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Quantum spherical XY model with orthorhombic anisotropy in two dimensions

Yu.A. Fridman[a] and D.V. Spirin

Theoretical Physics Chair, Physical Faculty, Tavrida National University, Yaltinskaya st. 4, Simferopol, 95007, Crimea, Ukraine

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Abstract. The quantum spherical XY model with orthorhombic anisotropy is investigated. It is shown that in contradiction with the results of reference [9], the long-range magnetic order is stabilized in two dimensions. Both analytical and numerical results are presented. The incorrect results of the work [9] are explained to be the result of improper choice of quantization axis.

PACS. 75.10.-b General theory and models of magnetic ordering

1 Introduction

Quantum spin models have been widely studied over the last few years. Quantum XY model is still attracting interest because it is used for description of liquid helium, high-temperature superconductors and other systems. Since the Mermin-Wagner theorem [1] states that there is an absence of long-range magnetic ordering in two-dimensional (2D) systems, it is of fundamental interest and has been extensively studied by different methods. The 2D spin one-half XY model was investigated by renormalization group method [2], Monte Carlo simulations [3], perturbation theory [4], exact finite lattice calculations [5], variational methods [6], spin-wave theory [7,8].

Quantum 2D XY models with $S > 1/2$ were also studied. Ma and Figueiredo (MF) [9] considered a spin-one quantum ferromagnetic XY model with single-site orthorhombic anisotropy in the form $-\frac{D}{2}[(S_i^x)^2 - (S_i^y)^2]$ and with exchange Hamiltonian including interactions between nearest neighbor operators S_i^x and S_i^y. This form of anisotropy is believed to describe the anisotropy in some magnetic materials, $MnCl_2 \cdot 4H_2O$ for instance [10]. MF used a spherical constraint $\sum_i \lfloor (S_i^x)^2 + (S_i^y)^2 \rfloor = N$ where N is the number of lattice sites. In boson language this constraint becomes a mean hard-core boson constraint [9]. These authors found that in spite of the presence of a symmetry-breaking anisotropic term the long-range order is stabilized only for $d > 2$ which is the lower critical dimensionality for this system.

These results seem to be curious. Fifteen years ago Gomez-Santos and Joannopoulos [7] showed that while considering quantum systems it is important to choose a proper direction of quantization axis (*i.e.* z-axis). For the spin one-half XY model they used the usual Holstein-Primakoff spin-wave theory and obtained results in much better agreement with numerical ones than results of spin wave theory with incorrectly chosen quantization axis.

Our purpose is to show that the same takes place for quantum spherical XY ferromagnet with anisotropy. Precisely, here the improper choice of quantization axis has led to completely incorrect results obtained by MF.

We found that $d = 2$ is not the lower critical dimensionality. In two dimensions there exists long-range ferromagnetic order with nonzero Curie temperature.

2 Self-consistent spin-wave theory for a 2D ferromagnet

We begin with the Hamiltonian:

$$H = -\frac{1}{2}J \sum_{r,r+\delta} \left(S_r^x S_{r+\delta}^x + S_r^z S_{r+\delta}^z \right) - \frac{D}{2} \sum_r \left[(S_r^z)^2 - (S_r^x)^2 \right], \quad (1)$$

where J is the strength of exchange interaction between nearest neighbors. This Hamiltonian coincides with that of MF (Eq. (1) in Ref. [9]) if we replace $x \to y$, $z \to x$. Because of the symmetry-breaking term of single-site anisotropy the long-range ferromagnetic order is expected to be stabilized in the system under study. This means that each spin of the lattice has the projection on the quantization axis close to 1. The only quantum operators with macroscopically measurable averages are S^z and S^2. This justifies the choice of Hamiltonian in the form (1).

