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Reentrant phenomena in a three-dimensional spin-1 planar ferromagnet with easy-axis single-ion anisotropy

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ABSTRACT

The two-time Green function method is employed to explore the phase diagram and the magnetic-field-induced quantum criticality of a three-dimensional spin-one planar ferromagnet with easy-axis single-ion anisotropy. We adopt the Tyablikov and Anderson-Callen decouplings for higher order exchange and single-ion anisotropy Green functions, respectively. The central finding is that, within a characteristic range of the anisotropy parameter values, reentrant phenomena occur in the phase diagram close to the quantum critical point producing a sensible change of the conventional quantum critical scenario.

1. Introduction

The Heisenberg model with different types of exchange anisotropies has been the subject of intensive studies to describe the properties of several magnetic compounds. In this context, experiments have shown that in complex magnetic materials crystal anisotropy fields exist which play an important role in determining their thermodynamics properties [1–7]. Theoretically, a suitable description of such materials can be performed including, in the Heisenberg model with exchange anisotropy, additional anisotropic crystal fields as easy-plane or easy-axis single-ion anisotropy [6,8–12]. In this context, the planar ferromagnet (PFM), i.e. a XXZ model with in-plane exchange interactions greater than the longitudinal ones, is of broad interest as a starting point due to its numerous applications [13–23]. This model, without any further anisotropy, exhibits a magnetic-field induced quantum phase transition (QPT) and the related quantum critical properties, including the low-temperature phase diagram, have been studied with different approaches [13–23]. It is, however, inadequate for a more accurate study of magnetic materials with a complex crystalline structure and may be very useful for practical situations to investigate the effects of single-ion anisotropy on the magnetic-field-induced quantum criticality (QC) of PFM.

In the present work we perform such a study by using the two-time Green function (GF) method at the level of the Tyablikov decoupling (TD) [24,25] for the exchange interaction contribution, and the Anderson-Callen decoupling (ACD) [26] for the single-ion anisotropy, to close the chain of equations of motion. Interestingly we will show that, within this approximation, a non-conventional quantum critical scenario involving reentrant phenomena emerges when the easy-axis crystal-field anisotropy parameter ranges within a peculiar interval of values.

Reentrant phenomena are found to occur in the phase diagrams of a wide variety of materials stimulating recently a lot of experimental and theoretical interest. The term "reentrant" refers to a phase transition to an ordered phase (OP) at some temperature followed by a transition to a disordered phase (DP) at a lower temperature. Reentrant phase diagrams have been observed, for instance, in complex ferromagnetic and antiferromagnetic systems with different types of anisotropies and applied magnetic fields, [27–29], superconducting compounds [30–33], liquid crystals [34] and in many other systems [35–39]. From a theoretical point of view it is not easy to find suitable models providing reentrancies in the phase diagrams so that the proper description of reentrant phenomena poses challenges to microscopic physics for a variety of condensed matter systems. In order to construct an appropriate model, the strategy is to consider in the Hamiltonian suitable competing terms which are expected to generate the microscopic mechanism underlying the specific nature of the reentrant behavior under study. In spite of the intrinsic difficulties typical of these complex phenomena, different mechanisms for reentrance in the phase diagrams have been suggested depending on the physical situations. As selected examples, we mention here models for solid hydrogen with quantum fluctuation-induced reentrance [40], semiconductors with reentrant ferromagnetism [41], reentrant charging energy effects in granular superconductors [42], spin-glass [43] and

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random-bond spin lattices [44] with frustration, doped lamellar antiferromagnets [36], complex spin systems with uniform [45] and random [46] fields with single-ion anisotropy. Here, we will show that the PFM with easy-axis single-ion anisotropy in the presence of a longitudinal magnetic field provides an instructive example for the possible occurrence of reentrant phenomena in the influence domain of magnetic-field induced QCPs. The outcome is particulary interesting because it points out that the competition between the quantum critical fluctuations and the single-ion anisotropy ones is responsible for the reentrance in the phase diagram. In spite of the lack of a direct experimental evidence of this reentrant mechanism, we believe that it may be adopted in exploring other magnetic systems which exhibit a field-induced QCP at fixed values of the single-ion anisotropy parameter.

