Ground state properties of the classical two-dimensional frustrated Heisenberg magnet

1990 J. Phys.: Condens. Matter 2 1037

(http://iopscience.iop.org/0953-8984/2/4/024)

J. Phys.: Condens. Matter 2 (1990) 1037–1041. Printed in the UK

LETTER TO THE EDITOR

Ground state properties of the classical two-dimensional frustrated Heisenberg magnet

K Y Szeto† and Yihren Wu‡

† Department of Physics, York University, Toronto, Ontario M3J 1P7, Canada

‡ Department of Mathematics, Hofstra University, Hempstead, NY 11550, USA

Received 13 November 1989

Abstract. The ground state of the classical Heisenberg magnet on a square lattice with dilute frustrated bonds is discussed in the context of the homotopy group. It is shown that in general the ground state of the two-dimensional frustrated Heisenberg system is *XY*-like. In the special case of one frustrated bond an analytical expression for the ground state is given. A relation to high-temperature superconductivity in La_2CuO_4 is suggested.

The ground state of a classical Heisenberg magnet on a square lattice is well known, as is the corresponding topological analysis of the local energy minimum states in terms of instanton numbers [1]. However, as soon as frustrated bonds are introduced, such as in the model of Aharony *et al* [2, 3] for La_2CuO_4, the ground state properties are found to be drastically different. Instead of the isotropic Ising-like ground state of uniform magnetisation, we find that static frustrated bonds force the Heisenberg system to behave like an *XY* magnet with frustration. This is in fact what we observed in the magnetic ordering of the Cu spins in La_2CuO_4 from neutron scattering experiments [4], which is also in agreement with a high-temperature series analysis of the susceptibility data [5]. In this letter, we provide a mathematical justification of the *XY* nature of the ground state of the frustrated Heisenberg system. In particular, for a system with only one frustrated bond, the ground state spin configuration is explicitly given.

We first consider a classical nearest-neighbour Heisenberg ferromagnet on a square lattice with the following Hamiltonian:

$$\tilde{H}_0(s) = -J \sum_{\langle r,r'\rangle} s(r) \cdot s(r'). \tag{1}$$

Here $r = m_x\hat{x} + m_y\hat{y}$ defines a discrete point on a square lattice on which sits a unit-magnitude classical three-component spin s. Thus a spin configuration is a map $s : \mathscr{X}^2 \to \mathscr{S}^2$ where $\mathscr{X}$ denotes the set of integers and $\mathscr{S}^2$ the sphere. Since the ground state of a classical ferromagnet is given by a state of uniform magnetisation, we assume that for an unfrustrated system the ground state is given by the spin configuration,

0953-8984/90/041037 + 05 $03.50 © 1990 IOP Publishing Ltd

$I = \{s(r) = \hat{i}, \forall r\}$. Here $(\hat{i}, \hat{j}, \hat{k})$ form a standard Cartesian basis for $\mathscr{R}^3$. A normalised Hamiltonian is given by

$$H_0(s) = \tilde{H}_0(s) - \tilde{H}_0(I) = \frac{J}{2} \sum_{\langle r, r' \rangle} (s(r) - s(r'))^2 \tag{2}$$

which, in the continuum limit, is

$$H_0 = \frac{J}{2} \int \mathrm{d}^2 r \left(\frac{\mathrm{d}s(r)}{\mathrm{d}x}\right)^2 + \left(\frac{\mathrm{d}s(r)}{\mathrm{d}y}\right)^2. \tag{3}$$

By a stereographic projection $\mathscr{S}^2 \to \mathscr{C}$, Belavin and Polyakov [1] have shown that the Euler–Lagrange equation becomes the Cauchy–Riemann equation, and the corresponding instanton solutions are analytic.

If there is one frustrated bond of strength K joining $r_0 = (0, 0)$ and $r_1 = (1, 0)$, the Hamiltonian in equation (1) becomes

$$\tilde{H}_1 = -J \sum_{\langle r, r' \rangle} s(r) \cdot s(r') + (K + J) s(r_0) \cdot s(r_1). \tag{4}$$

We will only consider the special case where $K \gg J$, which is the case most relevant to La_2CuO_4 [2, 3]. In this case the minimum energy spin configuration must have $s(r_0) = -s(r_1)$. By normalisation similar to equation (2), we have

$$H_1(s) = \tilde{H}_1(s) - \tilde{H}_1(I) = \frac{J}{2} \sum_{\langle r, r' \rangle} (s(r - s(r'))^2 - 2(K + J). \tag{5}$$

To determine the ground state configuration, we can normalise further by dropping the last term in equation (5). Thus the resulting expression is the same as for the unfrustrated case (equation (2)), with the understanding that now the spin configuration satisfies the boundary condition $s(r_0) = -s(r_1)$. Let us define the spin space coordinate axis $\hat{k}$ by $s(r_0)$ for this frustrated spin system. The other two axes $\hat{i}$ and $\hat{j}$ are defined arbitrarily to form an orthogonal system. We now claim that the minimum energy spin configuration of (4) is XY-like.

