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Tutorial : Dynamical spin susceptibility : From Kondo relaxation to quantum criticality

S. Raymond
CEA-Grenoble, raymond@ill.fr

I. MAGNETIC INELASTIC NEUTRON SCATTERING

We propose to study several aspects of the dynamical spin susceptibility $\chi"(\mathbf{Q},\omega)$ of $4f$ electron systems. This quantity is directly measured in an inelastic neutron scattering experiment. The neutron cross section is proportional to the scattering function $S(\mathbf{Q},\omega)$, which is proportional to the Fourier transform in space and time of the spin-spin correlation function :

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S^{\alpha,\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\sum_{i,j}\int_{-\infty}^{+\infty} exp\{i\mathbf{Q}.(\mathbf{R}_i\text{-}\mathbf{R}_j)\} < S_i^{\alpha}(0)S_j^{\beta}(t) > exp\{-i\omega t\}dt \tag{1}$$

$S(\mathbf{Q},\omega)$ is related to $\chi"(\mathbf{Q},\omega)$ via the fluctuation-dissipation theorem.

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\mathbf{Q},\omega) = \frac{1}{1-exp(-\hbar\omega/k_BT)}\chi"(\mathbf{Q},\omega) \tag{2}$$

We are interested in a heavy fermion system for which magnetic order ordering occurs at T=0 K as a function of pressure or chemical substitution. This tutorial gives some flavor of the Spin Fluctuation theory of Moriya and its application to heavy fermion systems (Moriya and Takimoto, J. Phys. Socc. Japan 64 (1995) 960).

II. KONDO RELAXATION

We consider a single $4f$ moment that is quenched by the conduction electrons, hence the (auto)-correlation function is written in the relaxation time approximation :

$$< S(t)S(0) >= S^2(0)e^{-(\Gamma_L/\hbar)t} \tag{3}$$

Γ_L is proportional to the Kondo temperature ($\Gamma_L \approx k_BT_K$). In the following, we will use the notation : $S^2(0) = T\chi_L$
By using the Kubo formula in the classical limit :

$$\chi(\omega) = -\frac{1}{T}\int_0^{\infty} dte^{i\omega t} < S'(t)S(0) > \tag{4}$$

Calculate the dynamical susceptibility $\chi_L(\omega)$ and $\chi"_L(\omega)$ for such a case. Draw a sketch of $\chi"(\omega)$ using the asymptotic limits $\omega \to 0$ and $\omega \to \infty$. At which ω, $\chi"(\omega)$ is maximum ? Is it an eigen-energy of the system ? What is the width at half maximum of $\chi''(\omega)$. Draw a sketch of $S(\omega)$ for $T \ll \hbar\omega$ and $T \gg \hbar\omega$. Give some physical interpretation in term of neutron energy loss and neutron energy gain. Justify why we do not consider any $\mathbf{Q}$ dependence here.

III. MAGNETIC INTERACTIONS

For a rigorous treatment see e.g. J. Jensen and A.R. Macintosh, Rare Earth Magnetism, Clarendon Press, 1991. We will now take into account the RRKY exchange interactions that arise between local $4f$ electrons. We consider an exchange Hamiltonian :

$$\hat{H}_{ex} = -\sum_{i,j} J_{i,j}S_iS_j \tag{5}$$

For simplicity S_i is the component of the spin along the z quantification axis defined by the direction of an applied field. We define the Fourier component $S_Q = \sum_j S_j exp(iQ.R_j)$.
Rewrite $\hat{H}_{ex}$ in Q space with $J(Q) = \sum_{i,j} J_{i,j} exp(iQ(R_j - R_i))$.
In the so-called Random Phase Approximation (RPA), S_{-Q} is replaced by its mean value $< S_{-Q} >$ in $\hat{H}_{ex}$ (while S_Q is kept as it is). Write the corresponding internal effective field $H^{eff}(-Q)$ acting on S_Q.
We define $M(Q) = - < S_Q >$. In the following, we consider only the component at the frequency ω of $M(Q)$ that we note $M(Q,\omega)$. In a mean-field approach like the RPA, it is also assumed that $M(Q,\omega) = \chi_0(Q,\omega)H^{eff}(Q,\omega)$ where $\chi_0(Q,\omega)$ is the non interacting susceptibility and $H^{eff}(Q,\omega)$ is an effective field that includes the external field, $H(Q,\omega)$, and the internal field calculated with the assumption made above.
Show that the total (or interacting susceptibility), defined as usually by $M(Q,\omega) = \chi(Q,\omega)H(Q,\omega)$, writes as

