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Minireview

Phase diagrams of the transverse Ising antiferromagnet in the presence of the longitudinal magnetic field

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ABSTRACT

In this paper we study the critical behavior of the two-dimensional antiferromagnetic Ising model in both uniform longitudinal (H) and transverse (Ω) magnetic fields. Using the effective-field theory (EFT) with correlation in single site clusters we calculate the phase diagrams in the $H - T$ and $\Omega - T$ planes for the square lattice. We have only found second order phase transitions for all values of fields and reentrant behavior was not observed.

Contents

1. Introduction

In the last decade there has been an increasing number of works dealing with magnetic models to study quantum phase transitions. In particular, considerable interest has been directed to the transverse Ising model (TIM) used to describe a variety of physical systems [1–3]. It was originally introduced by de Gennes [1] as a pseudospin model for hydrogen-bonded ferroelectrics such as KH_2PO_4 in the order–disorder phenomenon with tunneling effects. It has been successfully used to also study a number of problems of phase transitions associated with order–disorder phenomena in other systems [4,5]. It provides a good description to analyze some real anisotropic magnetic materials in a transverse field [6].

Theoretically, various methods have been employed to study the criticality of the TIM such as renormalization group (RG) [7], effective field theory (EFT) [8–10], mean field theory (MFA) [11], cluster variation method (CVM) [12], pair approximation (PA) [13], Monte Carlo (MC) simulations [14], and so on. The critical behavior of the one-dimensional TIM has already been established through exact results, where the ground-state energy, the elementary excitations and the correlation functions were obtained [15]. The TIM is among the simplest conceivable classes of quantum models in statistical mechanics to study quantum phase transitions [16,17]. The ferromagnetic TIM has been studied intensively [7–10,13,14]. The critical and thermal properties of the ferromagnetic and antiferromagnetic TIM are equivalent, but the properties of

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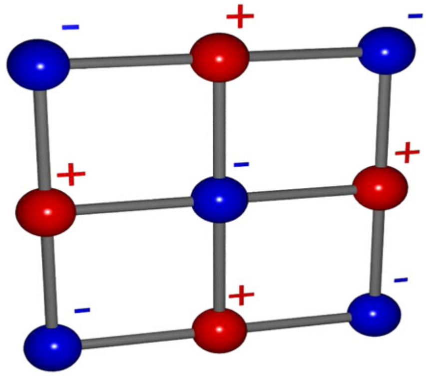

Fig. 1. Ground state of the quantum Ising antiferromagnet on an square lattice described by the Hamiltonian given in Eq. (1).

these two models are very different at not null longitudinal field ($H \neq 0$). For example, the ground-state phase transition in the ferromagnetic TIM is smeared out by the longitudinal field in contrast to the antiferromagnetic TIM for which the phase diagram remains qualitatively the same at $H \neq 0$.

Experimental investigations on the metamagnetic compounds such as $FeBr_2$ and $FeCl_2$ [18] and $Ni(NO_3)_2 2H_2O$ [19,20], under hydrostatic pressure, have been performed. For example, in the $FeBr_2$ compound a sharp peak was observed in magnetization measurements under a field inclined by 33° with the c axis (perpendicular to the plane) of the crystal. They concluded that the peak was affected by the ordering of the planar spin components. It is obvious that the field can be decomposed into the longitudinal and transverse components. The model is described by the Ising Hamiltonian to which is added a term which represents the effects of the transverse field part. Due to the non-commutativity of the operators in the Hamiltonian, deriving eigenvalues is a very difficult problem. Therefore, many theoretical methods have been used to investigate this system [21–25].

From a theoretical point of view it is known that the effect of the transverse field in the Ising model TIM is to destroy the long-range order of the system. Many approximate methods [7–14,21–30] have been used to study the critical properties of this quantum model. Some years ago, a simple and versatile scheme, denoted by the differential operator technique [31], was proposed and has been applied exhaustively to study a large variety of problems. In particular, this technique was used to treat the criticality of the TIM [32] obtaining satisfactory quantitative results in comparison with more sophisticated methods (for example, MC). This method is used in conjugation with a decoupling procedure which ignores all high-order spin correlations (EFT). The EFT included correlations through the use of the van der Waerden identity and provided results which are much superior than the ones coming from the MFA. The TIM was first studied by using EFT [32] for the case of spin $S = 1/2$, and generalized [26] for arbitrary spin-$S \geqslant 1/2$.

