Physica A 388 (2009) 21–27

Contents lists available at ScienceDirect

Physica A

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

Quantum phase transition in the two-dimensional XY model with single-ion anisotropy

A.S.T. Pires [a,*], M.E. Gouvea [b]

[a] Departamento de Fisica, Universidade Federal de Minas Gerais, CP 702, Belo Horizonte, MG, 30123-970, Brazil

[b] Centro Federal de Educação Tecnológica de Minas Gerais, Av. Amazonas 7675, Belo Horizonte, MG, Brazil

ARTICLE INFO

Article history:
Received 21 August 2008
Available online 1 October 2008

PACS:
75.10.Jm
75.40.-s

Keywords:
Quantum-phase transition
XY model
Two-dimensional

ABSTRACT

In this paper we study the quantum phase transition and low temperature behavior in a square lattice quantum two-dimensional XY model with single-ion anisotropy and spin $S = 1$. Starting with the Villain representation, a Landau–Ginzburg expression is written. The large D phase is studied using the bond operator formalism.

1. Introduction

Although quantum phase transitions (QPT) in low-dimensional magnetic models have been studied extensively [1–5], some problems still deserve attention. Most of the work done has focused on the zero-temperature properties of the QPT system. In contrast to the classical critical point where scaling is observed only in a narrow range around the critical point, the influence of a quantum critical point extends over a wide region at finite temperatures. Here we will be interested in the low temperature behavior of the two-dimensional anisotropic quantum XY model described by the following Hamiltonian:

$$H = J \sum_{\langle n,m \rangle} (S_n^x S_m^x + S_n^y S_m^y) + D \sum_n (S_n^z)^2, \tag{1}$$

where $\langle n, m \rangle$ represents the sum over nearest neighbors on the sites, n, of a square lattice and $0 \le D < \infty$. We consider the antiferromagnet, since, in general, this is the case of more interest. However, the Hamiltonian (1) is invariant under the transformation $J \to -J$, $k \to k + \pi$. Due to the form of the single-ion anisotropy we take $S > 1/2$. We will be particularly interested in the case $S = 1$, where we can use the bond operator formalism presented in Section 3. The standard procedure for treating the XY model, is to start with the Villain representation [6]:

$$S_n^+ = \mathrm{e}^{\mathrm{i}\phi_n} \sqrt{(S + 1/2)^2 - (S_n^z + 1/2)^2},$$
$$S_n^- = \sqrt{(S + 1/2)^2 - (S_n^z + 1/2)^2}\, \mathrm{e}^{-\mathrm{i}\phi_n}, \tag{2}$$

where ϕ is the operator corresponding to the azimuthal angle of the spin around the z axis.

* Corresponding author. Tel.: +55 31 3499 6624; fax: +55 31 3499 6600.
E-mail address: antpires@fisica.ufmg.br (A.S.T. Pires).

0378-4371/$ – see front matter
doi:10.1016/j.physa.2008.09.030

Using the self-consistent harmonic approximation (SCHA) described in [7], we can write the Hamiltonian (1) as

$$H = \sum_r \left[\frac{\tilde{S}^2 \rho}{2} (\phi_r - \phi_{r+a})^2 + b(S_r^z)^2 \right], \quad (3)$$

where $b = 1 + D$, $\tilde{S}^2 = S(S+1)$, ρ is the stiffness renormalized by thermal and quantum fluctuations, and we have set $J = 1$.

As is well known, a Kosterlitz–Thouless phase transition occurs when D is less than a critical value D_C, resulting from the unbinding of vortex–anti-vortex pairs [8]. In this region, the critical behavior of the quantum XY model is of the KT-type, as in the classical case. Quantum fluctuations at finite T can change the quantitative behavior of the model, but the qualitative picture of the classical system persists [9].

