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1989 J. Phys. A: Math. Gen. 22 4257

(http://iopscience.iop.org/0305-4470/22/19/018)

J. Phys. A: Math. Gen. **22** (1989) 4257-4261. Printed in the UK

COMMENT

Ground state properties of a quantum antiferromagnet with infinite-range interactions

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Received 5 June 1989

Abstract. We discuss the order of a Heisenberg antiferromagnet in the ground state for isotropic and anisotropic exchange with and without a staggered field.

Heisenberg quantum antiferromagnets in two dimensions have been the subject of quite a few recent studies. Of main interest here is the nature of the ground state and its possible order. In this context, a solvable model can be quite useful in order to understand general aspects of the symmetry breaking. This has been pointed out by Kaplan *et al* [1]. They proposed to study a model with infinite-range interactions introduced by Lieb and Mattis [2-4]. In this comment we want to treat this model in some detail both for isotropic and anisotropic exchange. The choice of the interaction has interesting implications. For the isotropic model there is a simple angular momentum representation of the ground state and including a staggered field one can produce the order parameter directly. We show that this problem is closely related to the quantum harmonic oscillator. We also comment on the character of the isotropic ground state in the resonant valence-bond (RVB) picture.

Consider two 'sublattices' A and B, each containing N spins one-half. Each spin interacts with all spins in the other sublattice via an exchange coupling of order $1/N$ to make the system extensive. Then the Hamiltonian, including a staggered field H_s, is (regardless of the dimension)

$$\mathcal{H} = \frac{J}{N}(\boldsymbol{S}_A \cdot \boldsymbol{S}_B - \lambda S_A^z S_B^z) - M_s^z H_s \tag{1}$$

Here $\boldsymbol{S}_A$, $\boldsymbol{S}_B$ are the total spins of the sublattices and $\boldsymbol{M}_s = \boldsymbol{S}_A - \boldsymbol{S}_B$ is the staggered magnetisation.

Consider first the isotropic case, $\lambda = H_s = 0$. We are then dealing with a sort of free atom where two large spins are coupled to a total spin $\boldsymbol{S} = \boldsymbol{S}_A + \boldsymbol{S}_B$. The lowest eigenstates of $\mathcal{H}$ are those where the sublattice spins are maximal, $S_A = S_B = N/2$, and will be denoted by $|S, M\rangle$ where M is the z component of $\boldsymbol{S}$. Their energy is given by

$$E_S = -\frac{J}{2}\left(\frac{N}{2}+1\right) + \frac{J}{2N} S(S+1) \qquad 0 \leq S \leq N. \tag{2}$$

The ground state $|0, 0\rangle$ is a singlet as usual [2], which can easily be written down here [5]. Equation (2) shows that for $N \to \infty$, infinitely many of the other states become degenerate with it. This is what one expects for such a system with continuous symmetry

0305-4470/89/194257+05$02.50

[6]. The states $|S, M\rangle$ are also exact eigenstates of $\boldsymbol{M}_s^2 = 2(\boldsymbol{S}_A^2 + \boldsymbol{S}_B^2) - \boldsymbol{S}^2$. In the ground state one obtains for $\boldsymbol{m}_s = \boldsymbol{M}_s / N$

$$\langle \boldsymbol{m}_s^2 \rangle = 3\langle (m_s^z)^2 \rangle = 1 + \frac{2}{N}. \tag{3}$$

The deviation from the classical value 1 is a quantum correction due to the finite length of $\boldsymbol{S}_A$ and $\boldsymbol{S}_B$. Either $\boldsymbol{m}_s^2$ or $(m_s^z)^2$ can be used to measure the order but the values differ by a factor of three. This has caused some debate on the proper choice of the order parameter [1, 7, 8]; see below.

We now include the field H_s. Then the states $|S, M\rangle$ are coupled via the matrix elements [9]

$$\langle S-1, M | M_s^z | S, M \rangle = \sqrt{f(S, M)} \tag{4}$$

where

$$f(S, M) = \frac{(S^2 - M^2)[(2S_A+1)^2 - S^2]}{4S^2 - 1}. \tag{5}$$

The new ground state lies in the subspace with $M = 0$ and is of the form $\Sigma_S \Phi(S)|S, 0\rangle$ where $\Phi(S)$ is a solution of the equations

$$-h_{S-1}\Phi(S-1) + \lambda_S \Phi(S) - h_S \Phi(S+1) = \varepsilon \Phi(S) \tag{6}$$

