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DYNAMICS OF IMPURITY SPIN ABOVE THE KONDO TEMPERATURE

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Recently the dynamics of impurity spin contained by nonmagnetic host metal has attracted great interest [1-4]. Doniach and Spencer [1] called the attention to the fact that a Kondo anomaly might be observed in the g-shift of impurity spin, $S = 1/2$. They calculated the g-shift up to the second order of the exchange coupling in the limit of small external magnetic field. Wang and Scalapino [4] obtained logarithmic terms in the line-width carrying out the calculation up to the third order in the high field limit.

A study of dynamics of the localized momentum is reported here making use of the Abrikosov's diagram technics [5] to calculate the highest power of logarithmic terms in any order of the perturbation theory. These calculations are correct only well above the Kondo temperature.

1/. The transverse dynamic retarded susceptibility can be written as

$$\chi^{-+R}(t-t') = i\theta(t-t') \lim_{\lambda\to\infty} \frac{\left\langle \left[a_\alpha^+ \, S_{\alpha\beta}^-(t) \, a_\beta, \; a_{\alpha'}^+ \, S_{\alpha'\beta'}^+(t') \, a_{\beta'} \right]_- \right\rangle}{\langle a_\alpha^+ \, a_\alpha \rangle} \qquad /1/$$

where operators a_α^+ , a_β stand for the peseudo-fermion representation of spin, λ is the fictitious pseudofermion energy, $S_{\alpha\beta}^+$ and $S_{\alpha'\beta'}^-$ are the impurity spin matrixes, and a summation over double indices is implied. The static magnetization of the impurity spin is

$$\langle S^z \rangle = \lim_{\lambda\to\infty} \frac{\langle a_\alpha^+ \, S_{\alpha\beta}^z \, a_\beta \rangle}{\langle a_\alpha^+ \, a_\beta \rangle} \qquad /2/$$

where z is the direction of the magnetic field. In both expressions the numerator and denominator are calculated separately making use of the linked cluster expansion.

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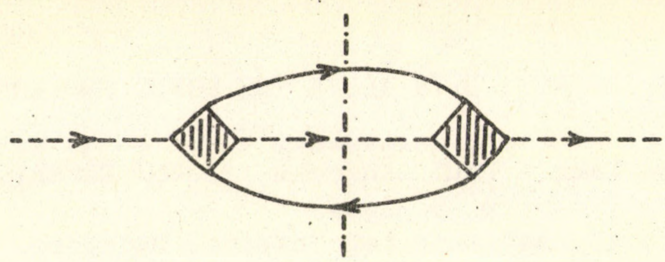
2/ The real and imaginary part of the pseudofermion Green function is determined calculating the contribution of the following diagram



where the solid and dotted lines represent the electron and pseudofermion propagators, the squares the renormlaized vertexes [5], and the cut refers to the smallest values of the energy variables /for $\mathrm{Re}\ \Sigma(\omega)$ / and to the imaginary part of the contributions of the cut lines /for $\mathrm{Im}\ \Sigma(\omega)$ /, respectively. In the logarithmic appoximation the following results are obtained:

$$\mathrm{Re}\ \Sigma_{\alpha\alpha'}(\omega) = -S(S+1)\,\gamma\left(\omega\delta_{\alpha\alpha'} - S^z_{\alpha\alpha'}\,\omega_o\right) - \gamma\omega_o\,S^z_{\alpha\alpha'} \qquad /3/$$

where ω_o is the unrenormalized resonance frequency and

$$\gamma = \frac{1}{2}\,\frac{\left(2\,\frac{J}{N}\,\rho_o\right)^2 \log\frac{D}{kT}}{1 + \frac{2J\rho_o}{N}\log\frac{D}{kT}} \qquad /4/$$

