Spin fluctuations in itinerant electron antiferromagnetism and anomalous properties of $Y(Sc)Mn_2$

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An analysis of spin-fluctuation (SF) effects in itinerant electron magnets with antiferromagnetic instabilities is presented in two well-distinguished regimes of SF's. One, related to soft-mode (SM) fluctuations, is dominated by strongly coupled low-frequency SF's giving rise to the increase of the unsaturated local magnetic moments with temperature. The other, the localized moments (LM) regime, is characterized by dispersionless SF's, local in the real space, and by saturated thermally induced moments giving rise to the Curie-Weiss susceptibility. It is shown that both thermal and zero-point SF's play an important role in SM as well as in LM regimes. The presented description of the SF behavior generalizes the conventional mode-mode coupling theory based on a weak-coupling constraint and establishes a link between SM and LM regimes of SF's. The results are shown to give a quantitative description of the SF behavior and effects of frustration in the $Y(Sc)Mn_2$ system. [S0163-1829(96)00245-7]

I. INTRODUCTION

During the past two decades investigations of itinerant electron magnetism were focused on studies of spin-fluctuation (SF) effects in metals close to a magnetic instability which are strongly influenced by overdamped fluctuations of the magnetic order parameter.[1] The overdamped SF's were directly observed in a series of weakly ferromagnetic metals by inelastic neutron scattering[2,3] which was centered mainly near the origin of the Brillouin zone, presenting evidence for softening of the characteristic frequency of long-wavelength SF's. Another example of the soft-mode SF's is presented by the antiferromagnetic itinerant electron system $Y(Sc)Mn_2$ exhibiting a heavy fermion behavior, where the paramagnetic state is stabilized by doping with small amounts of Sc. The previous neutron-scattering measurements on powder samples revealed a strong magnetic response peaked around the antiferromagnetic wave vector $Q \approx 1.5$ Å^{-1},[4–7] and allowed us to estimate local magnetic moments on Mn atoms M_L being at low temperatures about $1.3\mu_B$ (where μ_B is the Bohr magneton) due to strong zero-point SF's.[6] Recently performed neutron-scattering experiments on single crystals of $Y(Sc)Mn_2$ discovered strongly anisotropic and flat SF spectrum near the wave vector $\vec{Q} \approx (1.25,1.25,0)$ (in reciprocal-lattice units), described by the SF frequency $\omega_{SF}(\vec{Q})$ almost linearly dependent on temperature.[8] The unusual SF spectrum was related to the effects of geometrical frustration and to the heavy fermion behavior exhibited by the $Y(Sc)Mn_2$ system.[8–10]

So far the descriptions of itinerant magnets close to a magnetic instability within both the phenomenological Ginzburg-Landau[11,12] and microscopic Hubbard[1,12,13] or Fermi-liquid[14] models were based on two important constraints. Namely, (i) mode-mode coupling of SF's was considered to be weak and SF effects were described in the lowest order approximation in SF amplitudes, and (ii) only soft-mode SF's with wave vectors close to $\vec{q} \sim \vec{Q}$ were taken into account. However, neutron-scattering experiments[6] and theoretical estimates[15,16] for itinerant magnets close to an instability present the direct evidence for strong spin anharmonicity characterized by the dimensionless parameter g_0 which at low temperatures is not small,

$$g_0 \sim M_L^2/\mu_B^2 N_e^2 \sim 1, \tag{1}$$

(where N_e is the density of itinerant electrons) due to effects of zero-point SF's. Thus constraint (i) perhaps does not hold in real materials. Condition (ii) is fulfilled below a certain temperature T_L where the SF $\omega_{SF}(\vec{Q})$ frequency softens. Above T_L $\omega_{SF}(\vec{Q})$ increases proportionally to the inverse susceptibility, and the soft-mode features of SF's disappear.

To account for strong mode-mode coupling and soft-mode behavior of SF's a soft-mode (SM) theory[15,16] based on a variational approach was recently worked out extending the conventional SF theory of itinerant magnets[1,11–14] beyond a weak-coupling limit. So far the SM theory was used to describe itinerant magnets close to a ferromagnetic instability with an isotropic spectrum of SF's. The compound $Y(Sc)Mn_2$ presents an example of a different SF system with highly anisotropic spectrum of antiferromagnetic fluctuations strongly influenced by effects of frustration. In the present paper we analyze the effects of anisotropic SF's in itinerant magnets with antiferromagnetic instabilities. A particular emphasis is made on the anomalous properties of the Y(Sc)Mn_2 system in the paramagnetic state. In Sec. II basing on recent inelastic neutron-scattering experiments in Y(Sc)Mn_2,[8] we introduce a model for an anisotropic SF's spectrum. Then in Sec. III we use the fluctuation-dissipation theorem to distinguish between different SF regimes: a SM one governed by low-frequency SF's with strong spatial dispersion, and localized moments (LM) regime characterized by almost dispersionless SF's related to fluctuating localized atomic moments. To describe SF behavior in the SM regime in Sec. IV we use the SM theory of SF's,[15,16] and in Sec. V we apply the fluctuation-dissipation theorem to discuss quantum effects of SF's in the LM regime and the crossover from the SM to the LM regime. The results are applied in Sec. VI to describe the SF behavior of the Y(Sc)Mn_2 system which exhibits heavy fermionlike behavior due to 3*d* electrons.[9] Finally, Sec. VII is devoted to a summary.

