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Critical dynamics of Heisenberg antiferromagnets: correlation functions above Néel point

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Abstract

Theory describing critical behavior of isotropic Heisenberg antiferromagnets (AF) is proposed for a temperature range above the Néel point. It is shown that the critical dynamics of AF should be described in terms of relaxation-diffusion mode coupling and the scaling behavior of spin diffusion coefficient is determined by the scaling law for relaxation kinetic coefficient. The method based on analysis of diagrammatic expansion for diffusion and relaxation constants allows incorporation of nonlocal spin-liquid correlations. Applications of the method to heavy-fermion (HF) materials are briefly discussed.

Keywords: Heavy fermions; Critical dynamics; Antiferromagnets

In recent years there had been considerable activity, both experimental and theoretical, in the field of critical phenomena of antiferromagnets with Heisenberg and RKKY interactions. This increase of interest was stimulated by new experiments in high-T_c superconductors and heavy-fermion compounds. In particular, the critical spin fluctuations are supposed to be responsible for the crossover from Fermi-liquid (FL) to Non-FL (NFL) low-temperature behavior of the heat capacity and resistivity in $CeCu_{6-x}Au_x$ [1] and $Ce_{1-x}La_xRu_2Si_2$ [2] in the vicinity of the quantum critical point (QCP).

The scaling behavior of critical fluctuations in Heisenberg AF is described in terms of wave number $\boldsymbol{k}$ and inverse coherence length ξ^{-1} [3,4,9], and the critical fluctuations of the order parameter $\boldsymbol{N} = \boldsymbol{M}_1 - \boldsymbol{M}_2$ (the difference in the moments of the sublattices) are characterized by the wave vectors $q \gg \xi^{-1}$, where $q = |\boldsymbol{k} - \boldsymbol{Q}|$ and $\boldsymbol{Q} = \boldsymbol{Q}_{\mathrm{AF}}$. We are interested in hydrodynamic fluctuations with $q \ll \xi^{-1}$ which could be described in terms of relaxation modes. The scaling properties of these modes is governed by kinetic relaxation coefficient Γ_0 which diverges as $T - T_c \to 0$. It will be shown in this paper that the relaxation critical modes are coupled with diffusion critical modes characterized by the wave vectors $k \ll \xi^{-1}$. The diffusion modes describe the longitudinal fluctuations of total magnetization $\boldsymbol{M} = \boldsymbol{M}_1 + \boldsymbol{M}_2$. These fluctuations do not lead to any singularities in spin correlators. Nevertheless, the macroscopic equations which describe the temporal evolution of the vectors $\boldsymbol{N}$ and $\boldsymbol{M}$ in the long-wavelength limit,

$$\frac{\partial \boldsymbol{M}}{\partial t} = D_0 \nabla^2 \boldsymbol{M}, \quad \frac{\partial \boldsymbol{N}}{\partial t} = -\frac{\Gamma_0}{\chi}\boldsymbol{N}. \qquad (1)$$

are not independent, and the relaxation kinetic coefficient Γ_0 is coupled with the spin diffusion coefficient D_0 by a scaling relation. Derivation of this relation is the main content of the paper.

To derive the kinetic coefficients microscopically, we consider the dynamical susceptibility of a cubic Heisenberg antiferromagnet with nearest-neighbor interaction V_{ij} in zero magnetic field above the Néel temperature. As is known, the susceptibility χ is related to the retarded Green's function (GF) by the following equality: $\chi(\boldsymbol{k}, \omega) = (g\mu_0)^2 K^{R}_{SS}(\boldsymbol{k}, \omega)$ (g is the Lande factor, μ_0 is the Bohr

