wegner, Ann. Phys 3, 77('94)

Look for unitary transformation *U(l)* such that

$$H(l)=U(l)\ H\ U^{dagger}(l)\overset{l\to\infty}{\approx} diagonal$$

Convenient way to construct *U(l)*

$$U(l)=T_l\exp\left(\int_0^l dl'\,\eta(l')\right)$$

$$\frac{dH(l)}{dl}=\left[\eta(l),H(l)\right]$$

How to choose $\eta(l)$?

Wilson, RMP 47, 773('75)

Successively eliminate high energy scales with increasing *l*

Wegner's suggestion:

Wegner, Ann. Phys. 3, 77('94)

$$H=H_0+H_{int}$$

$$\eta(l)=\left[H_0(l),\ H_{int}(l)\right]$$

Guaranteed: $\frac{d}{dl}Tr\,H_{int}^2\leqslant 0$ $\Rightarrow$ transformed Hamiltonian becomes „more diagonal“

Not guaranteed:

- $H_{int}(l\to\infty)=0$
- Calculate correlation functions for physical observables: $O\to O(l),\ \ \partial_l O(l)=\left[\eta(l),\ O(l)\right]$

Successfully applied:

- Sine- Gordon model — Kehrein, PRL 83, 4914('98)
- Kondo model, spin- boson model — Kehrein & Mielke, Phys. Lett. A 219, 313('96); Hofstetter & Kehrein, PRB 63, 140402('01)
- Spin- 1/2 chain (construction of approximations) — Knetter & Uhrig, EPJ B 13, 209('00)

Flow- equations for Kondo model:

Hofstetter & Kehrein, PRB 63, 140402('01)
Slezak, Kehrein, TP, Jarrell, cond- mat/0208539

$$H=\underbrace{\sum_{k\sigma}\epsilon_{k\sigma}c^{dagger}_{k\sigma}c_{k\sigma}}_{H_0}+J_{parallel}S_z s_z(0)+\frac{J_{bot}}{2}\left(S_+s_-(0)+h.c.\right)$$

Elimination of term with $J_{||}$:

Bosonization (Schotte, Z. Phys. 230, 99('70))
+ unitary transformation

$$H=H_0+\int d\epsilon\, g^{(0)}_\epsilon\left(C^{dagger}_\epsilon(\lambda_0)S_-+h.c.\right)+\int d\epsilon\,\omega^{(0)}_\epsilon\left[C^{dagger}_\epsilon(\lambda_0),C_\epsilon(\lambda_0)\right]+\delta J_{parallel}S_z s_z(0)+\dots$$

$$g^{(0)}_\epsilon=\frac{J_{bot}}{4\pi}\sqrt{\rho_c(\epsilon)},\quad \lambda_0=\sqrt{2}-\frac{J_{parallel}\rho_c(0)}{\sqrt{8\pi^2}} \qquad \lambda_0\rightarrow\lambda(l)$$

Perform initial infinitesimal unitary transformation with Wegner's η $\Rightarrow$ final flowing Hamiltonian

$$H(l)\approx H_0+\int d\epsilon\, g_\epsilon(l)\left(C^{dagger}_\epsilon(\lambda(l))S_-+h.c.\right)+\int d\epsilon\,\omega_\epsilon(l)\left[C^{dagger}_\epsilon(\lambda(l)),C_\epsilon(\lambda(l))\right]$$

Resulting „flow equations“ for the parameters:

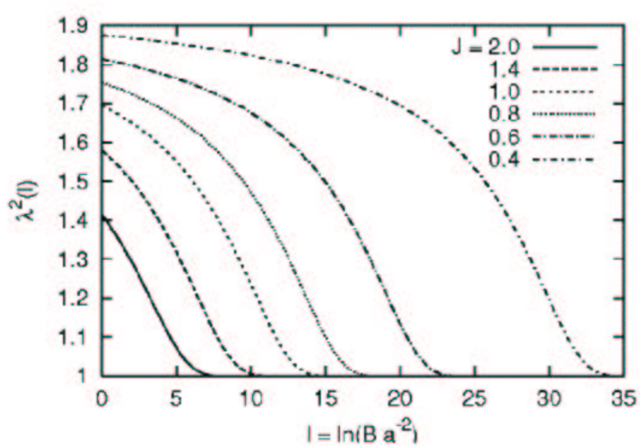
$$\frac{d\,g_\epsilon}{d\,l}=-\epsilon^2 g_\epsilon+\frac{2\pi}{\Gamma(\lambda^2)}P\int d\epsilon'\,\frac{\epsilon+\epsilon'}{\epsilon-\epsilon'}g_\epsilon g_{\epsilon'}^2|\epsilon'|^{\lambda^2-1}+\frac{1}{4}g_\epsilon\ln(l)\frac{d\,\lambda^2}{d\,l}$$