II. SF SPECTRUM: EFFECTS OF FRUSTRATION

SF spectra in metallic magnets influenced by frustration may essentially differ from those in isotropic itinerant magnets.[10] Frustration resulting either from competing exchange interactions or due to the crystallographic structure may give rise to a degenerate ground state and to a highly anisotropic SF spectrum, flat in one or several directions. The effects of frustration were studied mainly in the case of the Heisenberg model on Kagomé or pyrochlore lattices,[17,18] but they are also expected to play an important role in metallic magnets of the YMn_2 type: the lattice structure of these Laves phase compounds is similar to the pyrochlore structure. To account for effects of frustration in itinerant magnets we use the model for the dynamical magnetic susceptibility $\chi(\vec{q},\omega)$ which was recently suggested to describe anomalous properties of Y(Sc)Mn_2,[10]

$$\chi^{-1}(\vec{Q}+\vec{q},\omega)=\chi^{-1}(\vec{Q}+\vec{q})-i\frac{\omega}{\Gamma}=\chi_Q^{-1}+c(\vec{q})-i\frac{\omega}{\Gamma}. \tag{2}$$

Here we assume that $\chi(\vec{q},\omega)$ has a maximum at a finite wave vector $\vec{q}=\vec{Q}$, around which $c(\vec{q})$ may be expanded in powers of $\vec{q}$,

$$c(\vec{q})=a_1q_\perp^2+a_2q_z^4, \tag{3}$$

where $q_\perp^2=q_x^2+q_y^2$, and the relaxation rate is almost constant, $\Gamma=$const. The model defined by Eqs. (2) and (3) describes overdamped SF's with the characteristic frequency

$$\omega_{\rm SF}(\vec{q})=\Gamma[\chi_Q^{-1}+c(\vec{q})], \tag{4}$$

softening around $\vec{q}=\vec{Q}$ and is supported by the neutron-scattering measurements in Y(Sc)Mn_2,[8] where a flat in the [001] direction [which is related to the z axis in Eq. (3)] spectrum was reported near the wave vector $\vec{Q}=(1.25,1.25,0)$ r.l.u.

Below we limit the phase volume of SF's by introducing a cutoff wave vector $\vec{q}_C=(\vec{q}_{\perp C},\vec{q}_{zC})$,

$$c(\vec{q})\leqslant c(\vec{q}_C)=c_C, \tag{5}$$

where $\vec{q}_c$ is defined by the volume of the Brillouin zone

$$N_0=\frac{1}{2\pi^2}q_{\perp C}^2q_{zC}. \tag{6}$$

We also introduce a frequency cutoff, $\omega\leqslant\omega_C$, where ω_C should be inferred from the experimental data.

III. LOCAL MAGNETIC MOMENTS AND DIFFERENT SF REGIMES

One of the most important characteristics of SF's is the average squared amplitude of SF's, or squared local magnetic moment M_L^2 which is related to dynamical susceptibility $\chi(\vec{q},\omega)$ via the fluctuation-dissipation theorem (FDT),[19]

$$\begin{aligned}M_L^2&=12\hbar\sum_{\vec{q}}\sum_{\omega}\chi(\vec{q})\frac{\omega\omega_{\rm SF}(\vec{q})}{\omega^2+\omega_{\rm SF}^2(\vec{q})}\left(N_\omega+\frac{1}{2}\right)\\&=(M_L^2)_T+(M_L^2)_{\rm ZP}.\end{aligned} \tag{7}$$

Here $\chi(\vec{q})=\chi(\vec{q},0)$ is the static susceptibility, $\Sigma_{c(\vec{q})\leqslant c_C}=\int_{c(\vec{q})\leqslant c_C}d\vec{q}/(2\pi^3)$, $\Sigma_\omega=\int_0^{\omega_C}d\omega/2\pi$, and the factors $N_\omega=[\exp(\hbar\omega/k_BT)-1]^{-1}$ and 1/2 define thermal $(M_L^2)_T$ and zero-point $(M_L^2)_{\rm ZP}$ contributions to M_L^2, respectively.