The paper is organized as follows. In Section 2 we introduce the spin model and derive the basic relations arising from the GF framework. Section 3 is devoted to obtain the phase diagram of the model and to point out its peculiar reentrant structure by variation of the anisotropy parameter via both numerical findings and analytical estimates. In Section 4 QC for selected values of the single-ion anisotropy parameter involving reentrant phenomena is analyzed in detail. Finally, in Section. 5, concluding remarks are drawn.

2. The model and the two-time Green's function framework

The PFM with single-ion anisotropy here considered is described by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j=1}^{N}[J_{ij}(S_i^xS_j^x+S_i^yS_j^y)+K_{ij}S_i^zS_j^z]-D\sum_{i=1}^{N}(S_i^z)^2-h\sum_{i=1}^{N}S_i^z, \tag{1}$$

where $S_i^\alpha(\alpha=x,y,z)$ are the components of the vectorial spin operator $\vec{S}_i$ at site i of a three-dimensional cubic lattice with N sites and $[S_i^\alpha,S_j^\beta]=i\varepsilon_{\alpha,\beta,\gamma}\delta_{ij}S_i^\gamma$ ($\varepsilon_{\alpha,\beta,\gamma}$ is the usual Levi–Civita symbol) are the spin commutation relations. The FM exchange couplings J_{ij} and K_{ij} (with $J_{ii}=K_{ii}=0$) satisfy the inequality $K_{ij}<J_{ij}$, D is the single-ion uniaxial anisotropy parameter and h is the applied longitudinal magnetic field. We focus here on the easy-axis anisotropy with $D>0$. The easy-plane anisotropy case, with $D<0$, has been discussed in [47].

We now introduce the retarded two-time GF for commutator [24,25]

$$G_{ij}(t-t') = -i\theta(t-t')\langle[S_i^+(t-t'),S_j^-]\rangle \equiv \langle\langle S_i^+(t-t');S_j^-\rangle\rangle, \tag{2}$$

where $A(t)=e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}$, $\theta(x)$ is the step function, $\langle\cdots\rangle=\mathrm{Tr}(\cdots e^{-\beta\mathcal{H}})/\mathrm{Tr}(e^{-\beta\mathcal{H}})$ denotes a canonical average and $\beta=1/T$ is the inverse temperature.

The equation of motion for the time Fourier transform $G_{ij}(\omega)=\int_{-\infty}^{\infty}dt\, e^{-i\omega t}G_{ij}(t)\equiv\langle\langle S_i^+|S_j^-\rangle\rangle_\omega$ reads

$$(\omega-h)\langle\langle S_i^+|S_j^-\rangle\rangle_\omega = 2m\delta_{ij}-\sum_h[\langle\langle J_{hi}S_i^zS_h^+ - K_{hi}S_h^zS_i^+|S_j^-\rangle\rangle_\omega]+D\langle\langle S_i^zS_i^++S_i^+S_i^z|S_j^-\rangle\rangle_\omega, \tag{3}$$

where $m=\langle S_i^z\rangle$ is the longitudinal magnetization per spin.

For the higher order GFs in Eq. (3) we assume the TD [24,25] $\langle\langle S_h^zS_k^+|S_j^-\rangle\rangle_\omega\simeq\langle S_h^z\rangle\langle\langle S_k^+|S_j^-\rangle\rangle_\omega$ for the exchange interaction and the ACD [26] for spin-one to decouple the single-ion anisotropy term, $\langle\langle S_i^zS_i^++S_i^+S_i^z|S_j^-\rangle\rangle_\omega\simeq\langle S_i^z\rangle\langle(S_i^z)^2\rangle\langle\langle S_i^+|S_j^-\rangle\rangle_\omega$.