$$\chi(Q,\omega) = \frac{\chi_0(Q,\omega)}{1 - J(Q)\chi_0(Q,\omega)} \tag{6}$$

Using the noninteracting susceptibility of the Kondo problem, write the corresponding imaginary part of the total interacting susceptibility as :

$$\chi"(Q,\omega) = \frac{\chi_Q \Gamma_Q \hbar\omega}{(\hbar\omega)^2 + \Gamma_Q^2} \tag{7}$$

Give the relation between χ_Q and respectively Γ_Q and χ_L, Γ_L. Give the condition for magnetic ordering at $Q = k$ for which χ_k diverges. What happens to Γ_k ? Give an interpretation. Comment the value of $\chi_Q\Gamma_Q$. We now approximate $J(Q = k + q) = J(k) - Aq^2$ around the wave-vector of instability k. We will note $J^c(k)$ the critical value for magnetic order.
Express Γ_Q and $\chi_Q$as a function of q and define a correlation length ξ for antiferromagnetic fluctuations by the relation $\chi_Q = \frac{\chi_k}{(1+(\xi q)^2)}$ How is ξ on approaching the magnetic instability (write ξ as a function of $J(k) - J^c(k)$) ? Make a sketch of χ_Q as a function of Q for several $J(k)$.

IV. SPECIFIC HEAT

At low temperature, the contribution to the specific heat arising from the spin fluctuations given by (7) is :

$$\frac{C}{T} = \pi \sum_Q \frac{1}{\Gamma_Q} \tag{8}$$

Express Γ_Q as a function of q, ξ, χ_L Γ_L and χ_k. Calculate $\frac{C}{T}$ by replacing $\sum_q$ by an integral $\int_0^{q_B} \frac{4\pi q^2 dq}{(4\pi/3)q_B^3}$. You must find $C/T \propto \frac{1}{\chi_L \Gamma_L A q_B^2}\left[1 - \frac{\pi}{2\xi q_B}\right]$

V. EXPERIMENTAL RESULTS

Figure 1 shows a map of the spin fluctuations in the Brillouin zone of $CeRu_2Si_2$. Magnetic interactions lead to enhance the Kondo-like spin fluctuations (blue) around the vectors k_1, k_2 and k_3 (red/orange). When doping with La, magnetic orders occurs for $x > 0.075$ at the vector k_1.
Figure 3 shows the energy response in the blue region for x=0 and x=0.075. Give Γ_L and T_K for each compound (1 meV $\approx$ 11.6 K). Figure 4 shows the energy response at k_1 for x=0 and x=0.075. Give Γ_k for x=0. What about Γ_k for x=0.075
Figure 5 gives $J(k + q)$ for each compound. From these parameters, give the ratio of the Sommerfeld coefficients between x=0.075 and x=0 and compare with measurements (Figure 6).

For further information see
S. Kambe et al., J. Phys. Soc. Japan 65 (1996) 3294
H. Kadowaki et al., Phys. Rv. Lett. 92 (2004) 097204
W. Knafo et al., Nature Physics 5 (2009) 753