In the quantum temperature range when

$$k_BT\ll\hbar\omega_C, \tag{8}$$

the frequency integration in Eq. (7) yields the following explicit expression for the thermal contribution to M_L^2:[1,12]

$$\begin{aligned}(M_L^2)_T&=3k_BT\sum_{c(\vec{q})\leqslant c_C}\chi(\vec{q})G\left[\frac{\hbar\omega_{\rm SF}(\vec{q})}{2\pi k_BT}\right]\\&=3k_BT\sum_{c(\vec{q})\leqslant c(\vec{q}_T)}\chi(\vec{q}).\end{aligned} \tag{9}$$

Here

$$G(z)=2z[\ln z-1/2z-\Psi(z)] \tag{10}$$

[where $\Psi(z)$ is Euler's psi function] is a rapidly decreasing function of z accounting for quantum effects. This allows us to introduce a thermal wave vector cutoff $\vec{q}_T$ which can be estimated from $\hbar\Gamma c(\vec{q}_T)\sim\min\{k_BT,\hbar\Gamma c_C\}$. The integration of Eq. (9) [see below, formula (17)] yields a more precise definition,

$$c(\vec{q}_T)\equiv c_T=c_C\times\begin{cases}\dfrac{T}{T_m}, & T\leqslant T_m,\\ 1, & T>T_m,\end{cases} \tag{11}$$

where

$$T_m=\hbar\Gamma c_C/\alpha_0k_B \tag{12}$$

is the SF temperature and $\alpha_0\approx1.176$ is a dimensionless coefficient.

Formula (9) provides a natural separation of the SF behavior into two well-defined regimes: (i) the SM one, when

$$\chi_Q^{-1}(T) \ll c_T, \tag{13}$$

and (ii) the LM regime arising at higher temperatures when

$$\chi_Q^{-1}(T) \gg c_C. \tag{14}$$

As it follows from Eq. (9) the SM regime is dominated by thermally excited soft SF's with energies $\hbar\omega_{\rm SF}(\vec{q}) \leq k_B T$. On the other hand, in the LM regime SF's are almost dispersionless, $\hbar\omega_{\rm SF}(\vec{q}) \approx \Gamma\chi_Q^{-1}$, and local in real space, which allows us to describe them in terms of LM. In the intermediate-temperature range defined by $c_T \leq \chi_Q^{-1}(T) \leq c_C$ a crossover from SM to LM regimes takes place. Here we do not discuss the low-temperature regime, $c_T \ll \chi_Q^{-1} \approx {\rm const}(T)$, where SF's give rise to a conventional Fermi-liquid behavior.

Analogously, one can estimate the zero-point contribution to M_L^2,

$$(M_L^2)_{\rm ZP} = \frac{3}{\pi}\hbar\Gamma N_0 \alpha_1\left[f, \frac{\chi_Q^{-1}}{c_C}\right], \tag{15}$$

where $f = \omega_C/\Gamma c_C$ and

$$\alpha_1 = \frac{1}{N_0}\sum_{c(\vec{q}) \leq c_C} \ln\left[1 + \frac{\omega_C^2}{\omega_{\rm SF}^2(\vec{q})}\right]. \tag{16}$$

As it follows from Eqs. (15) and (16) the zero-point contribution to M_L^2 dominates at low temperatures and vanishes in the high-temperature limit. Temperature dependences of local magnetic moments in the different SF regimes are illustrated by Fig. 1.