[a] e-mail: frid@tnu.crimea.ua

Instead of constraint $\sum_i \lfloor (S_i^x)^2 + (S_i^y)^2 \rfloor = N$ we use other one:

$$\sum_i \left\lfloor (S_i^x)^2 + (S_i^z)^2 \right\rfloor = N. \tag{2}$$

This is a quantum version of the original concept of spherical model [11]. Introducing the Holstein-Primakoff transformation [12] and performing the Fourier transformation of equations (1, 2) one obtains:

$$H = \sum_q A_q a_q^+ a_q + \frac{1}{2}\sum_q B_q \left(a_q^+ a_{-q}^+ + a_q a_{-q}\right), \tag{3}$$

$$\sum_q \left[a_q^+ a_q - \frac{1}{2}\left(a_q^+ a_{-q}^+ + a_q a_{-q}\right)\right] = \frac{1}{2}, \tag{4}$$

where coefficients A_q and B_q are determined as follows:

$$A_q = J\left(1 - \frac{1}{2}\gamma_q\right) + \frac{3}{2}D + \mu,\ B_q = \frac{1}{2}D - \frac{1}{2}J\gamma_q - \mu, \tag{5}$$

with $\gamma_q = \frac{1}{2}(\cos q_x + \cos q_z)$ the structure factor. Here in equations (3–5) we introduced chemical potential μ to satisfy equation (4) on an average. This quantity should be found self-consistently.

Using Bogoliubov transformation:

$$a_q^+ = u_q \alpha_q^+ + v_q \alpha_q, \quad a_q = u_q \alpha_q + v_q \alpha_q^+, \tag{6}$$

with

$$u_q = \sqrt{\frac{A_q + \varepsilon_q}{2\varepsilon_q}}, \quad v_q = -\frac{B_q}{|B_q|}\sqrt{\frac{A_q - \varepsilon_q}{2\varepsilon_q}},$$

$$\varepsilon_q = \sqrt{(J(1-\gamma_q) + 2D)(J + D + 2\mu)} \tag{7}$$

the Hamiltonian (3) can be easily diagonalized:

$$H = \sum_q \varepsilon_q \alpha_q^+ \alpha_q. \tag{8}$$

Condition (5) in the 2D case can be rewritten as:

$$\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\sqrt{\frac{A_q - B_q}{A_q + B_q}}\left(n_q + \frac{1}{2}\right)\mathrm{d}q_x\,\mathrm{d}q_z = 1,$$

$$n_q = (\exp(\varepsilon_q/T) - 1)^{-1}. \tag{9}$$

The second term in the brackets of the first equation is a part of quantum fluctuation corrections. Discarding this term one has:

$$\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\sqrt{\frac{A_q - B_q}{A_q + B_q}} n_q\,\mathrm{d}q_x\,\mathrm{d}q_z = \frac{1}{2}\cdot \tag{10}$$

The equation (10) can be solved analytically in the low-temperature limit. One obtains:

$$\mu \approx T - \frac{J + D}{2}\cdot \tag{11}$$

The mean magnetization is given by:

$$M_z = \frac{3}{2} - \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{A_q}{\varepsilon_q}\left(n_q + \frac{1}{2}\right)\mathrm{d}q_x\,\mathrm{d}q_z. \tag{12}$$

Substituting equation (11) into (12) and neglecting the second term in the brackets, for low temperatures we have:

$$M_z \approx 1 - \frac{T}{2\pi J}\left(1 + \frac{D}{T}\right)\ln\left(1 + \frac{\pi J}{2D}\right)\cdot \tag{13}$$

At zero temperature M_z is less than 1 due to the presence of single-site anisotropy:

$$M_z(T=0) \approx 1 - \frac{D}{2\pi J}\ln\left(1 + \frac{\pi J}{2D}\right)\cdot \tag{14}$$

Equation (14) is correct for small $D \ll J$. The critical temperature of the phase transition from ferromagnetic phase into paramagnetic one is given by:

$$T_C \approx \frac{2\pi J M_z(T=0)}{\ln\left(1 + \frac{\pi J}{2D}\right)}\cdot \tag{15}$$

3 Numerical calculations

Equation (9) can be solved numerically without approximations like those made in the previous section. Then one substitutes numerical solution $\mu(T, D)$ into equation (12) and obtains dependence of the magnetization on temperature or anisotropy.

We performed such numerical calculations in the range of anisotropy values $D \in [0.001J; 0.1J]$. The results of the calculation of chemical potential μ (below solid horizontal line) and magnetization M (upper lines) for $D = 0.001J$ and $D = 0.01J$ are shown at Figure 1. Dotted lines depict mean magnetization for $D = 0.001J$ (lower line) and $D = 0.01J$ (upper line) the one calculated with the use of equation (13). One can see that the crude formula (13) is just a linear approximation of mean magnetization. However, equation (11) is much more appropriate because from Figure 1 one can see that chemical potential i) depends on D weakly, ii) it is almost a linear function up to temperatures $T \propto J$.