On the other hand, the critical and thermal properties of the transverse Ising antiferromagnet in the presence of a longitudinal magnetic field have been somewhat studied in the literature [33,34]. Using the classical approach MFA and the density-matrix renormalization-group method (DMRG) [34], the ground state phase diagram in the $(H - \Omega)$ plane was studied for a one-dimensional lattice. A critical line separates the antiferromagnetic (AF) phase with long-range order (LRO) from the paramagnetic (P) phase with uniform magnetization. The quantum critical point $\delta_c \equiv \left(\frac{\Omega}{J}\right)_c$ decreases as $h_c \equiv \left(\frac{H}{J}\right)_c$ increases, and is null at $h_c = 2.0$. The MFA approach does not give the correct qualitative description of the critical line [34]. Firstly, the quantum fluctuations shift the ground critical point $\delta_c = 1.0$ to $\delta_c = 2.0$ at $h = 0$ which underestimates the critical value. Second, the form of the critical line shows an incorrect behavior around the critical point $h_c = 2.0$.

By using the EFT approach, Neto and Ricardo de Sousa [35] have studied the ground-state phase diagram of this quantum model on two-dimensional (honeycomb ($z = 3$) and square ($z = 4$)) lattices, and discussed the possibility of the existence of a reentrant behavior around the $h_c = z$ critical value. The spin correlation effects are partially taken into account in EFT, while they are entirely neglected in MFA. The differences of results given by using EFT and MFA show that the spin correlation is important on the phase diagram. The ground-state phase diagram in the $(H - \Omega)$ plane is qualitatively similar to the results of Fig. 1 in Ref. [34], but the reentrant behavior found by MFA occurs near $h_c = z$.

In the present paper, using EFT we investigate the quantum phase transitions of the Ising antiferromagnet in both external longitudinal and transverse fields. This work is organized as follows. In Section 2 we outline the formalism and its application to the transverse Ising antiferromagnet in the presence of a longitudinal magnetic field; in Section 3 we discuss the results; and finally, in Section 4 we present our conclusions.

2. Model and formalism

The model studied in this work is the nearest-neighbor (nn) Ising antiferromagnet in a mixed transverse and longitudinal magnetic field divided into two equivalent interpenetrating sublattices A and B, that is described by the following

Hamiltonian

$$H = J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - H\sum_i \sigma_i^z - \Omega\sum_i \sigma_i^x, \tag{1}$$

where J is the AF exchange coupling, $\langle i,j\rangle$ denoted the sum over all pairs of nearest-neighbor spins (z) on a d-dimensional lattice (here we treat the square lattice), σ_i^ν is the $\nu(=x,z)$ component of the spin-1/2 Pauli operator at site i, and $H(\Omega)$ is the longitudinal (transverse) magnetic field.

The σ_i^x and σ_i^z spin-1/2 Pauli operators do not commute, then a nonzero field (Ω) transverse to the spin direction causes quantum tunneling between the spin-up and spin-down eigenstates of σ_i^z and quantum spin fluctuations. These fluctuations decrease the critical temperature T_c at which the spins develop long-range order. At a critical field Ω_c, T_c vanishes, and a quantum phase transition between the AF ordered state and a quantum paramagnetic state occurs. To the best of our knowledge, the model (1) at finite temperature ($T\neq 0$) has not yet been examined in the literature. In particular, the ground-state phase diagram was studied by Neto and Ricardo de Sousa [35]. In this work we generalize it to analyze the field effects at finite temperature by using EFT.

The ground-state of the model (1) is characterized by an antiparallel spin orientation in the horizontal and vertical directions and so it exhibits Néel order within the initial sublattices A and B (see Fig. 1), that is denoted by the AF state.

The competition between the antiferromagnetic exchange field leads to interesting properties in the phase diagram. In particular, the model (1) has an AF (ordered) phase in the presence of a field, with a decreasing transition temperature as the field intensity increases, where at $T=0$ (ground-state) a second-order transition occurs at both critical fields with $H_c(=zJ)$ and Ω_c.