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magneton). Using Eq. (1), one can rewrite an expression for the retarded GF in the fluctuation region in the form

$$K^{R}_{SS}(\boldsymbol{k},\omega)=\frac{i\gamma(\boldsymbol{k},\omega)}{\omega+iG_0^{-1}(\boldsymbol{k})\gamma(\boldsymbol{k},\omega)},\tag{2}$$

where $G_0(\boldsymbol{k})$ is static susceptibility. Then $D_0=\lim_{k\to0}\lim_{\omega\to0}k^{-2}\gamma(\boldsymbol{k},\omega)G_0^{-1}(\boldsymbol{k})$, $\Gamma(\boldsymbol{k},\omega)=\gamma(\boldsymbol{k},\omega)$. Using the properties of spin operators and equation of motion [5] one can obtain the relation between the Kubo functions [4] and the spin-current correlator at Matsubara frequencies:

$$K_{\dot{S}\dot{S}}(\boldsymbol{k},\omega_n)=\frac{(a^2T_c\alpha)^2}{6N}\int_0^{1/T}d\tau e^{i\omega_n\tau}\sum_{p_1,p_2}(\nabla V(\boldsymbol{p}_1)\boldsymbol{k})(\nabla V(\boldsymbol{p}_2)\boldsymbol{k})\times\langle T_\tau(S^{\mu}_{p_1+k}S^{\rho}_{-p_1})_\tau(S^{\mu}_{-p_2-k}S^{\rho}_{p_2})_0\rangle,\tag{3}$$

where a is a lattice constant and $\alpha\sim1$ is a numerical coefficient.

The generalized kinetic coefficient can be rewritten in terms of irreducible spin-current self-energy part as follows: $\gamma(\boldsymbol{k},\omega)=(1/i\omega)(\sum^{R}_{\dot{S}\dot{S}}(\boldsymbol{k},\omega)-\sum^{R}_{\dot{S}\dot{S}}(\boldsymbol{k},0))$. The contributions to $\sum^{R}_{\dot{S}\dot{S}}$, in turn, can be classified with respect to the number of intermediate states. To begin with, we take into account only contributions with two-particle intermediate states (see Fig. 1a and b):

$$\sum^{(2)}_{\dot{S}\dot{S}}(\boldsymbol{k},i\omega)=\frac{(T_ca^2\alpha)^2}{\sqrt{N}}T\sum_{\varepsilon}\sum_{p}(\boldsymbol{k}\Lambda^{(2)}(\boldsymbol{p},\boldsymbol{k},i\omega,i\varepsilon,i(\omega-\varepsilon)))\times(\boldsymbol{k}\Lambda^{(2)\dagger}\boldsymbol{P},\boldsymbol{k},i\varepsilon,i(\omega-\varepsilon),i\omega))\times K_{SS}(\boldsymbol{p},i\varepsilon)K_{SS}(\boldsymbol{k}-\boldsymbol{p},i\omega-i\varepsilon),\tag{4}$$

where $K^{R}_{SS}(\boldsymbol{k}\to0,\omega)=K(\boldsymbol{k},\omega)$ and $K^{R}_{SS}(\boldsymbol{q}=(\boldsymbol{k}-\boldsymbol{Q})\to0,\omega)=\mathscr{L}(\boldsymbol{q},\omega)$ correspond to "diffuson" and "relaxon" GF, respectively. In the fluctuation region the spin GF can be expressed in terms of scaling function F as follows: $K^{R}_{SS}(\boldsymbol{k},\omega)=G_0(\boldsymbol{k})\,F(k\xi,\omega/(T_c\tau^{\nu z}))$, where the standard notations for the critical exponents are used (the Fisher critical index η is set equal to 0).

Since the vertex functions $\Lambda^{(2)}$ are analytical functions of all three frequencies [5], we can restrict ourselves by static vertex corrections. Substituting Eq. (2) into Eq. (4) and taking into account the Ward identity and the property of vertices at $k\to Q$:

$$\Lambda^{(2)}(\boldsymbol{p},\boldsymbol{k},0)\sim\partial G_0^{-1}/\partial\boldsymbol{p},\ \Lambda^{(2)}(\boldsymbol{p},\boldsymbol{Q},0)\sim\partial V/\partial\boldsymbol{p}\sim\boldsymbol{p},\tag{5}$$

one can obtain the self-consistent system of equations for kinetic coefficients:

$$D_0^{(2)}=\frac{A}{4}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\sinh^{-2}\left(\frac{\varepsilon}{2T}\right)\sum_{p}(\nabla G_0^{-1}(\boldsymbol{p}))^2[(\mathrm{Im}\,\mathscr{K}(\boldsymbol{p},\varepsilon))^2+(\mathrm{Im}\,\mathscr{L}(\boldsymbol{p},\varepsilon))^2]$$

