Kondo model with magnetic anisotropy terms for magnetic impurities on surfaces

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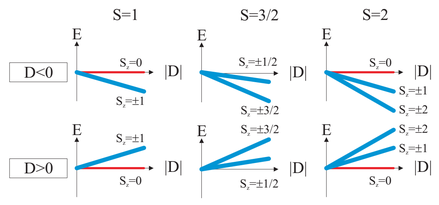
Motivation

Magnetic impurities (Fe, Mn, Co) on normal metal surfaces (Cu) with a decoupling layer (CuN) behave as high-spin Kondo impurities with strong magnetic anisotropy [1].
Spin-excitation spectroscopy [2] using a scanning tunneling microscope (STM) shows direction-dependent shifts of magnetic excitations and direction-dependent splitting of the Kondo resonance in magnetic fields [1].



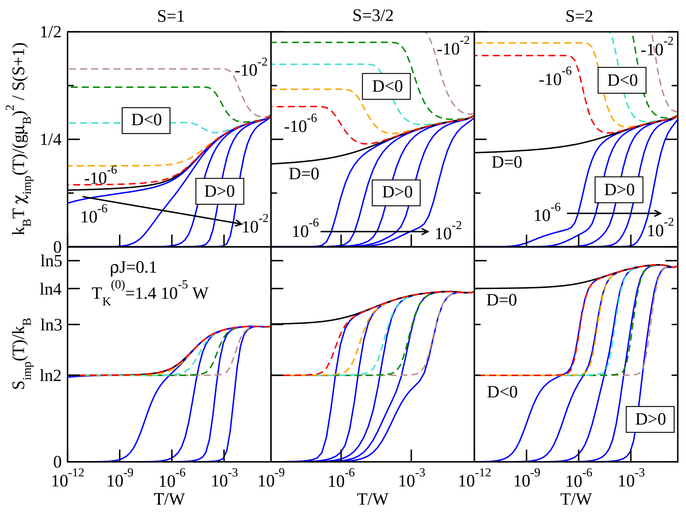
Model and Method

We study the anisotropic Kondo model [3, 4, 5]

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J\mathbf{s}\cdot\mathbf{S} + DS_z^2 + E(S_x^2 - S_y^2)$$

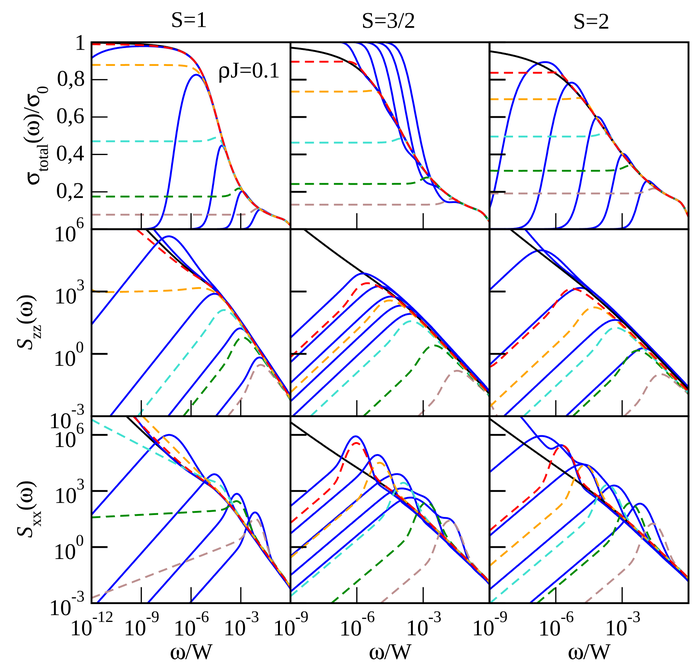
using the numerical renormalization group technique [6, 7].