To treat the model (1) on two-dimensional lattices by the EFT approach, we consider a simple example of a cluster on a lattice consisting of a central spin and z perimeter spins being the nearest-neighbors of the central one. The nearest-neighbor spins are substituted by an effective field produced by the other spins, which can be determined by the condition that the thermal average of the central spin is equal to that of its nearest-neighbor ones. The Hamiltonian for this cluster is given by

$$\mathcal{H}_{1A} = \left(J\sum_{\delta}^{z}\sigma_{(1+\delta)B}^z - H\right)\sigma_{1A}^z - \Omega\sigma_{1A}^x, \tag{2}$$

and

$$\mathcal{H}_{1B} = \left(J\sum_{\delta}^{z}\sigma_{(1+\delta)A}^z - H\right)\sigma_{1B}^z - \Omega\sigma_{1B}^x, \tag{3}$$

where A and B denote the sublattice.

From the Hamiltonians (2) and (3), we obtain the average magnetizations in sublattices A, $m_A=\langle\sigma_{1A}^z\rangle$, and B, $m_B=\langle\sigma_{1B}^z\rangle$, using the approximate Callen–Suzuki relation [32], which are given by

$$m_A = \left\langle \frac{H-a_{1A}}{\sqrt{(H-a_{1A})^2+\Omega^2}}\tanh\beta\sqrt{(H-a_{1A})^2+\Omega^2}\right\rangle, \tag{4}$$

and

$$m_B = \left\langle \frac{H-a_{1B}}{\sqrt{(H-a_{1B})^2+\Omega^2}}\tanh\beta\sqrt{(H-a_{1B})^2+\Omega^2}\right\rangle, \tag{5}$$

where $a_{1A}=J\sum_\delta^z \sigma_{(1+\delta)B}^z$ and $a_{1B}=J\sum_\delta^z \sigma_{(1+\delta)A}^z$.

Now, using the identity $\exp(\alpha D_x)F(x)=F(x+a)$ (where $D_x=\frac{\partial}{\partial x}$ is the differential operator) and the van der Waerden identity for the two-state spin system (i.e., $\exp(a\sigma_i^z)=\cosh(a)+\sigma_i^z\sinh(a)$) Eqs. (4) and (5) are rewritten as

$$m_A = \left\langle \prod_{\delta\neq 0}^{z}(\alpha_x+\sigma_{(1+\delta)B}^z\beta_x)\right\rangle F(x)|_{x=0}, \tag{6}$$

and

$$m_B = \left\langle \prod_{\delta\neq 0}^{z}(\alpha_x+\sigma_{(1+\delta)A}^z\beta_x)\right\rangle F(x)|_{x=0}, \tag{7}$$

with

$$F(x) = \frac{H-x}{\sqrt{(H-x)^2+\Omega^2}}\tanh\beta\sqrt{(H-x)^2+\Omega^2}, \tag{8}$$

where $\alpha_x = \cosh(JD_x)$ and $\beta_x = \sinh(JD_x)$. Eqs. (6) and (7) are expressed in terms of multiple spin correlation functions. The problem becomes unmanageable when we try to treat exactly all boundary spin–spin correlation functions present in Eqs. (6) and (7). In this work we use a decoupling of the right-hand sides in Eqs. (6) and (7), namely

$$\left\langle \sigma_{iA}^z \sigma_{jB}^z \ldots \sigma_{lA}^z \right\rangle \backsimeq m_A m_B \ldots m_A, \tag{9}$$

where $i \neq j \neq \cdots \neq l$ and $m_\mu = \left\langle \sigma_{i\mu}^z \right\rangle (\mu = A, B)$. The approximation (9) neglects correlations between different spins but takes relations such as $\left\langle \left(\sigma_{i\mu}^z\right)^2 \right\rangle = 1$ exactly into account, while in the usual MFA all the self- and multispin correlations are neglected. Using the approximation (9), Eqs. (6) and (7) are rewritten as

$$m_A = \sum_{p=0}^{z} A_p(T_N, H, \Omega) m_B^p, \tag{10}$$

and

$$m_B = \sum_{p=0}^{z} A_p(T_N, H, \Omega) m_A^p, \tag{11}$$

with

$$A_p(T_N, H, \Omega) = \frac{z!}{p!(z-p)!} \alpha_x^{z-p} \beta_x^p F(x)|_{x=0}, \tag{12}$$

where the coefficients $A_p(T_N, H, \Omega)$ are obtained by using the relation $\exp(\alpha D_x)F(x) = F(x + a)$.