Fig.1

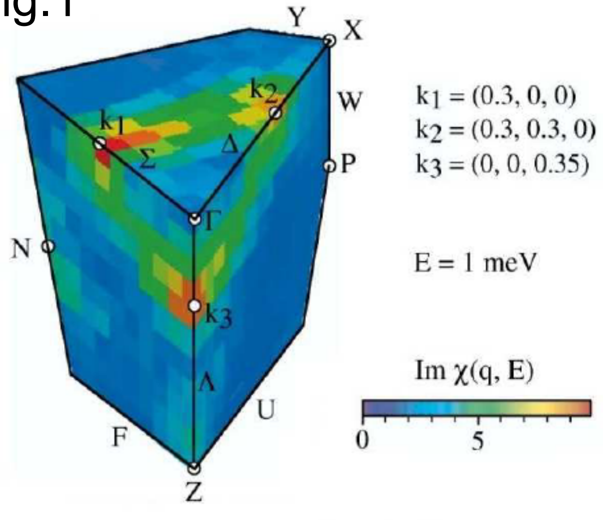

Fig.3

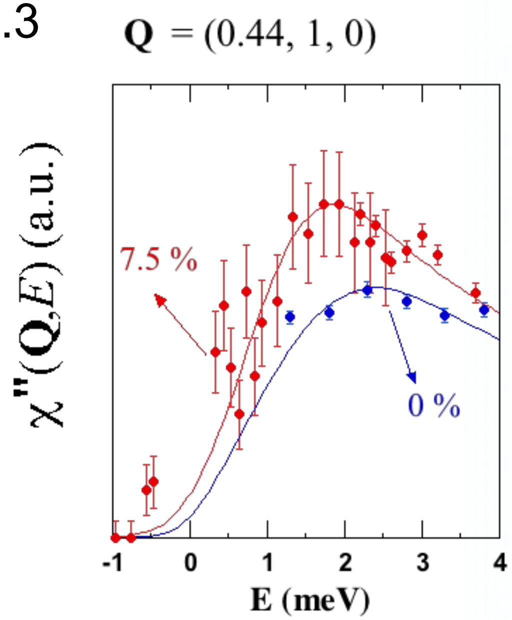

Fig.4

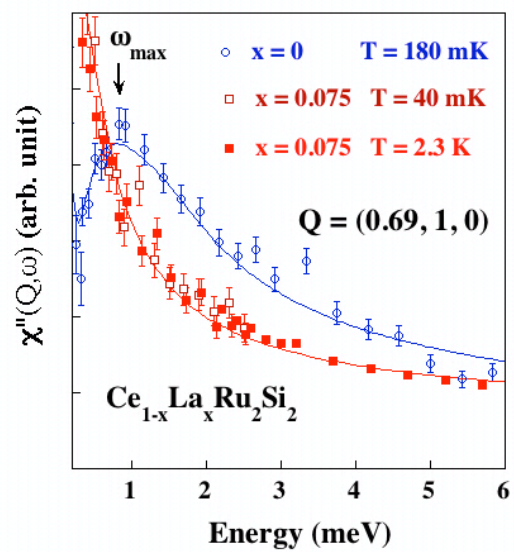

Fig.5

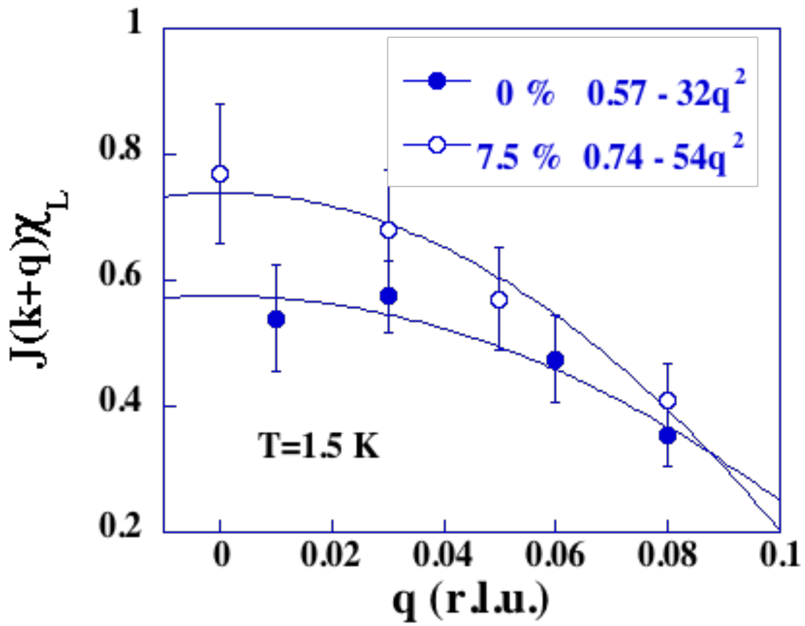

Fig.6