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Generalized theory of spin fluctuations in itinerant electron magnets: Crucial role of spin anharmonicity

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ABSTRACT

The paper critically overviews the recent developments of the theory of spatially dispersive spin fluctuations (SF) in itinerant electron magnetism with particular emphasis on spin-fluctuation coupling or spin anharmonicity. It is argued that the conventional self-consistent renormalized (SCR) theory of spin fluctuations is usually used aside of the range of its applicability actually defined by the constraint of weak spin anharmonicity based on the random phase approximation (RPA) arguments. An essential step in understanding SF in itinerant magnets beyond RPA-like arguments was made recently within the soft-mode theory of SF accounting for strong spin anharmonicity caused by zero-point SF. In the present paper we generalize it to apply for a wider range of temperatures and regimes of SF and show it to lead to qualitatively new results caused by zero-point effects.

1. Introduction

Spin fluctuations (SF) with strong spatial dispersion in itinerant electron magnets are in the focus of condensed matter physics for more than half a century and play an important role in many classes of metallic systems including, e.g., weak itinerant magnets [1], heavy fermion compounds [2], Invar alloys [3] and magnetoresistive manganites [4]. Recently they were also found in high-temperature superconductors [5] and newly discovered Fe-based superconductors [6] strongly suggesting their possible effect on mechanisms of unconventional superconductivity. However, up to now understanding of physics of SF in itinerant magnets and their role in superconductivity is not clear.

One of the most important problems of the SF theory in itinerant electron magnets is caused by strong coupling of SF (spin anharmonicity) induced by zero-point effects which cannot be treated within conventional perturbative schemes based on the random phase approximation (RPA) arguments (or Gaussian approximation in the high-temperature limit). This problem is somewhat unique because SF are probably the only type of strongly coupled Bose excitations in the solid state physics. First attempts to treat SF go back to 1960s when the theory of paramagnons, uncoupled overdamped Bose excitations in the electron–hole continua, was introduced based on the RPA (see Ref. [1]). In 1970s Murata and Doniach [7] and Moriya and Kawabata [8] generalized the paramagnon theory in a self-consistent manner accounting for coupling of paramagnons. The formulated then a self-consistent renormalized (SCR) theory of SF established both microscopically and phenomenologically (see Refs. [9,10]) treated overdamped long wavelength SF basing on the RPA-like arguments. The initial version of the SCR theory where zero-point SF were neglected successfully explained many properties of weak itinerant magnets including the Curie–Weiss behavior of the magnetic susceptibility [1,10]. The further version of the SCR theory partly incorporated zero-point SF and their temperature dependence [11,12]. However, the authors [11,12] used the same RPA arguments neglecting strong spin anharmonicity induced by zero-point effects. The improved version of the SCR theory was argued to lead to a simple renormalization of the parameters of the SCR theory treated within the phenomenological approach.

The alternative approach to the theory of SF in itinerant electron magnets was based on the functional integral arguments and was successful in explaining metallic magnets with SF of mainly local single-site nature (see the book [1]). However, this approach is usually based on uncontrolled approximations and does not account for the effects of strong spin anharmonicity intrinsic for itinerant magnets.

A new trend in the description of SF in itinerant magnets started in 1990s when it was realized that in the vicinity of

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magnetic instabilities SF soften similarly to softening of phonons near the structural transitions. However, unlike phonons soft SF give rise to giant amplitudes of zero-point SF [13] and to strong spin anharmonicity [14] which cannot be described within perturbative approaches based on the RPA arguments. To account for large zero-point SF amplitudes and strong spin anharmonicity a soft-mode (SM) theory of SF was formulated using both microscopic [15] and phenomenological [16] approaches. In the present paper we formulate a generalized theory of SF extending the SM theory [15–18] for a wider range of temperatures and regimes of SF. Zero-point SF are shown to lead to new qualitative effects including enhancement of low-temperature specific heat.

2. Model for spin fluctuations

To account for various types of magnets with itinerant electrons instead of using microscopic models we start with the following phenomenological form for the inverse dynamical magnetic susceptibilities [1,10]

$$\chi_\nu^{-1}(\mathbf{k},\omega)=\chi_\nu^{-1}(T)+c(\mathbf{k})-i\frac{\omega}{\Gamma(\mathbf{k},\omega,T)} \tag{1}$$

as a function of the wavevector $\mathbf{k}$, frequency ω, temperature T and polarization ν ($\nu=t$ marks the transverse and $\nu=l$ longitudinal ones), which was supported both theoretically and experimentally [1,10]. Here $\chi_\nu(T)$ are static susceptibilities, which coincide with the thermodynamic ones

$$\chi_t^{-1}=\frac{1}{M}\frac{\partial F}{\partial M},\quad \chi_l^{-1}=\frac{\partial^2 F}{\partial M^2}, \tag{2}$$