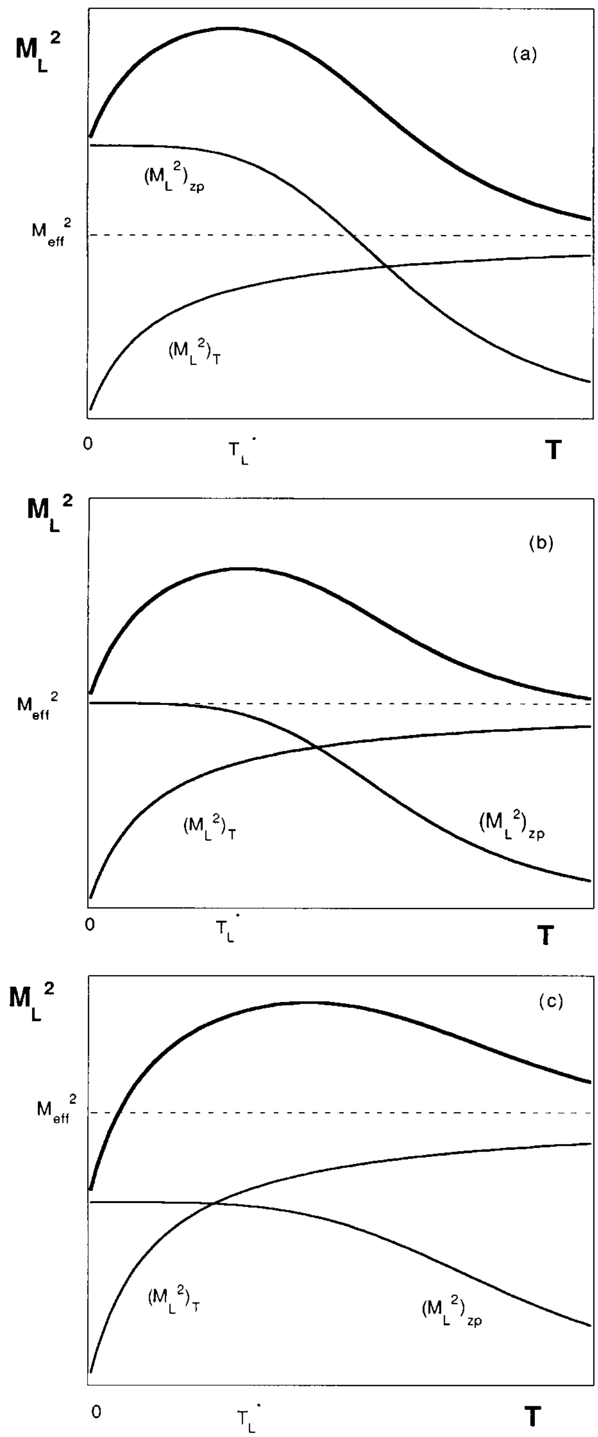

FIG. 1. Temperature dependence of local magnetic moments. $(M_L^2)_{\rm ZP}$ and $(M_L^2)_T$ correspond to zero-point and thermal SF contributions, respectively, $M_{\rm eff}^2$ is the squared saturated moment, the temperature T_L^* indicates the crossover to the localized moments regime of SF's. The upper curves describe the temperature dependence of the total squared local moment M_L^2: (a) when $M_{\rm eff}^2/M_L^2(T=0)<1$, (b) when $M_{\rm eff}^2/M_L^2(T=0)=1$, and (c) when $M_{\rm eff}^2/M_L^2(T=0)>1$.

IV. SF BEHAVIOR IN THE SOFT-MODE REGIME

As it follows from Eq. (9) the thermally excited magnetic moments increase with temperature in the SM regime,

$$(M_L^2)_T = 15 k_B T \frac{N_0 c_T^{1/4}}{c_C^{5/4}}, \tag{17}$$

as $\sim T^{5/4}$ in the quantum temperature range, $T < T_m$, and as $\sim T$ in the classical limit, $T > T_m$, where T_m is defined by Eq. (12) with $\alpha_0 = [\Gamma(5/4)/4\cos(\pi/8)]^4$. It should be emphasized that in the frustrated systems with an anisotropic SF spectrum the temperature dependence $(M_L^2)_T \sim T^{5/4}$ for $T << T_m$ is close to a linear one whereas for isotropic antiferromagnetic fluctuations with a quadratic dispersion $c(\vec{q}) \sim \vec{q}^2$ one has[1] $(M_L^2)_T \sim T^{3/2}$.

The zero-point contribution to M_L^2 according to Eqs. (15) and (16) is slowly changing with temperature due to the variation of $\chi_Q(T)$,

$$(M_L^2)_{\rm ZP} = M_{L0}^2 - 3g[\gamma_0 \chi_Q(T)]^{-1}, \tag{18}$$

where M_{L0}^2 is given by Eq. (15) with $\chi_Q^{-1} = 0$ and

$$g_0 = \frac{5}{\pi}\frac{\hbar\gamma_0 \Gamma N_0}{c_C}\alpha_2\left(\frac{\omega_C}{\Gamma c_C}\right) \tag{19}$$

is the spin anharmonicity parameter.[15,16] Here $\alpha_2(f) = f^2\int_0^1 dx/(x^8 + f^2) \leq 1$ is a dimensionless parameter, and $\gamma_0 = 2\partial^2 F_0/\partial(M_Q^2)^2$ is the SF coupling constant defined by the Hartree-Fock free energy $F_0(M_Q)$ (where M_Q is the magnetic order parameter). Using the approximations $\gamma_0 \sim (\mu_B^2 N_e^2 \chi_p)^{-1}$, $\hbar\Gamma \sim \mu_B^2 N_e$, and $c_C \sim \chi_p^{-1}$ (where χ_p is the Pauli susceptibility) following from the microscopic model of Moriya,[1] we come to the previous estimate Eq. (1) for the spin anharmonicity parameter.

The temperature dependence of the susceptibility $\chi_Q(T)$ in the SM regime arises due to mode-mode coupling of soft SF's. However, the conventional SF theory of mode-mode coupling in weak itinerant antiferromagnets[1] is based on the weak-coupling constraint and cannot be applied to real magnets where spin anharmonicity is expected to be strong $g_0 \sim 1$. To account for the effects of strong spin anharmonicity we use the SM theory of SF's (Refs. 15 and 16) based on a variational procedure. According to Ref. 15 the free energy of an anharmonic itinerant magnet is given by

$$F = F_0 + \frac{1}{\zeta} \Delta F_{\mathrm{RPA}}(\chi_Q), \tag{20}$$

where $\Delta F_{\mathrm{RPA}}(\chi_Q)$ is the SF contribution to the free energy in the random-phase approximation (RPA) (see, e.g., Ref. 1). The factor $\zeta = \partial(\chi_Q^{-1})/\partial(\chi_{Q0}^{-1})$, where χ_{Q0} is the Hartree-Fock magnetic susceptibility, accounts for the anharmonic effects beyond RPA. A minimization of Eq. (20) with respect to χ_Q yields

$$\chi_Q^{-1}(T) = \chi_Q^{-1}(0) + \frac{5}{3} \gamma \langle M_L^2 \rangle_T . \tag{21}$$