Renormalization group analysis shows that at the Kosterlitz–Thouless transition temperature, T_{KT}, the stiffness exhibits a universal jump given by $2T_{KT}/\pi\tilde{S}^2$. The KT temperature for the XY model, described by the Hamiltonian (1), can be determined [10] by the crossing between the curve $\rho(T)$, and the line $\gamma = 2T/\pi\tilde{S}^2$. Using this procedure, $T_{KT}(D)$ was calculated in Ref. [4]. The discontinuous drop in ρ in figure 3 of this reference, can be considered to be a spurious effect. If we extrapolate the curve continuously to zero, we can estimate D_C as about 5.3.

At $T = 0$, the energy of the first term in Eq. (3) is minimized by the magnetically ordered state in which all spins are oriented in the same direction. One has a gapless phase described by the spin wave formalism. The energy of the second term is minimized when the orientation of the spins are maximally uncertain (by the uncertainty principle), and this term leads to a quantum paramagnetic state in which the spins do not have a definite orientation. This phase consists of a unique ground state with total magnetization $S^z_{\text{total}} = 0$, separated by a gap from the first excited states which lie in the sectors $S^z_{\text{total}} = \pm 1$. The elementary excitations are called excitons, with $S = 1$ and an infinite lifetime at low energies.

Using the equation of motion for ϕ:

$$\dot{\phi}_r = -\mathrm{i}[\phi_r, H] = -2\mathrm{i}bS_r^z, \quad (4)$$

we obtain, in the continuum limit

$$H = \frac{1}{2} \int \mathrm{d}x\mathrm{d}y \left[\rho\tilde{S}^2 (\nabla\phi)^2 + \frac{1}{2b} \left(\frac{\partial\phi}{\partial t} \right)^2 \right], \quad (5)$$

which is the O(2) non-linear sigma model. We note that in the above equation, ϕ is an angle variable. The KT transition, as was said before, is caused by topological excitations and is obtained only when we consider ϕ as an angle. It can not be obtained using only the spin wave formalism. However, the behavior of the spin correlation function is correctly given by the harmonic Hamiltonian using the expression:

$$\begin{aligned} \langle (S_0^x S_r^x + S_0^y S_r^y) \rangle &\approx \langle [S(S+1) - (S_r^z)^2] \rangle \langle \cos(\varphi_0 - \varphi_r) \rangle \\ &= \langle [S(S+1) - (S_r^z)^2] \rangle \exp\left[-\frac{1}{2} \langle (\varphi_0 - \varphi_r)^2 \rangle \right]. \end{aligned} \quad (6)$$

This happens because in (6) we have effectively bypassed the higher order perturbative theory.

In this paper we will be interested in the region $D \geq D_C$, since the region $D < D_C$ has already been well studied. In Section 2 we present a Landau–Ginzburg theory for the model. In Section 3 we introduce the bond-operator representation and present results, at finite temperature, of a self-consistent mean field calculation. The calculation of Section 3, although in agreement with the one calculated in Section 2, is more general, since it leads to quantitative results.

2. Landau–Ginzburg approach

In the low temperature phase of the region $D < D_C$ we have a power-law decay of the correlations but no broken symmetry. This phase is not described by a simple order parameter in the Landau–Ginzburg (LG) theory of phase transitions. We can, however, use the LG formalism to study the quantum-phase transition if, for $D < D_C$, we restrict ourselves to the $T = 0$ limit only. The finite temperature behavior in the KT region is well known. Thus we write

$$F = \int \mathrm{d}^d r \mathrm{d}\tau \left[(\nabla\phi)^2 + (\partial_\tau \phi)^2 + \delta\phi + \frac{V}{2}\phi^4 \right], \quad (7)$$

where here ϕ is a field variable (and not an angle) and τ is an imaginary time.

In a path integral formulation we use the Hubbard–Stratanovich transformation to decouple the quartic term, introducing an auxiliary field λ. In the saddle-point approximation, λ is a constant. All this is standard procedure [1,11]. Minimization with respect to λ leads to:

$$\lambda = VT \sum_n \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{\delta + k^2 + \omega_n^2 + \lambda}, \quad (8)$$