ARTICLE IN PRESS

Physica B xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Reentrant behaviors in the phase diagram of spin-1 planar ferromagnet with single-ion anisotropy

I. Rabuffo[a], L. De Cesare[a], A. Caramico D'Auria[b], M.T. Mercaldo[a,*]

[a] Dipartimento di Fisica "E. R. Caianiello", Università di Salerno and CNISM, Unità di Salerno, I-84084 Fisciano, Salerno, Italy
[b] Dipartimento di Fisica, Università di Napoli Federico II, I-80125 Napoli, Italy

ARTICLE INFO

Keywords:
Quantum criticality
Planar ferromagnet
Single-ion anisotropy
Reentrant phenomena
Two-time Green's functions

ABSTRACT

We used the two-time Green function framework to investigate the role played by the easy-axis single-ion anisotropy on the phase diagram of ($d > 2$)-dimensional spin-1planar ferromagnets, which exhibit a magnetic field induced quantum phase transition. We tackled the problem using two different kind of approximations: the Anderson-Callen decoupling scheme and the Devlin approach. In the latter scheme, the exchange anisotropy terms in the equations of motion are treated at the Tyablikov decoupling level while the crystal field anisotropy contribution is handled exactly. The emerging key result is a reentrant structure of the phase diagram close to the quantum critical point, for certain values of the single-ion anisotropy parameter. We compare the results obtained within the two approximation schemes. In particular, we recover the same qualitative behavior. We show the phase diagram, close to the field-induced quantum critical point and the behavior of the susceptibility for different values of the single-ion anisotropy parameter, enhancing the differences between the two different scenarios (i.e. with and without reentrant behavior).

1. Introduction

The study of quantum magnetic systems is a very active research subject in condensed matter physics [1,2]. Experiments have shown that, in complex magnetic materials, crystal anisotropy fields exist which play an important role in determining their thermodynamics properties [2–5]. 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 [2,6–10]. 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 [11–20]. 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 [11–20]. It is, however, inadequate for a more accurate study of magnetic materials with a complex crystalline structure. Indeed in recent years, the quantum criticality in magnetic systems with different types of anisotropies [16–21], in particular single-ion anisotropy (SIA) measured by a parameter D, have attracted a great deal of experimental [22–26] and theoretical interest [27–32].

In this paper we use the two-time Green function (GF) method to study the PFM and the influence of SIA on its magnetic field induced QPT. This method has been proved through several decades to be one of the most powerful tools in the theory of magnetism, but it has attracted less attention in exploring quantum critical properties close to a QPT of spin models with crystal-field anisotropies. Usually, for conventional finite-temperature phase transitions one uses decouplings for single-sites higher order GFs in the equations of motion, as the Anderson-Callen decoupling (ACD) [35], which were proved to be adequate only for sufficiently small D [36,2]. For the Heisenberg model with SIA, Devlin [36] showed explicitly that the difficulties arising for large D can be overcome since the single-ion higher order terms in the equations of motion can be treated exactly. Indeed he found that for spin $S \geq 1$ the problem can be reduced to a closed system of $2S$ equations of motion. In the present work we are going to use both approaches to determine the phase boundary for the spin-($S = 1$) XXZ model with additional single-ion anisotropy, and we compare the results.

Remarkably, within both approximation schemes, we find a non-conventional quantum critical scenario involving reentrant phenomena, which appears when the easy axis crystal field exceeds a certain threshold value. These 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

* Corresponding author.
E-mail address: mtm@physics.unisa.it (M.T. Mercaldo).

https://doi.org/10.1016/j.physb.2017.10.064
Received 30 June 2017; Accepted 16 October 2017

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 [37–39], superconducting compounds [40–42] and in many other systems [43–47].

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

We study the following Heisenberg Hamiltonian with magnetic anisotropies:

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

where $S_i^\alpha(\alpha = x, y, z)$ are the spin components at site i of a d-dimensional hypercubic lattice with N sites and unit lattice spacing, J_{ij} and K_{ij} (with $J_{ii} = K_{ii} = 0$) are the FM exchange couplings, $D > 0$ is the easy-axis SIA parameter and H is the applied magnetic field along the longitudinal direction. For $D = 0$, the anisotropic exchange interactions may compete providing: the easy-axis FM if $K_{ij} > J_{ij}$ with the extreme limit $J_{ij} = 0$ (Ising model); the isotropic Heisenberg model if $K_{ij} = J_{ij}$; and the easy-plane (or planar) ferromagnet if $K_{ij} < J_{ij}$, with the extreme limit $K_{ij} = 0$ defining the XY model. We limit ourselves to the easy-plane exchange ($K_{ij} < J_{ij}$) case [14,17,20].

We now introduce the retarded two-time GF [33,34]

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

where $A(t) = e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}$, $\theta(x)$ is the step function, $\langle\cdots\rangle = \mathrm{Tr}(\cdots e^{-\beta\mathcal{H}})/Tr(e^{-\beta\mathcal{H}})$ 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

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

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

The equation of motion for $G_{ij}(\omega)$ is not in a closed form, due to the presence of higher order GFs. In order to get a closed equation of motion for $G_{ij}(\omega)$, the higher order Green's functions on the right hand side of Eq. (3) have to be properly decoupled. We have used two different decoupling schemes [33–36] and in the present paper we want to stress the differences in the phase diagram obtained.