Then, working with the Fourier transforms $G_{ij}(\omega)=(1/N)\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)]G_\perp(\mathbf{k},\omega)$ and $X(\mathbf{k})=\sum_{\mathbf{r}}X(|\mathbf{r}|)e^{i\mathbf{k}\cdot\mathbf{r}}$ (where $X=J,K$), with the wave-vectors $\mathbf{k}$ ranging within the first Brillouin zone (1BZ), the equation of motion for the transverse GF in the $(\mathbf{k},\omega)$-Fourier space $G_\perp(\mathbf{k},\omega)$ can be easily diagonalized providing the solution

$$G_\perp(\mathbf{k},\omega)=\frac{2m}{\omega-\omega_{\mathbf{k}}}, \tag{4}$$

with $\omega\to\omega+i\varepsilon$ $(\varepsilon\to0^+)$ for retarded GF. In this equation

$$\omega_{\mathbf{k}}=\omega_0+m\,[J(0)-J(\mathbf{k})] \tag{5}$$

is the energy spectrum of the undamped spin-excitations and

$$\omega_0=h-m[J(0)-K(0)-\langle(S_i^z)^2\rangle D] \tag{6}$$

provides the energy gap.

Using the identity $(S_i^z)^2=2-S_i^z-S_i^-S_i^+$, the spectral theorem [24,25] provides

$$\langle(S_i^z)^2\rangle=2-m(1+2\Phi), \tag{7}$$

with

$$\Phi=\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{e^{\beta\omega_{\mathbf{k}}}-1}\overset{N\to\infty}{=}\int_{1BZ}\frac{d^3k}{(2\pi)^3}\frac{1}{e^{\beta\omega_{\mathbf{k}}}-1}. \tag{8}$$

Then, the energy gap can be conveniently written as

$$\omega_0=h-mH(m), \tag{9}$$

where

$$H(m)=J(0)-K(0)-2D+mD(1+2\Phi). \tag{10}$$

For next developments it is essential to obtain an explicit expression for m in terms of correlation functions related to the original GF. This can be obtained by using the Callen method [48] originally proposed for the isotropic Heisenberg model. It is based on the introduction of the generalized GF $\langle\langle S_i^+(t-t');e^{aS_j^z}S_j^-\rangle\rangle$ where a is an arbitrary parameter to be set to zero at the end of calculations. For our anisotropic XXZ model with spin $S=1$ the suitable relation for m is [47]

$$m=1-\Phi+\frac{3}{(1+\Phi^{-1})^3-1}=B(\Phi) \tag{11}$$

with the asymptotic expansions for the function

$$B(\Phi)\simeq\begin{cases}1-\Phi+3\Phi^3+\cdots, & \Phi\ll1\\ \frac{2}{3\Phi}\left(1-\frac{1}{2\Phi}+\frac{1}{6\Phi^2}+\cdots\right), & \Phi\gg1,\end{cases} \tag{12}$$

which will play a relevant role. Eqs. (8)–(11) constitute a set of self-consistent equations to determine $G_\perp(\mathbf{k},\omega)$, $\omega_{\mathbf{k}}$, m, and other relevant thermodynamic quantities [24,25] as functions of T and h, for fixed single-ion anisotropy parameter D.

The basic quantity to explore the static and dynamic in-plane properties of our spin model is the transverse GF (4). This provides the dynamical transverse susceptibility

$$\chi_\perp(\mathbf{k},\omega)=-G_\perp(\mathbf{k},\omega)=\frac{2m}{\omega_{\mathbf{k}}-\omega}, \tag{13}$$

and the static one

$$\chi_\perp(T,h)=\chi_\perp(\mathbf{k}=0,\omega=0)=\frac{2m}{\omega_0}, \tag{14}$$

where stability $(\chi_\perp>0)$ requires $\omega_0\geq0$, $\omega_0=0$ defining the stability boundary. By inspection of Eq. (9), it follows that the equality $\omega_0=0$ is physically possible for $h>0$ and $m>0$ only if $H(m)>0$, which is the basic condition for the existence of a field-induced QCP.

When $m(T,h)$ is known, the longitudinal susceptibility will be given by $\chi_\parallel(T,h)=(\partial m/\partial h)_T$ and other relevant quantities, as the free energy, specific heat, etc. can be easily derived by using known thermodynamic relations [24,25]. One can also obtain the transverse correlation length $\xi_\perp$ which, for short-range