The temperature-dependent susceptibility Eq. (21) has the same form as in the rotationally invariant form of the conventional mode-mode coupling theory.[1,12,14] However, the ground-state susceptibility $\chi_Q(0)$ and the coupling constant are strongly renormalized compared to the Hartree-Fock values, χ_{Q0} and γ_0

$$\chi_Q^{-1} = \zeta \chi_{Q0}^{-1} + \frac{5}{3} \gamma M_{L0}^2 , \tag{22}$$

$$\gamma = \gamma_0 \frac{1-5g}{1+6g}, \tag{23}$$

where $\zeta = 1-5g$, and $g = g_0 \gamma/\gamma_0$ is the renormalized spin anharmonicity parameter. It should be mentioned that the factor $0 < \zeta < 1$ is always positive and is vanishing $\sim g_0^{-1}$ in the limit of strong anharmonicity ($g_0 \gg 1$).

Using Eqs. (18) and (21) we get the following explicit expression for the total local moment Eq. (7):

$$M_L^2 = M_L^2(T=0) + (1-5g) \langle M_L^2 \rangle_T . \tag{24}$$

As it follows from Eq. (24), though the variations of the zero-point and thermal contributions to M_L^2 are of different signs, they are not compensated and M_L^2 strongly depends on temperature. We emphasize once more that in itinerant magnets with SM fluctuations local magnetic moments M_L are not conserved as it is often assumed in descriptions of strongly correlated electron systems.[20,21] This assumption is not born out of thermodynamics and according to Ref. 16 holds only in nearly Heisenberg systems.

Substituting Eq. (17) into Eq. (21) we get the explicit temperature dependence of the staggered susceptibility in the paramagnetic state

$$\chi_Q^{-1}(T) = \chi_Q^{-1}(0) \left[1 + \left(\frac{T}{\Theta} \right)^{\beta} \right], \tag{25}$$

with the paramagnetic Néel temperature

$$\Theta = T_m [\eta c_C \chi_Q(0)]^{-1/\beta}, \tag{26}$$

where $\beta = 5/4$ for $T < T_m$ and $\beta = 1$ for $T > T_m$. Here

$$\eta = \frac{\alpha_0 \alpha_2(f)}{5\pi g} \tag{27}$$

is a dimensionless parameter expected to be of order unity in anharmonic itinerant magnets.[16]

The temperature dependence of the susceptibility Eq. (25) in the SM regime may be interpreted in terms of the Curie-Weiss law

$$\chi_Q(T) = \frac{C_{\mathrm{eff}}(T)}{T + \Theta} \tag{28}$$

with a temperature-dependent effective Curie constant $C_{\mathrm{eff}}(T)$. For $T > T_m$, C_{eff} is temperature independent and may be related to the low-temperature local magnetic moment Eq. (18),

$$C_{\mathrm{eff}} = \frac{\alpha_2(f)}{15 g \alpha_1(f,0)} \frac{M_{L0}^2}{k_B N_0}. \tag{29}$$

It should be emphasized that the Curie-Weiss law defined by Eqs. (28) and (29) arises due to strong mode-mode coupling of SF's, as was anticipated in the early mode-mode coupling theory of Murata and Doniach.[11]

Following Moriya[1] we can also estimate the temperature dependence of the nuclear spin-lattice relaxation rate in the SM regime of SF's. Using the model Eqs. (2) and (3) for the SF spectrum of a frustrated magnet we have

$$(T_1 T)^{-1} \sim \sum_{c(\vec{q}) \leqslant c_C} \frac{\mathrm{Im}\chi(\vec{q}, \omega_0)}{\omega_0} \sim \chi_Q^{3/4}(T), \tag{30}$$

where ω_0 is the nuclear resonance frequency and the susceptibility $\chi_0(T)$ is given by Eq. (25). According to Eq. (30) in frustrated systems nuclear relaxation has a stronger temperature dependence, as $\chi_0^{3/4}(T)$, instead of $\chi_0^{1/2}(T)$ arising in itinerant magnets with a quadratic dispersion of antiferromagnetic fluctuations.[1]

Finally, using Eqs. (11) and (25) we estimate the temperature T_L defined by

$$\chi_Q^{-1}(T) = c_T , \tag{31}$$

above which the SM regime does not hold. E.g., when Θ, $T_L > T_m$ the temperature T_L is related via

$$\Theta + T_L = \eta T_m \tag{32}$$

to the characteristic SF temperature T_m. It should be also mentioned that Eq. (31) has another, low-temperature solution defining a crossover to the Fermi-liquid regime of SF's, which we do not discuss here.