with $\lambda_S = S(S+1)/2N^2$, $h_S = h\sqrt{f(S, 0)}/2$, $h = H_s/J$ and $\varepsilon = (E - E_0)/JN$. We are interested in the thermodynamic limit, i.e. a large system and a small field. This is the standard way to determine the order parameter. Now for $h \gg 1/N^2$, a large number of states $|S, 0\rangle$ will be involved and $\Phi(S)$ will vary smoothly with S. This suggests taking a continuum limit in (6). Since for $1 \ll S \ll N$, h_S is practically constant, $h_S \simeq h/2$, this leads to the equation

$$-\frac{1}{2}\frac{d^2\Phi}{dS^2} + \frac{1}{2}\omega^2 S^2 \Phi(S) = \nu \Phi(S) \tag{7}$$

where $\omega^2 = 1/N^2 h$, $\nu = (\varepsilon + h)/h$. This is the Schrödinger equation for the harmonic oscillator. Our solutions have to vanish at $S = 0$, so the lowest eigenvalue is $\nu = 3\omega/2$ or

$$\varepsilon = -h + \frac{3}{2}\frac{\sqrt{h}}{N}. \tag{8}$$

Then $\langle m_s^z \rangle$ follows from $-\partial\varepsilon/\partial h$ and is

$$\langle m_s^z \rangle = 1 - \frac{3}{4N}\frac{1}{\sqrt{h}}. \tag{9}$$

The results of the continuum limit change only slightly if one diagonalises the exact equations (6) numerically. The exact $\Phi(S)$ has essentially the same form as the first oscillator function. From a finite-size scaling analysis one then finds for $N \gg 1$ and $1/N^2 < h \ll 1$

$$\langle m_s^z \rangle = 1 + \frac{a}{N} - \frac{b}{N}\frac{1}{\sqrt{h}} \tag{10}$$

with $a \simeq 0.8$, $b \simeq 0.5$.

We see that in the thermodynamic limit $\langle m_s^z \rangle = 1$, which is the same as $\sqrt{\langle \boldsymbol{m}_s^2 \rangle}$ without a field. Thus the calculation confirms the classical picture that the vector length $\boldsymbol{m}_s^2$ is the proper order parameter here and that the field just turns $\boldsymbol{m}_s$ in the right direction [1, 7]. For this, however, one needs more than just the first excited state.

Consider now the anisotropic system, $\lambda \neq 0$, $H_s = 0$. The special cases $\lambda = -\infty$, 1, 2 correspond to the Ising limit, the XY model and the isotropic ferromagnet. Again the states $|S, M\rangle$ are coupled, this time via the matrix elements (which follow from (4))

$$\langle S, M | S_A^z S_B^z | S, M \rangle = \tfrac{1}{4}(M^2 - f(S, M) - f(S+1, M)) \tag{11}$$

$$\langle S, M | S_A^z S_B^z | S+2, M \rangle = -\tfrac{1}{4}\sqrt{f(S+1, M) f(S+2, M)}. \tag{12}$$

The spectrum of $\mathscr{H}$ can be obtained as before. The qualitative features, however, can already be seen from first-order perturbation theory. In the planar region ($\lambda > 0$) from each S-multiplet the states evolving from $|S, \pm S\rangle$ are shifted towards the ground state and become exactly degenerate with it at the ferromagnetic point. In the uniaxial region ($\lambda < 0$) only the state $|1, 0\rangle$ moves down and for $N \to \infty$ one has the usual twofold degeneracy of the Ising model. The ground state again lies in the subspace $M = 0$.

In figure 1 we show numerical results for $\langle (m_s^z)^2 \rangle$ as a function of λ. We see the expected behaviour, namely a rapid increase in the uniaxial region, where $\langle m_s^z \rangle$ is the proper order parameter, and a rapid decrease in the planar region, where $\boldsymbol{m}_s$ will lie in the xy plane. The curves become rapidly steeper as the size of the system increases. The vector length $\langle \boldsymbol{m}_s^2 \rangle$ is roughly independent of λ. In the two limiting cases, one can derive analytical results, namely Ising case: $\langle (m_s^z)^2 \rangle = 1$, $\langle \boldsymbol{m}_s^2 \rangle = 1 + 1/2S_A$; isotropic ferromagnet: $\langle (m_s^z)^2 \rangle = 1/(4S_A - 1)$, $\langle \boldsymbol{m}_s^2 \rangle = 1 + 1/2S_A + 1/(4S_A - 1)$. Thus the corrections to the asymptotic values are of the order $1/N$. This also holds for general λ.