In general, we can represent $s(r)$ by $(\varphi(r), \theta(r))$ with respect to $(\hat{i}, \hat{j}, \hat{k})$ so that

$$s(r) \cdot s(r') = \cos(\varphi(r) - \varphi(r')) \sin(\theta(r)) \sin(\theta(r')) + \cos(\theta(r)) \cos(\theta(r')). \tag{6}$$

Note that $0 \leqslant \sin(\theta(r)) \sin(\theta(r'))$ because $0 \leqslant \theta \leqslant \pi$. The minimum of $\tilde{H}_1$ is achieved when the prefactor $\cos(\varphi(r) - \varphi(r'))$ in equation (5) is equal to 1. This implies that

$$s(r) \cdot s(r') = \cos(\theta(r) - \theta(r')) \tag{7}$$

is a necessary condition for the minimum energy spin configuration. Thus the ground state is XY-like. Note also that in the ground state the spins span only half of a circle $0 \leqslant \theta \leqslant \pi$. For the case with n static frustrated bonds of strength $K \gg J$, the corresponding Hamiltonian is adjusted by $2n(K + J)$ instead of $2(K + J)$ and all the spins on the frustrated bonds are antiparallel and along some common direction $\hat{k}$. The ground state of a Heisenberg magnet with n frustrations is again XY-like.

In the continuous limit, the spin configuration $\{s(r')\}$ is discontinuous at the frustrated bonds. Since homotopy theory is not equipped to handle discontinuous functions, it is not possible to recover the analogous statement of Belavin and Polyakov on the analyticity of the local minimum states and their classification by instanton numbers. We now present a normalisation procedure to circumvent this problem of discontinuity of s at frustrated bonds. We define the *core size of the frustration* to be the disk centred at the midpoint of the frustrated bond with radius ε. Furthermore, we assume that the energy E_c within the core is the same for any local minimum energy spin configuration, thereby allowing us to *normalise the energy by subtracting off* E_c. This assumption is a physical one since the frustrated bonds only produce small perturbations to the unfrustrated system and the local minimum energy spin configuration should therefore be determined by some global spin arrangement. The normalised energy expression for a frustrated system is thus the same as equation (3) with specific boundary conditions to be defined around the cores of frustrated bonds.

Since the ground state is XY-like, we may assume $s(\boldsymbol{r}) = (\cos(\psi(\boldsymbol{r})), \sin(\psi(\boldsymbol{r}))$ with $\psi(\boldsymbol{r}) \to 0$ as $|\boldsymbol{r}| \to \infty$. We may further assume that there is one frustrated bond centred at the origin along the $\hat{x}$ direction and the bond length is 2ε. In the continuous limit, $\varepsilon \to 0$ and the statement $s(\boldsymbol{r}_0) = -s(\boldsymbol{r}_1)$ implies that the spin angle ψ changes discontinuously,

$$\psi(x = -\varepsilon, y = 0) = \pi + \psi(x = \varepsilon, y = 0). \tag{8}$$

Treating the frustrated bond as a source term $\rho(\boldsymbol{r})$ at the origin, and recalling that without frustration, the Green function G in two dimensions is

$$G(\boldsymbol{r}) = -(1/2\pi) \log r + c \tag{9}$$

where c is a constant, we can then write in a general form the solution for ψ as

$$\psi(\boldsymbol{r}) = \int \mathrm{d}x' \, \mathrm{d}y' \, G(x - x', y - y')\rho(x', y') \tag{10}$$

so that

$$\nabla^2 \psi(\boldsymbol{r}) = \begin{cases} 0 & \text{for } \boldsymbol{r} \neq \boldsymbol{0} \\ \rho(\boldsymbol{r}) & \text{for } \boldsymbol{r} = \boldsymbol{0}. \end{cases} \tag{11}$$

According to condition (8),

$$\nabla^2 \psi(\boldsymbol{r}) \Big|_{\boldsymbol{r}=\boldsymbol{0}} = \lim_{\varepsilon \to 0} \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} \Big|_{x = \pm\varepsilon, y=0} = \frac{\mathrm{d}\,\delta^{(2)}(\boldsymbol{r})}{\mathrm{d}x}. \tag{12}$$