$$\Gamma_0^{(2)}=\frac{B}{2T_c}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\sinh^{-2}\left(\frac{\varepsilon}{2T}\right)\sum_{p}(\nabla G_0^{-1}(\boldsymbol{p})\boldsymbol{Q})^2\times\mathrm{Im}\,\mathscr{K}(\boldsymbol{p},\varepsilon)\mathrm{Im}\,\mathscr{L}(\boldsymbol{p},\varepsilon),\tag{6}$$

where $A,B\sim1$ are numerical coefficients. These equations are the key results of the present paper. Solution of system (6) leads to the following scaling behavior of kinetic constants:

$$D_0/(T_ca^2)\sim\Gamma_0\sim(\xi/a)^{1/2}.\tag{7}$$

The behavior of $\Gamma_0(\xi)$ agrees with predictions of dynamic scaling theory [3,4] and with the renormalization group analysis [3]. Besides, we see that the scaling behavior of spin diffusion is determined by the intermediate relaxation processes. The correction to the coefficient D_0 owing to self-diffusion is of smallness $\delta D_0/D_0\sim\tau^{8/3}\ll1$. Calculation of dynamic critical exponent z in this approximation results in $z=\frac{3}{2}$. As is shown in Ref. [6], the intermediate states with more than two particles do not change the scaling dimensionality of kinetic coefficients.

The spin-liquid effects which are essential for nearly AF heavy-fermion systems [6], influence the behavior of spin correlation functions in the critical region. These effects can be taken into account by introducing anomalous intersite spinon-like correlations [7]. Nonlocal fermion correlations lead to emergence of a new characteristic length corresponding to short-range ordering. As a result, we expect changes in scaling behavior and in frequency and momentum dependence of spin susceptibility [6].

Next, to analyze the role of AF fluctuations in a framework of Kondo-lattice model we calculate the self-energy part [6] of conduction electrons with dispersion ε_p:

$$\sum_{el}(\boldsymbol{p},\varepsilon_n)=\frac{1}{N}\sum_{q}\frac{\mathscr{J}^2_{sf}\Gamma}{\pi}\frac{z}{z^2+b_q^2}\left[\psi\left(\frac{-iz}{2\pi T}\right)-\psi\left(\frac{b_q}{2\pi T}\right)+\frac{\pi T}{b_q}-\frac{\pi T}{-iz}-\frac{i\pi}{2}\tanh\frac{\varepsilon_{p-q}}{2T}\left(1+\frac{b_q}{-iz}\right)\right],\tag{8}$$

where $\mathscr{J}_{sf}$ is the s–f exchange integral, $z=i\varepsilon_n-\varepsilon_{p-q}$, $b_q=G_0^{-1}(\boldsymbol{q})\Gamma_0$ (see Eq. (7)) and $\psi(y)$ is a digamma

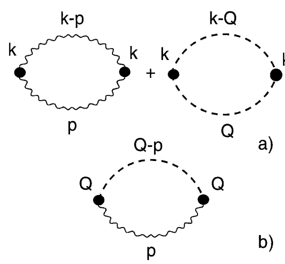

Fig. 1. Feynman diagrams for kinetic coefficients: (a) D_0, (b)Γ_0. The diffusion mode is represented by the wavy lines. Dashed lines stand for the relaxation mode. Dots represent the vertex parts from static scaling theory.

function. By calculating Eq. (8), the linear temperature behavior of resistivity $\Delta\rho \sim 1/\tau_{tr} \sim \mathrm{Im}\sum_{el}^{R}$ can be obtained in terms of spin-fluctuation model for T close to T_c [8]. In the case of 2D spin fluctuations in the vicinity of QCP [1] when the FL regime disappears, only $\Delta\rho \sim T$ contribution survives. Other NFL effects can be also analyzed in a framework of the method proposed.

To conclude, we have found that the scaling behavior of generalized kinetic coefficients in 3D isotropic Heisenberg antiferromagnets demands inclusion of diffusion-relaxation mode coupling in the theory of critical exponents. The main contribution to kinetic coefficients results from the processes with two-particle intermediate states. The method can be used for the explanation of unusual kinetic properties of heavy fermion compounds in FL and NFL regimes.

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