$$\frac{d\,\omega_\epsilon}{d\,l}=\frac{2\pi}{\Gamma(\lambda^2)}\epsilon\, g_\epsilon^2|\epsilon|^{\lambda^2-1}$$

$$\frac{d\,\lambda^2}{d\,l}=\frac{8\pi\lambda^2(1-\lambda^2)}{\Gamma(\lambda^2)}\int d\epsilon\, g_\epsilon g_{-\epsilon}|\epsilon|^{\lambda^2-1}$$

Solve the set of DGL:
Hofstetter & Kehrein, PRB 63, 140402('01)

- No spurious divergencies
- Quick flow of λ^2 towards 1



Meaning of λ=1?

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Specialty of $\lambda=1$:

$$\lambda=1 \Leftrightarrow \rho_c(0) J_{parallel} = 2\pi\left(2-\sqrt{2}\right)$$

$C_\epsilon(1)$ has fermionic anticommutation rules

$$\left\{C_\epsilon^{dagger}(1), C_{\epsilon'}(1)\right\} = \delta(\epsilon-\epsilon')$$

Well-known property of the asymmetric Kondo Hamiltonian: Toulouse & Seances, Acad. Sci. B 268, 1200('69)

$$\rho_c(0) J_{parallel} = 2\pi\left(2-\sqrt{2}\right)$$

Asymmetric Kondo model equivalent to Resonant Level model

$$H_{RLM} = \sum_k E_k c_k^{dagger} c_k + \epsilon_d d^{dagger} d + \sum_k V_k \left(c_k^{dagger} d + h.c.\right)$$

How does this equivalence show up in flow- equations?

Toulouse point of Kondo model

$$\frac{d\,g_\epsilon}{d\,l} = -\epsilon^2 g_\epsilon + 2\pi P \int d\epsilon' \frac{\epsilon+\epsilon'}{\epsilon-\epsilon'} g_\epsilon g_{\epsilon'}^2$$

$$\frac{d\,\omega_\epsilon}{d\,l} = 2\pi\epsilon g_\epsilon^2$$

Resonant level model (ϵ_d=0)

Kehrein & Mielke, Ann. Phys. 252, 1('96)

$$\frac{d\,V_\epsilon}{d\,l} = -\epsilon^2 V_\epsilon + P \int d\epsilon' \frac{\epsilon+\epsilon'}{\epsilon-\epsilon'} V_\epsilon V_{\epsilon'}^2$$

$$\frac{d\,E_\epsilon}{d\,l} = 2\epsilon V_\epsilon^2$$

Translation table

Toulouse	RLM
S_+	$d^\dagger$
S_z	$d^\dagger d$
$C_\epsilon(1)$	c_ϵ
$2\pi g_\epsilon^2$	V_ϵ^2
ω_ϵ	$E_\epsilon/2$

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Flow equations once again:

$$\frac{d\,g_\epsilon}{d\,l}=-\epsilon^2 g_\epsilon+\frac{2\pi}{\Gamma(\lambda^2)}P\int d\epsilon'\,\frac{\epsilon+\epsilon'}{\epsilon-\epsilon'}g_\epsilon g_{\epsilon'}^2|\epsilon'|^{\lambda^2-1}+\cancel{\frac{1}{4}g_\epsilon\ln(l)\frac{d\,\lambda^2}{d\,l}}$$

$$\frac{d\,\omega_\epsilon}{d\,l}=\frac{2\pi}{\Gamma(\lambda^2)}\epsilon\, g_\epsilon^2|\epsilon|^{\lambda^2-1}$$

$$\frac{d\,\lambda^2}{d\,l}=\frac{8\pi\lambda^2(1-\lambda^2)}{\Gamma(\lambda^2)}\int d\epsilon\, g_\epsilon g_{-\epsilon}|\epsilon|^{\lambda^2-1}$$