Axial anisotropy only ($D \neq 0$, $E = 0$)

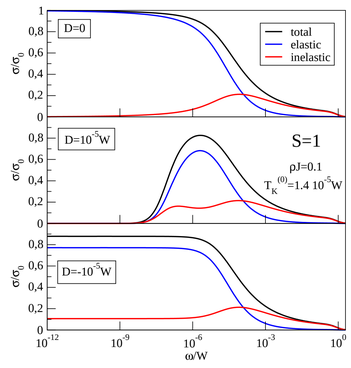


- Hard-axis ($D > 0$): spin always fully compensated
- Easy-axis ($D < 0$): residual spin (double degeneracy)

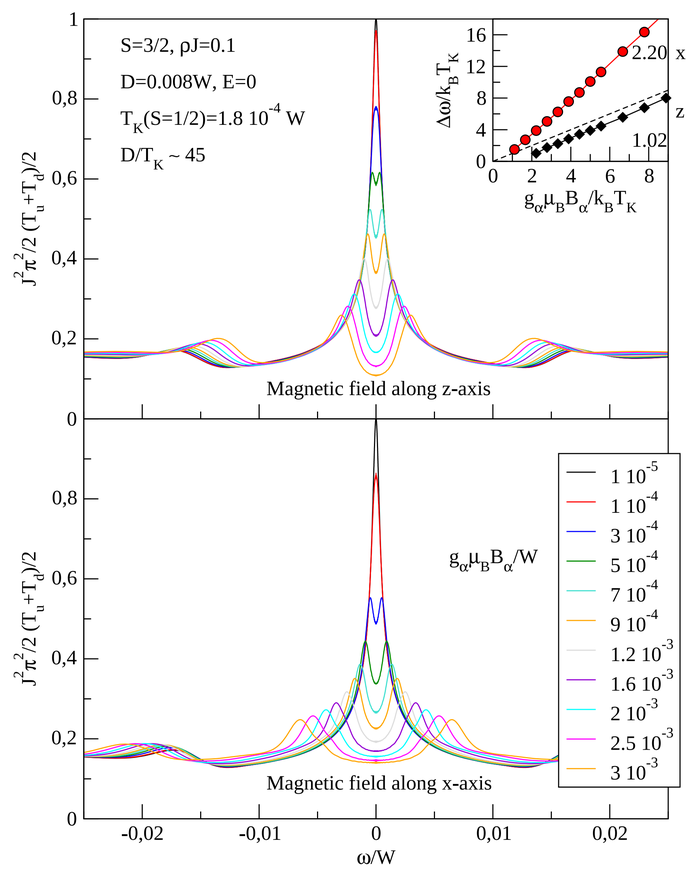
Dynamic properties ($D \neq 0$, $E = 0$)



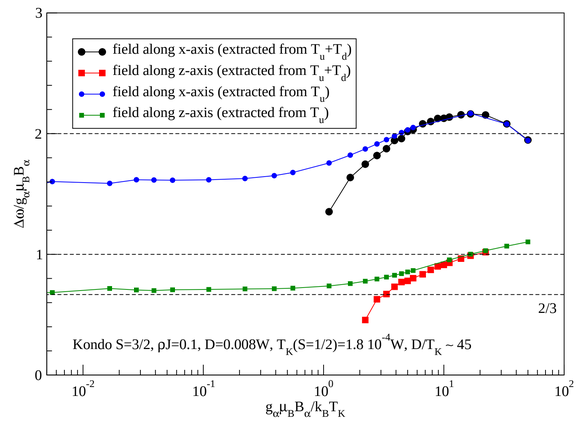
- Hard-axis ($D > 0$): regular Fermi-liquid behavior
- Easy-axis ($D < 0$): non-Fermi-liquid behavior [8]



Kondo resonance splitting (S=3/2)



- Coupling of the effective $S = 1/2$ impurity spin to the magnetic field is strongly anisotropic.



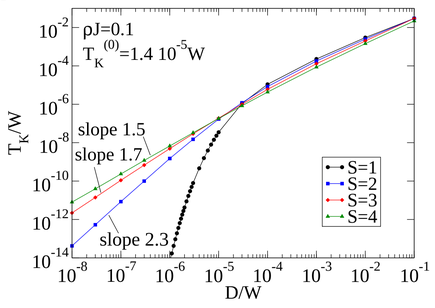
- At low fields, Fermi-liquid ratio 2/3 (after rescaling) is recovered.
- At high fields, $S_z = \pm 3/2$ states affect the splitting.