$c(\mathbf{k})$ accounts for their spatial dispersion (we neglect its frequency and temperature dependencies which do not lead to new physical results), $F=F(T,M)$ is the free energy dependent on the order parameter M. Here $\Gamma(\mathbf{k},\omega,T)$ is the relaxation rate defining the nature of SF. At relatively low temperatures [18,19] SF relaxation is defined by the linear Landau mechanism in the electron–hole continua and is ω- and T-independent. In this limit $\Gamma(\mathbf{k},\omega,T)\approx\Gamma_0(\mathbf{k})$ and SF have a conventional paramagnon nature. To account for the boundaries of electron–hole continua we introduce the wavevector k_c and frequency ω_c cutoffs being phenomenological parameters of the model. For the Stoner continuum we also introduce a low frequency cutoff wavevector k_0 below which no transverse SF exist [10]. At elevated temperatures the SF relaxation mechanism is different from the linear Landau one and is defined by the various non-linear mode–mode scattering processes which dominate the magnetic relaxation [18,19] and may result in the strong frequency and temperature dependent relaxation rate $\Gamma(\mathbf{k},\omega,T)$ and lead to a number of novel phenomena [21,22]. Here for simplicity we shall not discuss the effects of non-linear magnetic relaxation assuming that the temperature is sufficiently low and set $\Gamma(\mathbf{k},\omega,T)\approx\Gamma_0(\mathbf{k})\approx\Gamma_0(\mathbf{k}/k)^{Z-2}$, where the dynamical exponent z is 3 for ferro- and 2 for antiferromagnetic instabilities.

To find the free energy of itinerant electron magnets with strongly coupled SF models we adopt a physically transparent phenomenological approach based on the Ginsburg–Landau effective Hamiltonian

$$\hat{H}_{eff}=\frac{1}{2}\sum_{\mathbf{k}}\chi_0^{-1}(\mathbf{k})\,|\mathbf{M}(\mathbf{k})|^2+\frac{\gamma_0}{4}\sum_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4=0}(\mathbf{M}(\mathbf{k}_1)\mathbf{M}(\mathbf{k}_2))(\mathbf{M}(\mathbf{k}_3)\mathbf{M}(\mathbf{k}_4)) \tag{3}$$

which should be accompanied by the time-dependent equation

$$\frac{1}{\Gamma_0(\mathbf{k})}\frac{\partial\mathbf{M}(\mathbf{k})}{\partial t}=-\frac{\delta\hat{H}_{eff}}{\delta\mathbf{M}(-\mathbf{k})}. \tag{4}$$

Here $\mathbf{M}(\mathbf{k},t)=\mathbf{M}\delta_{\mathbf{k},0}+\mathbf{m}(\mathbf{k},t)$ is the time dependent magnetic order parameter, $\mathbf{m}(\mathbf{k},t)$ accounts for SF, $\chi_0^{-1}(\mathbf{k})=\chi_0^{-1}+c(\mathbf{k})$ and γ_0 define the static inhomogeneous paramagnetic susceptibility and mode-mode coupling constant not affected by SF. Here we treat (3) and (4) as a model describing both long and short wavelength SF at various temperatures and do not view them as expansions in powers of SF amplitudes which are not assumed to be small. The effective Hamiltonian was shown to arise from microscopic approaches after integrating out individual quasiparticles degrees of freedom and charge density fluctuations [9]. It was also widely used in the theory of critical phenomena near phase transitions [23].

Then the free energy is given by

$$F(M,T)=F_0(T)+\frac{1}{2\chi_0}M^2+\frac{\gamma_0}{4}M^4+\Delta F, \tag{5}$$

where $F_0(T)$ denotes the contribution independent on magnetization, terms with M^2 and M^4 are related to the Hartree–Fock approximation, and the SF contribution can be written using an integration of the equality $\partial\Delta F/\partial(\chi_0^{-1})=M_L^2/2$,

$$\Delta F\{\chi_\nu(\mathbf{k},\omega)\}=\frac{1}{2}\sum_\nu\int d\left(\chi_0^{-1}\right)M_L^2=\hbar\sum_\nu\sum_{\mathbf{k},\omega}\int d\left(\chi_0^{-1}\right)\mathrm{Im}\chi_\nu(\mathbf{k},\omega)[N_\omega+1/2]. \tag{6}$$

The squared local magnetic moment (averaged amplitudes of SF) $M_L^2=\left\langle\mathbf{m}^2\right\rangle$ is given by the fluctuation–dissipation theorem

$$M_L^2=\sum_{\mathbf{k},\omega}(M_L^2)_{\mathbf{k},\omega}=4\hbar\sum_\nu\sum_{\mathbf{k},\omega}\mathrm{Im}\chi_\nu(\mathbf{k},\omega)\left(N_\omega+\frac{1}{2}\right)\equiv\left(M_L^2\right)_T+\left(M_L^2\right)_{Z.P.}, \tag{7}$$

where $\sum_{\kappa,\omega}=\sum_{\mathbf{k}}\int_0^\infty(d\omega/2\pi)$, the factors $N_\omega=[\exp(\hbar\omega/k_BT)-1]^{-1}$ and 1/2 are related to thermal and zero-point SF, respectively, which provides a natural separation of M_L^2 into the zero-point $(M_L^2)_{Z.P.}$ and thermal $(M_L^2)_T$ contributions.

Integro-differential Eqs. (1), (2), (5), and (6) are the basic equations of the theory of SF that should be solved self-consistently. As it follows from Eq. (6) the key parameter defining the solution of these equations is the derivative

$$\zeta_\nu=\frac{\partial(\chi_\nu^{-1})}{\partial(\chi_0^{-1})} \tag{8}$$

which is the measure of the effects of SF on the magnetic susceptibilities.

3. Limitations of the self-consistent renormalized theory of spin fluctuations

In all versions of the SCR theory this parameter is set to unity

$$\zeta_\nu=1, \tag{9}$$

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