Returning to the isotropic model, we ask how the ground state $|0, 0\rangle$ looks in the RVB picture, i.e. in terms of singlet products (Rumer functions [10, 11]). It is then

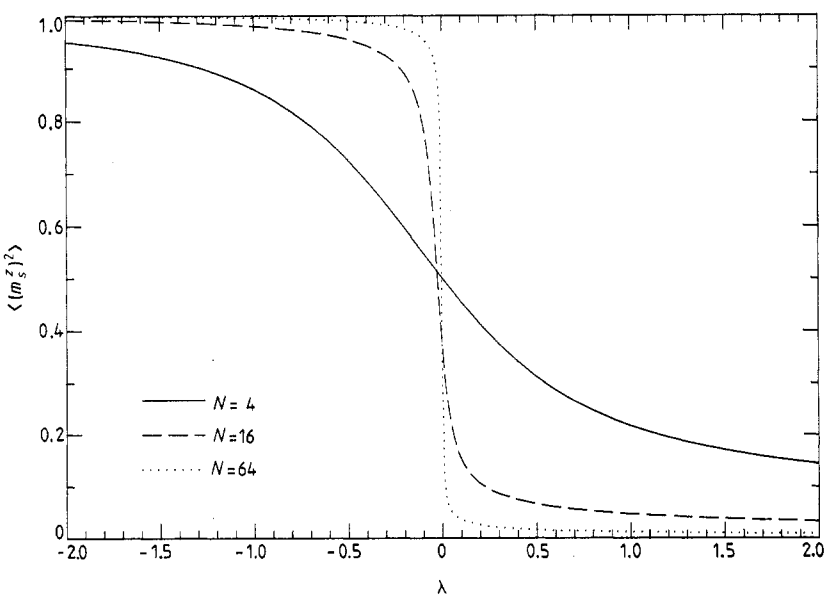

Figure 1. Expectation value of $(m_s^z)^2$ in the ground state as a function of the anisotropy.

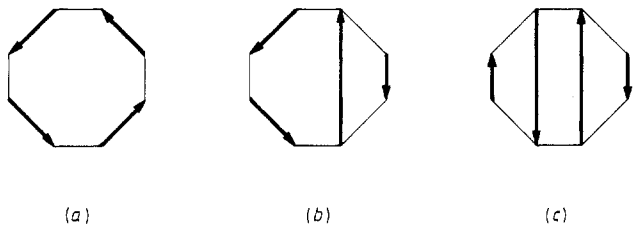

Figure 2. Types of Rumer functions for a ring of eight spins. The thick arrows denote singlet states between the two spins involved. Altogether there are 14 functions.

convenient to put the system on a ring with $A(B)$ spins on the even (odd) sites. Then for $N=4$ one has the three types of functions shown in figure 2. Because of the translational invariance of the ground state, all functions of one type occur with the same weight. The symmetry of $|0,0\rangle$ against permutations of sublattice spins then fixes the relative weight of the three classes. The result is

$$|0,0\rangle = \frac{2}{3\sqrt{5}}(|a\rangle - \tfrac{1}{2}|b\rangle - |c\rangle). \tag{13}$$

This should be compared with the ground state for the ring with nearest-neighbour interactions [12]. There the coefficients are $0.30\times(1, 0.36, 0.10)$. Thus in our case 'long singlets' appear with larger weight, which is quite reasonable. However, it is hard to draw conclusions just from the size of the coefficients since the Rumer functions are not orthogonal. For example, the spin correlation functions for the two systems with $N=4$ are not very different. For our model, it is easy to derive $\langle \boldsymbol{S}_i\boldsymbol{S}_j\rangle$ in the angular momentum representation (the function oscillates between $\frac{1}{4}$ and $-\frac{1}{4}-1/2N$ for even/odd separations). With the Rumer functions, the calculation is much more involved. Also the expansion of $|0,0\rangle$ for general values of N will be complicated since one expects that all classes of Rumer functions will enter with different weights. We have not solved this problem, but it would be of interest in connection with other calculations where long-range singlets play a role [13].

To sum up, we have studied a quantum mechanical model which can essentially be solved exactly and which allows one to study the thermodynamic limit in which classical behaviour is recovered. We should mention that recently the Hubbard model with infinite-range hopping has also been treated [14]. Our model with $\lambda = H_s = 0$ is a special case of that.

Acknowledgments

We thank Professor T Kaplan, Dr P Horsch and Dr P Tavan for various discussions and the Max-Planck-Institut für Festkörperforschung, Stuttgart, for its hospitality.

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