Identify:

$$\left.\begin{aligned}V_\epsilon^2&=\frac{2\pi}{\Gamma(\lambda^2)}g_\epsilon^2|\epsilon|^{\lambda^2-1}\\ E_\epsilon&=2\omega_\epsilon\end{aligned}\right\}\Rightarrow H_{Kondo}\rightarrow H_{RLM}(\lambda)$$

Translation table

Kondo	RLM
S_+	d^{dagger}
S_z	$d^{dagger}d$
$C_\epsilon(\lambda)$	$c_\epsilon+O(\lambda^2-1)$
$2\pi g_\epsilon^2$	V_ϵ^2
ω_ϵ	$E_\epsilon/2$

Further simplification:

Only

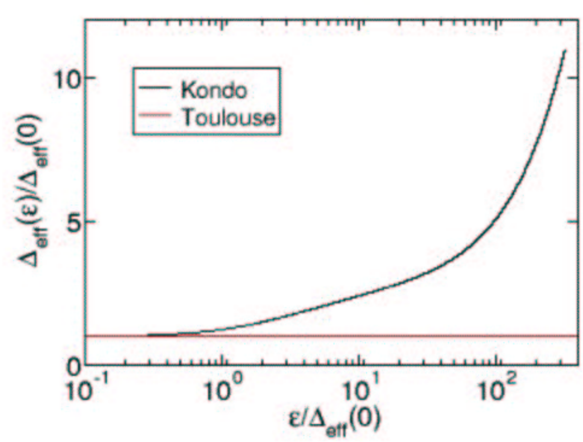
$$\Delta_{eff}(\omega)=\int d\epsilon\, V_\epsilon^2\,\delta(E_\epsilon-\omega)$$

needs to be considered

Actual procedure:

- Solve flow- equations for Kondo model
- Calculate simple correlation function, e.g. $<S_+(t)S_-(0)>$
- Match corresponding RLM correlation function, e.g. $<d^\dagger(t)d(0)>$, by adjusting $\Delta_{eff}(\omega)$
- Procceed with more complicated correlation functions via RLM

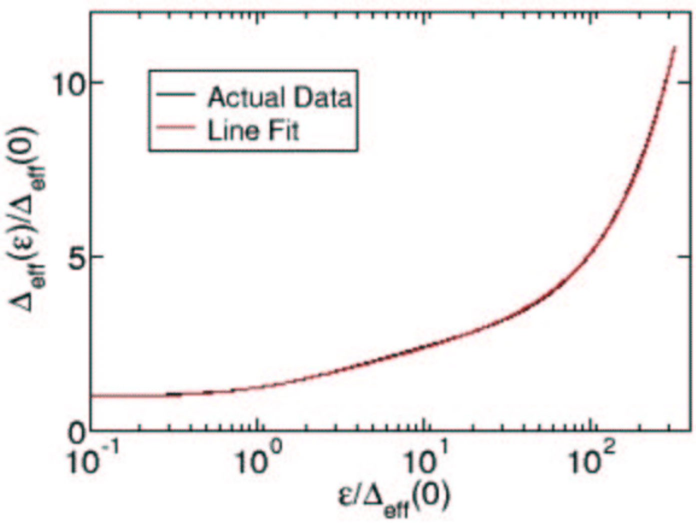
Result for $\Delta_{eff}(\omega)$:



Remarks:

- $\Delta_{eff}(\omega)$ thus constructed approximately accounts for $\lambda>1$ in intermediate energy range
- $\Delta_{eff}(\omega/\Delta_{eff}(0))/\Delta_{eff}(0)$ universal in weak-coupling $\rho_c(0)J_{\parallel} \to 0$
- Excellent fit:

$$\frac{\Delta_{eff}(x)}{\Delta_{eff}(0)} = 1+\frac{1}{4}\ln\left(1+\left(\frac{\pi^2 x}{8}\right)^2\right)+\frac{1}{10\pi^3}\left(\arctan\left|\frac{\pi^2 x}{8}\right|-\left|\frac{\pi^2 x}{8}\right|\right)\left(1-\ln\left|\frac{\pi^2 x}{8}\right|\right)$$