In terms of the uniform $m = \frac{1}{2}(m_A + m_B)$ and staggered $m_s = \frac{1}{2}(m_A - m_B)$ magnetizations, and near the critical point we have $m_s \to 0$ and $m \to m_0$, the sublattice magnetization m_A expanded up to linear order in m_s (order parameter) is given by

$$m_A = X_0(T_N, H, \Omega, m_0) + X_1(T_N, H, \Omega, m_0) m_s, \tag{13}$$

with

$$X_0(T_N, H, \Omega, m_0) = \sum_{p=0}^{z} A_p(T_N, H, \Omega) m_0^p, \tag{14}$$

and

$$X_1(T_N, H, \Omega, m_0) = -\sum_{p=0}^{z} p A_p(T_N, H, \Omega) m_0^{p-1}. \tag{15}$$

On the other hand, in this work only second-order transitions are observed, therefore, to study the phase diagram only we analyze Eqs. (14) and (15) in the limit of $m_{\mathbf{s}} \to 0$. We may then locate the second-order line and using the fact that $m_A = m_0 + m_s$ in Eq. (13), and therefore:

$$X_0(T_N, h, \delta, m_0) = m_0, \tag{16}$$

$$X_1(T_N, h, \delta, m_0) = 1, \tag{17}$$

at the critical point in which $m_s = 0$, $\delta \equiv \Omega/J$ and $h \equiv H/J$.

Thus, we can get an analytic solution for second-order transitions where m_s is the order parameter which is used to describe the phase transition of the model (1). The magnetizations of two sublattices are not equal for $m_s \neq 0$, and the system is in the antiferromagnetic phase. The magnetizations of two sublattices are equal for $m_s = 0$, and the system is in the saturated paramagnetic phase.

3. Results and discussion

The numerical determination of the phase boundary (second-order phase transition) is obtained by solving simultaneously Eqs. (16) and (17). We determined the phase diagrams of this quantum model in the $h - T$ and $\delta - T$ planes for the square ($z = 4$) lattice that comprises a field-induced AF phase ($m_s \neq 0$) at low fields and a P phase ($m_s = 0$) at high fields. In the case $h = 0$, we have $m_A = -m_B$ ($m_0 = 0$) and the critical behavior reduces to the transverse Ising ferromagnet analyzed in Ref. [32]. For $z = 3$ and $z = 4$, the values of the quantum critical point for $h = 0$ obtained are $\delta_c = 1.83$ ($\delta_c^{\text{MFA}} = 3.00$) and $\delta_c = 2.75$ ($\delta_c^{\text{MFA}} = 4.00$), respectively [35]. In the limit of vanishing fields $h = \delta = 0$, we have obtained the value $m_0 = 0$ and $k_B T_N/J = 3.085$ (square lattice) and $k_B T_N/J = 2.104$ (honeycomb lattice). The results for the critical temperature obtained by simple EFT with clusters of $N = 1$ spin (EFT-1) $k_B T_N/J = 3.085$, when compared with the exact solution $k_B T_N/J = 2.269\ldots$, for the Ising model on a square lattice, is not quantitatively satisfactory. On the other hand,

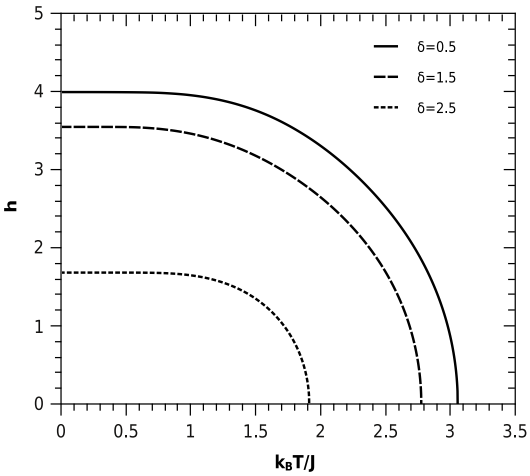

Fig. 2. Dependence of the reduced critical temperature k_BT/J as a function of the reduced magnetic field $h = H/J$ for a square lattice and several values of δ.