V. QUANTUM EFFECTS IN THE LOCALIZED MOMENTS REGIME OF SF'S

In the LM regime Eq. (14), the SM theory of SF's presented in Sec. IV does not hold due to the decreasing role of the spatial dispersion. In this limit the dispersion of SF's may be neglected: they behave as an ensemble of fluctuating localized moments. In this section we analyze the SF behavior in the LM regime using FDT, Eq. (7).

According to Eq. (9) the thermal contribution to M_L^2 in the LM regime of SF's is given by

$$(M_L^2)_T = 3k_B T N_0 \chi_Q(T) G\left[\frac{\hbar\Gamma\chi_Q^{-1}(T)}{2\pi k_B T}\right]. \tag{33}$$

If one assumes that the susceptibility $\chi_0(T)$ exhibits the Curie-Weiss behavior,

$$\chi_Q(T) = \frac{C}{T+\Theta_L} \tag{34}$$

[where the Curie constant C and temperature Θ_L are in principle different from $C_{\rm eff}$ and Θ in Eq. (28)] then according to Eq. (33) thermally induced local moments are going to be saturated at high temperatures $T \gg \Theta_L$, $(M_L^2)_T = M_{\rm eff}^2 = \text{const}$. And vice versa, saturation of M_L^2 gives rise to the Curie-Weiss susceptibility Eq. (34).

Up to now a reliable calculation of $M_{\rm eff}^2$ or C in the LM regime are still lacking. However, formula (33) provides a link between the squared saturated moment $M_{\rm eff}$ and the Curie constant C,

$$M_{\rm eff}^2 = 3k_B N_0 C G(z), \tag{35}$$

where

$$z = \frac{\hbar\Gamma}{2\pi k_B C} \tag{36}$$

is a constant. Relation (35) differs from a conventional one for Heisenberg magnets (see, e.g., Ref. 1) by a factor $G(z) \leqslant 1$ accounting for a quantum reduction of the SF phase space in the temperature range Eq. (8). Above $T \sim \hbar\omega_C/k_B$ quantum effects are negligible, and one should set $G(z) \to 1$.

Saturated moments $M_{\rm eff}^2$ may be compared with the low-temperature local moments $M_L^2(T=0)$ caused by zero-point motions. From Eqs. (15) and (35) we get

$$\frac{M_{\rm eff}^2}{M_L^2(T=0)} = \frac{G(z)}{2z\alpha_1[f,\chi_Q^{-1}/c_C]}. \tag{37}$$

Estimating roughly $\alpha_1 \sim 1$ we see that the parameter z given by Eq. (36) describes a measure of quantum zero-point effects. In the limit $z \ll 1$, when $G(z) \simeq 1$ and $M_{\rm eff}^2/M_L^2 \gg 1$, quantum zero-point effects in the ML regime may be neglected and SF's may be treated on a classical basis. When $z \sim 1$, according to Eq. (37) the zero-point contribution to M_L^2 may be comparable with the thermal one.

Using Eqs. (15) and (35) we have

$$(M_L^2)_{\rm ZP} = \frac{3}{\pi}\hbar\Gamma N_0 \ln\left[1 + \frac{\omega_C^2}{\Gamma^2}\chi_Q^2(T)\right]. \tag{38}$$

According to Eq. (38) the zero-point contribution to M_L^2 changes little with temperature when $\chi_0^{-1}(T) \leqslant \omega_C/\Gamma$. At high temperatures $(M_L^2)_{\rm ZP}$ decreases $\sim \chi_Q^2(T)$. In Fig. 1 we schematically show temperature dependences of the thermal $(M_L^2)_T$ and zero-point $(M_L^2)_{\rm ZP}$ contributions to M_L^2, and of the total squared local moment $M_L^2 = (M_L^2)_T + (M_L^2)_{\rm ZP}$ for different values of the ratio Eq. (37). It should be mentioned that according to Eq. (24) in the SM regime of a paramagnet the squared local moment increases with temperature and, except for the case when $M_{\rm eff}^2/M_L^2(T=0) > 1$, it has a maximum near the crossover temperature T_L^*. In the latter case M_L^2 may be a monotonically increasing function of temperature due to an interplay between $(M_L^2)_T$ and $(M_L^2)_{\rm ZP}$. The squared moment exhibits a maximum even when $M_L^2(T=0) = M_{\rm eff}^2$ [see Fig. 1(b)] and shows no signatures of conservation except for the limit of Heisenberg magnets.