- $\Delta_{eff}(0) \propto T_K \propto e^{-1/\rho J}$
- $\omega \leq T_K$ governed by „rescaled fermions“
- $T_K < \omega < 10^2\, T_K$ logarithmic regime
- Local magnetic field h:
  - RLM : $g\, \mu_B h \to g\epsilon_d$
  - $\Delta_{eff}(0) \to \Delta_{eff}(0,h)$

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Slezak, Kehrein, TP & Jarrell, cond- mat/0208539

Simplest observable to evaluate:

$$U_{imp}(h)=\langle H-H_0\rangle \Rightarrow \gamma_{imp}(h)=\left.\frac{\partial U(T,h)}{\partial T}\right|_{T\to 0}=\frac{\pi^2 k_B^2}{3}\rho_d(0,h)\left(1-\left.\frac{\partial \Lambda'(\omega,h)}{\partial \omega}\right|_{\omega=0}\right)$$

$$\Lambda(\omega,h)=\frac{1}{\pi}P\int d\epsilon\,\frac{\Delta_{eff}(\epsilon,h)}{\omega-\epsilon}$$

$$\rho_d(\omega,h)=\frac{1}{\pi}\frac{\Delta_{eff}(\omega,h)}{(\omega-gh-\Lambda(\omega,h))^2+\Delta_{eff}(\omega,h)^2}$$

Notable :

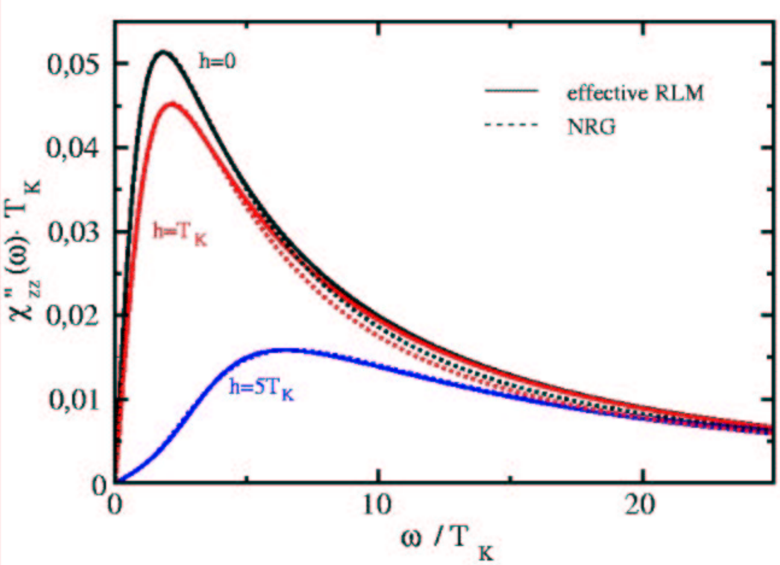
- Low T specific heat governed by spin- fluctuations: $S_+ \leftrightarrow d^\dagger$
- $\gamma_{imp}(0) \propto 1/T_K$ and $\gamma_{imp}(h) = \gamma_{imp}(h/T_K)$
- Correction factor crucial to obtain correct Wilson ratio
- h- dependence in Δ_{eff} important only for $h \gg T_K$

How about dynamics?

Simplest dynamical observable to evaluate:

$$\chi_{parallel}(z)=-\langle\langle S_z;S_z\rangle\rangle_z=-\langle\langle d^{dagger}d;d^{dagger}d\rangle\rangle_z$$

$$\chi''_{parallel}(\omega)=\pi\int_{-\omega}^{0}d\epsilon\,\rho_d(\epsilon)\rho_d(\omega+\epsilon)$$



- Small energies:
  $\chi''(\omega) \propto \omega/T_K$
- Large energies:
  $\chi''(\omega) \propto 1/\omega$ + logarithmic corrections
- Finite fields:
  - Shift of maximum due to ϵ_d
  - Additional shift + broadening due to Δ_{eff}