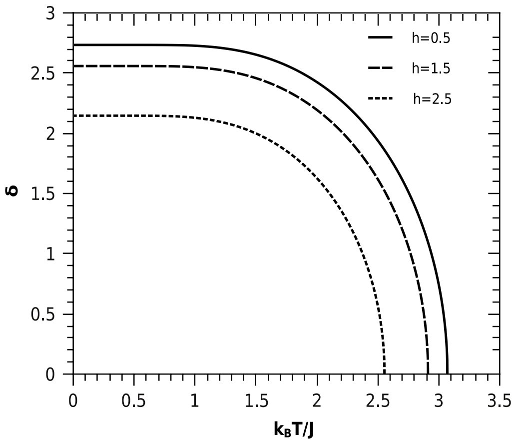

Fig. 3. Dependence of the reduced critical temperature k_BT/J as a function of the reduced magnetic field $\delta = \Omega/J$ for a square lattice and several values of h.

increasing the size of the cluster ($N = 2, 4, 9, \dots$) we have a possible convergence of the results for the critical temperature. In the present paper we are only interested in obtaining qualitative results for the phase diagram.

The study of quantum phase transitions is nowadays one of the main areas of research in condensed matter physics; most of the experimental and theoretical studies are related to the magnetic quantum critical point (QCP). For the square lattice ($z = 4$), the QCP for $h = 0$ obtained by using EFT [32], $\delta_c = 2.75$, can be compared with the results obtained using other methods, for example, $\delta_c = 4.00$ in the MFA, $\delta_c = 3.22$ of path-integral Monte Carlo simulations [36], $\delta_c = 3.05$ from the DMRG [37], $\delta_c = 3.08$ from the high-temperature series expansions [5], $\delta_c = 3.02$ using the effective-field renormalization group (EFRG) [38], $\delta_c = 3.00$ from the PA [13], and $\delta_c = 3.04$ using the cluster MC [39]. Increasing the size cluster we will possibly have a convergence to the rigorous results for δ_c [37,5,38,13,39].

In Fig. 2, the phase diagram in the $h - T$ plane is presented for the square lattice, with selected values of δ. In this figure, the phase transition between the AF and P phases is continuous for all values of the transverse field. The critical temperature decreases monotonically as the longitudinal field (H) increases, and vanishes at $h = h_c(\delta)$. and the critical behavior of h_c versus transverse field (δ) (ground-state phase diagram) has been analyzed by Neto and Ricardo de Sousa [35].

The same qualitative phase diagram is also observed in the $\delta - T$ plane in Fig. 3 for the square lattice, with selected values of h. When the longitudinal field increases the critical curve $T_c(\delta)$ decreases. We show that there is no reentrant behavior in the region of low temperature, and also the phase transition is of second order for all values of the fields h and δ. We hope that the present method can be employed for more complex models, for instance, the generalization of the model to treat three-dimensional lattices, where multicritical points in the phase diagrams are observed in MFT [40,41]. The results are qualitatively identical to the ones on the honeycomb lattice.

4. Conclusions

We have used the effective-field theory with correlation in single site clusters to obtain the state equations of the TIM antiferromagnet. We study the phase diagrams in $h-T$ and $\delta-T$ planes for the square ($z=4$) lattice. The transverse field δ has important effects on the phase diagrams because it destroys the long-range order of the system. The results show that for a given δ, the critical longitudinal magnetic field h decreases with increasing temperature. In the phase diagrams there are no reentrant phenomena. Our results (EFT) are consistent with second-order transitions from the antiferromagnetic phase to the paramagnetic phase at vanishing transverse field. The quantitative results for the phase diagrams can be obtained by using more reliable methods such as quantum Monte Carlo simulation and renormalization group approaches. Furthermore, the investigations of the same model on three-dimensional lattices are expected to show many characteristic phenomena. This will be discussed in future work.

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