2.1. "Devlin" framework

Within this approximation scheme we introduce another GF in order to treat the SIA term exactly

$$\Gamma_{ij}(\omega) = \langle\langle A_i|S_j^-\rangle\rangle_\omega, \quad (4)$$

where $A_i = S_i^zS_i^+ + S_i^+S_i^z$. The equation of motion for Γ_{ij} reads

$$(\omega - H)\Gamma_{ij}(\omega) = 2q\delta_{ij} - \sum_h\langle\langle J_{hi}q_i^zS_h^+ - K_{hi}S_h^zA_i|S_j^-\rangle\rangle_\omega + -\sum_h J_{ih}\langle\langle(S_i^+)^2S_h^-|S_j^-\rangle\rangle_\omega + DG_{ij}(\omega), \quad (5)$$

with $q_i^z = 3(S_i^z)^2 - 2$ and $q = \langle q_i^z\rangle = 3\langle(S^z)^2\rangle - 2$.

Eqs. (3) and (5) are exact but they still do not constitute a closed system of equations for $G_{ij}(\omega)$ and $\Gamma_{ij}(\omega)$. According to the suggestion by Devlin [36] we adopt, for the exchange contribution in Eqs (3) and (5), the simplest Tyablikov-like decouplings

$$\langle\langle S_h^zS_k^+|S_j^-\rangle\rangle_\omega \simeq \langle S_h^z\rangle\langle\langle S_k^+|S_j^-\rangle\rangle_\omega,$$
$$\langle\langle q_i^zS_h^+|S_j^-\rangle\rangle_\omega \simeq \langle q_i^z\rangle\langle\langle S_h^+|S_j^-\rangle\rangle_\omega,$$
$$\langle\langle(S_i^+)^2S_h^-|S_j^-\rangle\rangle_\omega \simeq 0, \quad (6)$$

which satisfy consistently the criterion to neglect the motion of spin at different sites as in the usual Tyablikov decoupling. In contrast, for the crystal-field anisotropy term with identical indices, we use exact transformations based on well known identities for spin-1 operators [2,36,48].

We stress that the Tyablikov-like approximations made in Eq. (6) for the exchange higher order terms in the equations of motion have been extensively used in literature providing reliable results in a clear way. Physically, with the first two decouplings we neglect correlations between spins located in different sites. Besides, the last approximation, suggested originally by Devlin [36], is quite reasonable since the operators S_i^+ and S_i^- represent the transverse motion of the spins and only S_i^z and q_i^z have finite ensemble averages, especially close to a QCP.

Working in the wave-vector-frequency $(\mathbf{k}, \omega)$-space ($\mathbf{k}$ ranging in the first Brillouin zone (1BZ)), with $G_{ij}(\omega) = \frac{1}{N}\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\vec{r_i} - \vec{r_j})]G_\perp(\mathbf{k}, \omega)$ and $J(\mathbf{k}) = \sum_{\vec{r}}J(|\vec{r}|)e^{i\mathbf{k}\cdot\vec{r}}$ (and analogously fot $\Gamma_{ij}(\omega)$ and K, respectively), we obtain for $G(\mathbf{k}, \omega)$ and $\Gamma(\mathbf{k}, \omega)$ the coupled equations of motion

$$\begin{cases}[\omega - H + m(J(\mathbf{k}) - K(0))]G(\mathbf{k}, \omega) - D\Gamma(\mathbf{k}, \omega) = 2m\\ [-D + qJ(\mathbf{k})]G(\mathbf{k}, \omega) + [\omega - H - mK(0)]\Gamma(\mathbf{k}, \omega) = 2q.\end{cases} \quad (7)$$

This constitutes now a closed system of two linear algebraic equations whose solutions, after some algebra, can be written in the polar form

$$G(\mathbf{k}, \omega) = \sum_{\nu=1}^{2}\frac{\lambda_\nu(\mathbf{k})}{\omega - \omega_\nu(\mathbf{k})}, \quad (8)$$

$$\Gamma(\mathbf{k}, \omega) = \sum_{\nu=1}^{2}\frac{\beta_\nu(\mathbf{k})}{\omega - \omega_\nu(\mathbf{k})}. \quad (9)$$

Here

$$\omega_{1,2}(\mathbf{k}) = (H + mK(0)) + \frac{1}{2}\{-mJ(\mathbf{k}) \pm \sqrt{\Delta(\mathbf{k})}\}, \quad (10)$$

are the dispersion relations (or resonance frequencies), with

$$\Delta(\mathbf{k}) = (mJ(\mathbf{k}))^2 + 4D^2\left(1 - q\frac{J(\mathbf{k})}{D}\right) \geq 0 \quad (11)$$

and

$$\lambda_{1,2}(\mathbf{k}) = m \pm \frac{1}{\sqrt{\Delta(\mathbf{k})}}(2qD - m^2J(\mathbf{k})), \quad (12)$$

$$\beta_{1,2}(\mathbf{k}) = q \pm \frac{1}{\sqrt{\Delta(\mathbf{k})}}(2mD - mqJ(\mathbf{k})). \quad (13)$$

From previous findings it is evident that for exploring the thermodynamics of our model within the GFs framework, one needs to know $m = \langle S^z\rangle$ and $q = 3\langle(S^z)^2\rangle - 2$ as functions of T and of the other parameters involved (such as H, J, K, D). This can be achieved by using appropriate spin-operator identities

$$S_i^-S_i^+ = 2 - S_i^z - (S_i^z)^2 \quad (14)$$

$$S_i^-A_i = 2 + S_i^z - 3(S_i^z)^2 = S_i^z - q_i^z, \quad (15)$$

for spin $S = 1$ and then determining the basic correlation functions via the spectral theorem [33,20]. Hence we get the exact relations

$$\langle S_i^-S_i^+\rangle = \frac{4}{3} - \frac{q}{3} - m \quad (16)$$

$$\langle S_i^-A_i\rangle = m - q. \quad (17)$$