S=1 model: two-stage Kondo screening

For $D < T_K^{(0)}$, S=1 Kondo screening at $T = T_K^{(0)}$, followed by S=1/2 Kondo screening at an exponentially reduced Kondo tempearture $T_K^{(2)}$.

Integer-spin models, $S \geq 2$

For $D < T_K^{(0)}$, effective $S = 1/2$ moment formed at $T \sim D$, screened at some lower $T_K = D^\alpha$, with a spin-dependent constant α.



Half-integer-spin models

S=3/2 model → S=1/2 XXZ anisotropic model

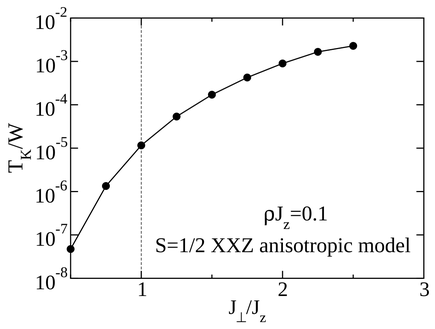
$$S_x = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \frac{\sqrt{3}}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$

Projection on the $S_z = \pm 1/2$ subspace:

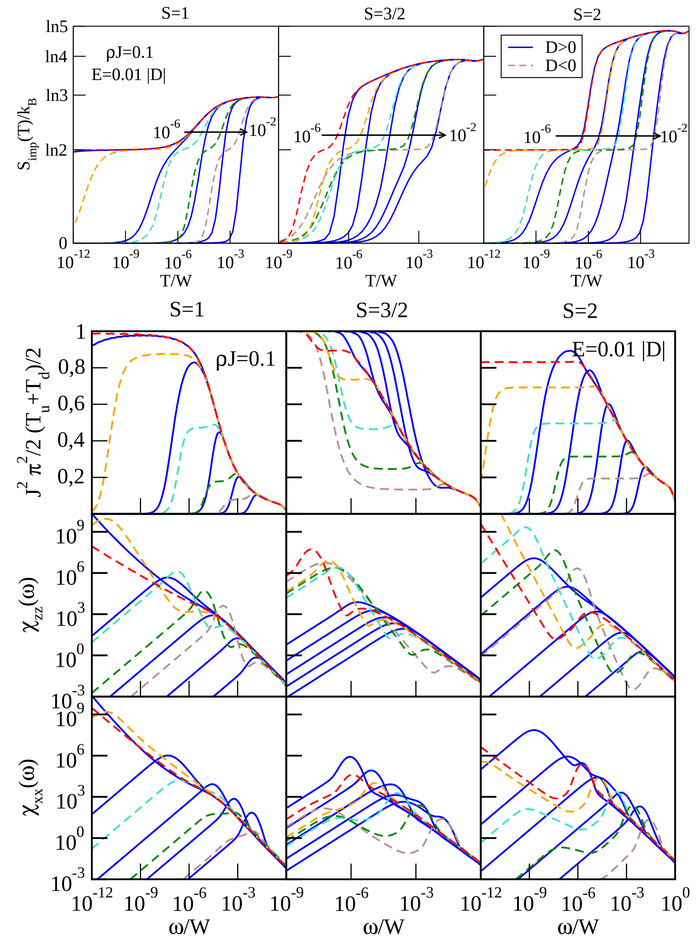
$$J_\perp \approx 2J, \quad J_z \approx J.$$

In general: $J_\perp = (S + 1/2)J$.
Enhancement of the Kondo temperature ($\alpha < 1$):

$$T_K \approx W \exp\left(-\frac{\alpha}{\rho J_z}\right), \quad \alpha = \frac{\arctan\gamma}{\gamma}, \quad \gamma = \sqrt{\left(\frac{J_\perp}{J_z}\right)^2 - 1}$$



Axial and transverse anisotropy ($E \neq 0$)



- Regular Fermi-liquid behavior restored
- For $D < 0$ and $E \ll |D|$, a temperature range where NFL behavior is perhaps observable

Acknowledgments

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