Analytical result:

$$S(\omega)=\frac{\chi''_{parallel}(\omega)}{\omega}$$

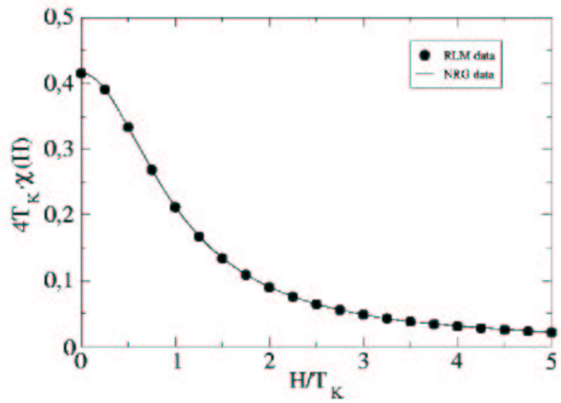
$$S(0)=\lim_{\omega\to 0} S(\omega)=\frac{1}{\pi}\frac{\Delta^2_{eff}(0,h)}{\left((gh)^2+\Delta_{eff}(0,h)^2\right)^2}$$

- Explicit demonstration of universality: $T_K^2\, S(0)=f(h/T_K)$
- Analytical formula for fitting e.g. $1/(T_1T)$ to extract T_K
- Independent of details of band structure

Missing piece of information: Value of T_K

Wilson's definition: $\chi_0(h=0)=\frac{w}{4T_K}\,,\quad w\approx 0.413$

From: $\chi_0=\frac{2}{\pi}\int_0^\infty d\omega \frac{\chi''_{parallel}(\omega)}{\omega}$

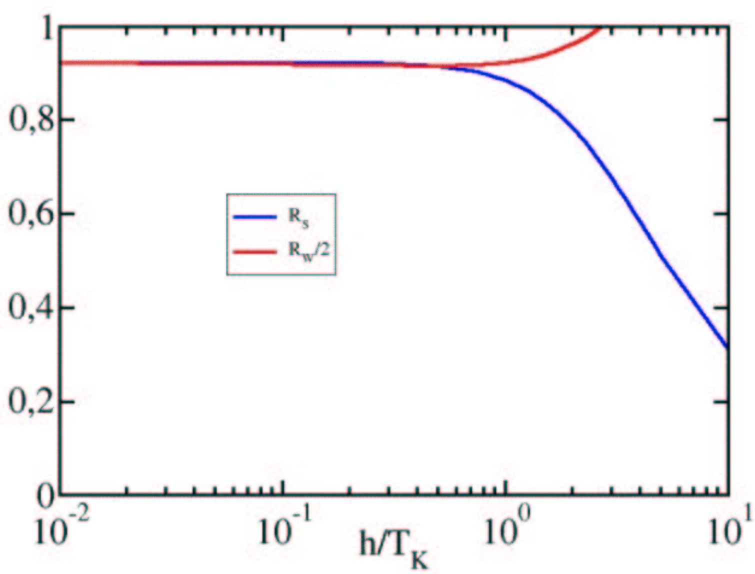


Wilson & Shiba relations:

$$R_W=\frac{4\pi^2k_B^2}{3(g\mu_B)^2}\frac{\chi_{imp}}{\gamma_{imp}}=2 \qquad R_S=\frac{(g\mu_B)^2}{2\pi\chi_0^2}=1$$

Note: $\chi_{imp}\neq\chi_0\,,\quad \chi_{imp}\approx\left[1-\rho_c(0)J\right]\chi_0$

Chen, Jayaprakash & Krishnamurthy, PRB 45, 5368('92)



- Toulouse limit:
  $R_w=4$, $R_S=1/2$
  $\Rightarrow$ energy dependence of Δ_{eff} crucial
- Absolute error 5% - 10%
- Strong field dependence
  Bethe ansatz: $R_w(h)=2$
- Not yet: Field dependence of Δ_{eff}

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- Analysis of flow-equation solution for Kondo model
  - Generated flow similar to that of a resonant level model
  - Low-energy fixed point Toulouse limit ≡ resonant level model
- Approximation: (controlled by small parameter)
  - Describe Kondo model by resonant level model with nontrivial hybridization function
  - Calculate static & dynamical correlation functions within this effective RLM
- Findings:
  - Good to excellent agreement of static and dynamical spin-susceptibility with e.g. NRG
  - Reasonable agreement of Wilson & Shiba relations with exact values
- Perspectives:
  - Calculate T-matrix: Evolution of fermionic operators under flow-equations?
  - Non-trivial band DOS: Low-energy fixed point of flow-equations?
  - Application to more complex „impurities“: A manageable effective low-energy model?