Assuming a Curie-Weiss behavior for the susceptibility Eq. (34) we can estimate the temperature T_L^* defined by

$$\chi_Q^{-1}(T_L^*) = c_C, \tag{39}$$

which defines a crossover from the SM to LM regimes. Analogously to Eq. (32) we get

$$\Theta_L + T_L^* = \frac{\alpha_0}{2\pi z} T_m. \tag{40}$$

It should be mentioned that for $T_L > T_m$ the temperatures T_L and T_L^* must be equal, though they are defined by different equations (32) and (40), the difference being due to the change of the Curie constant near $T = T_L$. From Eqs. (29) and (35) we get the ratio of the Curie constants defined by mode-mode coupling and LM mechanisms, respectively,

$$\frac{C_{\rm eff}}{C} = \frac{2\alpha_2 z}{5g}. \tag{41}$$

As we have seen in Secs. IV and V the SF temperature T_m defined by Eq. (12) plays an important role in itinerant magnets. According to Eqs. (26), (32), and (40) it scales the characteristic SF temperatures Θ, T_L, and T_L^* and thus defines the overall SF behavior. The temperature T_m also defines the low-temperature specific heat of SF's in the Fermi-liquid regime, which is inversely proportional to T_m.[10] Using a parabolic electron band model and assuming that the relaxation is defined by the linear mechanism due to Landau damping of SF's,[24] we can estimate $\Gamma \sim \chi_P \varepsilon_F/\hbar$, $c_C \sim \chi_P^{-1}$, and $k_B T_m \sim \varepsilon_F \sim m_{\rm eff}^{-1}$, where ε_F and $m_{\rm eff}$ are the Fermi energy and effective mass of quasiparticles, respectively. Thus, low values of T_m would imply a heavy fermion behavior. Moreover, if T_m is small both temperatures T_L and T_L^* defining the crossover from SM to LM regimes are also small. In other words, the heavy fermion behavior tends to suppress the SM regime of SF's shifting it to lower temperatures and favors the LM regime. As we shall see in the next section this situation is probably realized in the $Y(Sc)Mn_2$ system.

VI. SF BEHAVIOR IN $Y(Sc)Mn_2$ SYSTEM

Now we apply our model to discuss effects of SF's in the $Y(Sc)Mn_2$ system. Previously Shiga *et al.*.[9] have discussed

TABLE I. Soft-mode SF effects in itinerant electron magnets. The values of χ_l and c_C in weak ferromagnets MnSi, Ni_3Al, and $ZrZn_2$ are taken from Ref. 23.

	χ_l^{-1} or χ_Q^{-1} $(10)^3$	c_C $(10)^3$	χ_l^{-1}/c_C or χ_Q^{-1}/c_C	T_C or Θ_L (K)
Y(Sc)Mn_2			0.69	170
MnSi	7.0	0.155	0.45	29
Ni_3Al	2.3	1.65	0.013	41
$ZrZn_2$	3.3	3.31	0.010	28

anomalous properties of this system in terms of a quantum spin liquid using the constraint that the total squared local moment is a constant of motion, $M_L^2=\text{const}$. However, the presented above analysis suggests that in itinerant magnets with soft-mode SF's that is not the case (see Fig. 1).

According to the recent neutron-scattering data obtained by Ballou *et al.*[8] for a single crystal of $Y_{0.97}Sc_{0.03}Mn_2$ the SF spectra in this system is strongly anisotropic with the inverse correlation lengths being at 9 K equal to $\xi_\perp^{-1}=0.35$ Å and $\xi_Z^{-1}=0.58$ Å along [110] and [001] directions, respectively. The inelastic response was reported to have a Lorenzian shape with a characteristic SF energy $\omega_{\rm SF}(Q)$ linearly dependent on temperature and being equal to 5.00 meV at 9 K and 13.1 meV at 300 K. These data provide a new insight into the nature of SF's in this compound.

First, using the measured correlation lengths $\xi_{\perp,Z}^{-1}$ we estimate the proximity of this compound to a magnetic-nonmagnetic transition characterized by χ_Q^{-1}/c_C. According to our model Eq. (3) for the SF spectrum of frustrated systems, we use the following definitions of the correlation lengths:

$$\xi_\perp^2=a_1\chi_Q, \quad \xi_Z^2=a_2\chi_Q, \tag{42}$$

to get the ratio

$$\frac{\chi_Q^{-1}}{c_C}=(5\pi^2\xi_Z\xi_\perp^2N_0)^{-4/5}. \tag{43}$$

With the measured values of $\xi_{\perp,Z}^{-1}$ and $N_0^{-1}=4.41\times10^2$ Å^3,[4] one gets the estimate

$$\frac{\chi_Q^{-1}}{c_C}=0.69.$$

This value χ_Q^{-1}/c_C should be compared with the analogous value χ_l^{-1}/c_C for weak ferromagnets MnSi, Ni_3Al, and $ZrZn_2$, presented in Table I, where χ_l is the longitudinal susceptibility in the ferromagnetic ground state. As it follows from Table I the ratio χ_Q^{-1}/c_C in Y(Sc)Mn_2 is close to the value χ_l^{-1}/c_C in MnSi which was shown to exhibit well-defined soft-mode SF's,[2] and is much higher than in typical weak itinerant ferromagnets $ZrZn_2$ and Ni_3Al.