Here $\frac{J}{N}$ is the coupling in the Kondo Hamiltonian, D the cutoff energy and ρ_o the density of states. Furthermore,

$$\mathrm{Im}\ \Sigma_{\alpha\alpha'}(\omega) = -\,\mathrm{sg}(\mathrm{Im}\ \omega)\,\frac{1}{2}\,\pi\,S(S+1)\,\frac{\left(2\,\frac{J}{N}\,\rho_o\right)^2 kT}{\left(1 + 2\,\frac{J}{N}\,\rho_o\log\frac{D}{kT}\right)^2}\,\delta_{\alpha\alpha'} \qquad /5/$$

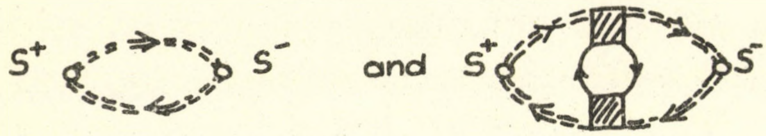
which is valid for $\omega < kT$, but in the case of $\omega > kT$ the temperature has to be replaced by $\omega\ (\omega > 0)$.

The spectral function of pseudofermion propagator consists of two parts, a Lorentzian one ρ_{Lor} for $\omega < kT$ and a long tail part ρ_{tail} for $(\omega > kT)$ whose integrals are

$$\int \rho_{Lor}(\omega)\,d\omega = z \qquad \text{and} \qquad \int \rho_{tail}(\omega)\,d\omega = \int \frac{\mathrm{Im}\ \Sigma(\omega)}{\pi\,\omega^2}\,d\omega = 1 - z \qquad /6/$$

where the renormalization constant is $z = \left(1 + S(S+1)\,\gamma\right)^{-1}$ and the sum rule $\int \rho(\omega)d\omega = 1$ is satisfied. The magnetization can be calculated on the basis of /2/ and the classical expression is obtained, but with a renormalized g factor $g_{eff} = g_o(1 - \gamma)$ where γ is given by /4/. This result is in agreement with the previous calculations which gave the first few terms of the power series [6]. The imaginary part of the pseudofermion /5/ and electron [5] self-energy has a ratio which can be derived by the classical argument of counting the number of collision.

3/ There are two diagrams which contribute to the dynamic susceptibility within logarithmic accuracy,



where the double dotted lines represent the renormalized pseudofermion propagator. The static susceptibility can be calculated from the dynamic one. The first diagram corresponds to the result obtained in Sec. 2, while the contribution of the second one vanishes exactly.

The symmetrical part of the final result is the following $\omega < kT$

$$\mathrm{Im}\,\chi^{-+R}_{(\omega)} = -2 \langle S^z \rangle \left\{ \frac{\frac{1}{T_2}}{(\omega-\omega_R)^2 + (\Delta\omega)^2} + \frac{[S(S+1)-1]\frac{(\Delta\omega)^2}{T_2}}{[(\omega-\omega_R)^2 + (\Delta\omega)^2]^2} \right\} \qquad /6/$$

where $\omega_R = \omega_o \frac{g_{eff}}{g_o}$, $\Delta\omega = 2\mathrm{Im}\Sigma(o)$ and $T_2^{-1} = \Delta\omega\,(S\,(S+1))^{-1}$ the transversal relaxation time of Korringa. It is worth mentioning that in /6/ at $\omega = o$ the total line-width occurs in the denominator.

4/ In a theory in which the spin dynamics is considered also, the exchange coupling constant would have to be replaced by a renormalized one Jeff = Jz which can be written as

$$\frac{J_{eff}}{J} = z = \left[1 + S(S+1)\,\frac{g_o - g_{eff}}{g_o}\right]^{-1}$$

If such an expression held below the Kondo temperature also, we would get an essential renormalization; e.g. at $T=o$ for $S = \frac{1}{2}$ $g_{eff} \equiv 0$ hence $\frac{J_{eff}}{J} \sim \frac{4}{7}$ which would lead to an important additional temperature dependence of the observable quantities.*

* More details will be published in Physics Letters.

61.801

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/The details will be published in Zeit.für Physik/.