In Figure 2 we present the phase diagram anisotropy – Curie temperature for a 2D ferromagnet. Note that the dependence of the critical temperature on anisotropy differs from that obtained by MF (however, their phase diagram was calculated for a 3D system).

4 Conclusion

We have investigated the quantum spherical 2D XY spin-1 model with orthorhombic anisotropy. Previously this system was considered by MF (Ref. [9]). We have shown that

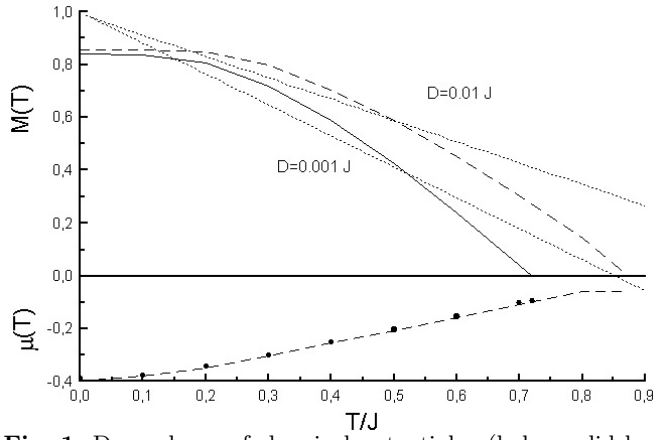

Fig. 1. Dependence of chemical potential μ (below solid horizontal line) and magnetization M (upper lines) on reduced temperature T/J of quantum spherical spin-one XY model in two dimensions. Case $D = 0.001J$: solid circles – chemical potential, solid line – mean magnetization. Case $D = 0.01J$: dashed lines. Dotted lines: mean magnetization for $D = 0.001J$ (lower line) and $D = 0.01J$ (upper line) calculated using approximation (13).

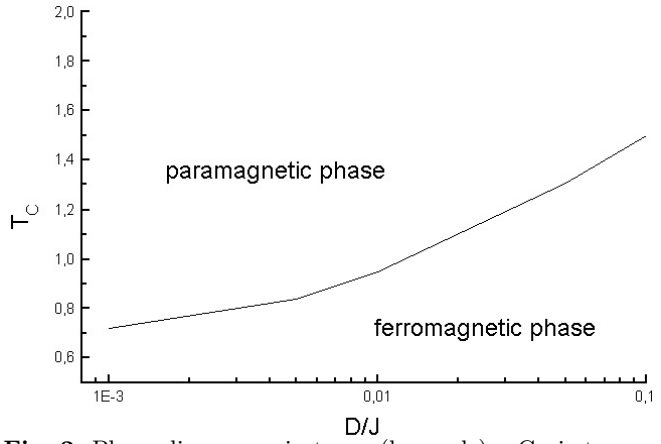

Fig. 2. Phase diagram anisotropy (log scale) – Curie temperature for 2D quantum spherical spin-one XY ferromagnet.

the proper choice of quantization axis leads to completely different results in comparison with those of MF. It was found that the long-range order in the 2D system exists up to the Curie temperature.

Note that the above-described method being applied to the same model but with the spin coordinated system chosen like in reference [9] gives for low temperatures the gapless spectrum of spin waves, and therefore the divergence of the integrals for $d < 3$ as in the work we criticize [9]. These incorrect results are caused by improper choice of quantization axis.

For XY spin-1/2 model such a mistake leads to significant overestimation of various quantities (see Ref. [7], Tabs. I, II, III). Therefore though there are few cases when improper choice of quantization axis leads to mistake we think it is dangerous to choose the x- or y- axis as the direction of (possible) long-range ordering, *i.e.* as the quantization axis, in quantum models. This question rises, for example, for the paper [13] where MF considered a quantum spherical XY model in a random field. They chose the x-axis as a direction of random magnetic field. We cannot state for certain that this paper is incorrect, however, similar calculations with the proper choice of quantization axis will shed light on this problem.

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