Assuming that the reported linear temperature dependence of $\omega_{\rm SF}(Q)=\Gamma\chi_Q^{-1}(T)$ (Ref. 8) can be described by a Curie-Weiss susceptibility Eq. (34), we estimate the temperature $\Theta=170$ K. This value is close to the estimate $\Theta_L=153$ K of Rainford *et al.*[7] but is somewhat larger than the one previously reported by Nakamura *et al.*,[22] which was inferred from the NMR measurements. This difference may arise from the interpretation of the nuclear spin-lattice relaxation based on Ref. 1, $T_1^{-1}\sim\sqrt{\chi_Q(T)}$. As we have shown in Sec. IV this relation is certainly not valid in Y(Sc)Mn_2. Then taking the measured value[8] for $\hbar\omega_{\rm SF}(Q)=5.00$ meV at 9 K and the estimated above ratio χ_Q^{-1}/c_C, we can evaluate the characteristic energy $\hbar\Gamma\ c_C=7.20$ meV and SF temperature $T_m=\hbar\omega_m/k_B\alpha_0=70$ K. This value for T_m inferred from neutron-scattering experiments[8] is in good agreement with the magnetic measurements in $Y_{0.95}Sc_{0.05}Mn_2$,[9] where an anomalous temperature dependence of the uniform magnetic susceptibility caused by SF's was reported about 70 K.

It is also possible to estimate the temperature T_L^* characterizing the crossover to the LM regime of SF's. First, we assume that in the temperature range $9<T<300$ K there is no significant change of the Curie constant and then directly get $T_L^*=88$ K from Eq. (39) using the measured linearly temperature dependent $\hbar\omega_{\rm SF}(\vec{Q})$.[8] We can also independently estimate T_L^* from Eq. (40). Extrapolating the linear temperature of $\hbar\omega_{\rm SF}(\vec{Q})$ reported in Ref. 8 to higher temperatures we evaluate the parameter $z=0.05$. Substituting it into Eq. (40) we arrive at the previous estimate for T_L^* which shows that the assumptions made above are reasonable.

Using these estimates we arrive at the following conclusions relating the SF behavior of the Y(Sc) Mn_2 system. First, the estimated value of $\chi_Q^{-1}/c_C<1$ at low temperatures presents strong evidence for the well-defined soft-mode behavior of SF's in the temperature range $T\leqslant T_L^*\sim100$ K. At higher temperatures Y(Sc) Mn_2 may be regarded as a LM system. This value of T_L^* together with relatively high-temperature Θ_L, compared to the Curie temperatures of weak itinerant ferromagnets (see Table I), suggests that this system is rather far from the second-order transition, and the first-order transition exhibited by this system is probably dominated by secondary mechanisms, e.g., by magnetoelastic coupling.

Second, our estimate of the SF temperature, which defines the low-temperature specific heat[10] and the effective mass of Fermi quasiparticles, shows that T_m is about 100 times less than the Fermi degeneracy temperature in conventional 3*d* metals and confirms the previous treatments[9,10] of Y(Sc)Mn_2 as a 3*d* heavy fermion system.

VII. SUMMARY

To summarize, we have analyzed the fluctuation effects in itinerant electron magnets with antiferromagnetic instabilities in different SF regimes defined with respect to the spatial dispersion of the dynamical susceptibility. To account for the influence of frustration reported in Y(Sc)Mn_2,[8,9] we used a simple model for an anisotropic and flat SF spectrum.[10] In the relatively low-temperature soft-mode regime the magnetic properties are shown to be defined by strongly $\vec{q}$-dependent soft-mode SF's. Strong coupling of SF's caused by zero-point effects makes it impossible to apply a conventional SF theory[1] based on the weak-coupling constraint. To calculate the temperature dependences of the staggered susceptibility and local magnetic moments we used the recently worked out soft-mode theory of SF's,[15,16] which accounts for strong spin anharmonicity arising due to zero-point SF's.

We have shown that with an increase of temperature the role of spatial dispersion of SF's decreases, and above some temperature T_L^* a crossover to the localized moments regime takes place, where SF's are almost dispersionless and localized in real space. Based on the fluctuation dissipation theorem we have shown that the saturation of thermally excited local magnetic moments gives rise to the Curie-Weiss magnetic susceptibility affected by quantum SF effects. As we have pointed out the overall SF behavior in the soft-mode and localized moments regime is determined by the SF temperature T_m related to the effective mass of Fermi quasiparticles. In the heavy fermion systems the temperature T_m is shown to be rather low, which favors the localized moments regime. This is probably realized in the $Y(Sc)Mn_2$ system as it follows from the neutron-scattering data.[8] Finally, we would like to emphasize that the presented description of SF's in itinerant magnets interpolating between the soft-mode and localized moments regimes is based on the phenomenological arguments resulting from the fluctuation-dissipation theorem. The main problem of the unified theory of itinerant magnetism—to work out thermodynamics valid both in the soft-mode and localized moments regimes—is still open for future investigations.

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