Using $\rho(\boldsymbol{r}) = (\mathrm{d}/\mathrm{d}x)\delta^{(2)}(\boldsymbol{r})$ in (10), we obtain

$$\psi(\boldsymbol{r}) = c_1 x/(x^2 + y^2) + c_2 \tag{13}$$

where c_1 and c_2 are constants. We must take $c_2 = 0$ so that $\psi(|\boldsymbol{r}| \to \infty) \to 0$. To relate to the size 2ε of the frustrated bond, we get for $\psi(x = \pm\, \varepsilon, y = 0) = \pm\pi/2$ the following solution for the ground state spin configuration of the Heisenberg system with one frustrated bond:

$$\psi(x, y) = (\pi/2)\, \varepsilon x/(x^2 + y^2). \tag{14}$$

Note that the range of ψ is the half circle $-\pi/2 \leqslant \psi \leqslant \pi/2$.

The ground state solution of equation (14) exhibits some obvious symmetries. First, we change to the usual coordinates on $\mathcal{S}^2$ by using $\theta = \psi + \pi/2$ and define the following map $\sigma : \mathcal{S}^2 \to \mathcal{S}^2$:

$$\sigma(s_i, s_j, s_k) = (s_i, s_j, -s_k). \tag{15}$$

The ground state $s(x, y)$ satisfies the following symmetries:

$$s(-x, y) = \sigma s(x, y) \tag{16a}$$

$$s(x, -y) = s(x, y). \tag{16b}$$

We denote by $\mathcal{D}$ the plane with the core removed, $\mathcal{D} = \{(x, y)|x^2 + y^2 \geq \varepsilon^2\}$, and by $\mathcal{B}$ the boundary $\mathcal{B} = \{(x, y)|x^2 + y^2 = \varepsilon^2\}$. All spin states are smooth on $\mathcal{D}$. The observation of the ground state configuration suggests that the symmetry properties (16*a*), (16*b*) should persist around the frustrated site for local minimum spin states, and we will henceforth assume this to be the case. That is, we assume that if $s : \mathcal{D} \to \mathcal{S}^2$ is a local energy minimum spin configuration, then we have $s(\varepsilon, 0) = \hat{k}$, $s(|r| \to \infty) = \hat{i}$ and $\{s(r)\}$ processes the symmetry properties (16*a*), (16*b*) on the core boundary $\mathcal{B}$.

By definition, two local energy minimum spin configurations are homotopic if they are homotopic *through* local minimum spin configurations. Explicitly, s_0 and s_1 are homotopic if there exists $s_t : \mathcal{D} \to \mathcal{S}^2$ such that $s_t = s_0$ at $t = 0$ and $s_t = s_1$ at $t = 1$, and satisfies for all $0 \leq t \leq 1$ the following four properties:

$$\begin{aligned} &\text{(a)} \quad s_t(|r| \to \infty) = \hat{i} \\ &\text{(b)} \quad s_t(\varepsilon, 0) = \hat{k} \perp \hat{i} \\ &\text{(c)} \quad s_t(-x, y) = \sigma s_t(x, y) \qquad \forall (x, y) \in \mathcal{B} \\ &\text{(d)} \quad s_t(x, -y) = s_t(x, y) \qquad \forall (x, y) \in \mathcal{B}. \end{aligned} \tag{17}$$

With this definition, we now show that the homotopy class is determined by an instanton number Q equal to the number of covers of the sphere, analogously to the unfrustrated situation.

Although the extended domain $\mathcal{D} \cup \{\infty\}$ is contractible to a point, this homotopy problem is non-trivial due to the boundary conditions on s. First we can use the conformal map $1/z$ to map $\mathcal{D} \cup \{\infty\}$ to a disk of radius $1/\varepsilon$. We can then glue the upper semicircle of this disk to the lower one by symmetry property (d). The resulting object is homotopic to a sphere, and the problem is reduced to the calculation of $\pi_2(\mathcal{S}^2) \cong \mathcal{Z}$. Note that the symmetry properties (a)–(d) prevent the functions s from being homotopic to a constant. The $Q = 0$ homotopy class is described by equation (14) and is the global minimum. Finally, it is anticipated that a local energy minimum spin configuration with lower instanton number has lower energy, since the instanton number arises from the topology of the spin arrangement outside the core.

For many frustrated bonds, as long as there is no hopping, the stationary situation can be treated as analogous to the case with one frustrated bond. Suppose that there are n frustrated bonds with midpoints located at $p_1, \ldots, p_n$ with orientations $v_i = \hat{x}$ or $\hat{y}$. Let the spins sitting on these frustrated bonds be $s(p_i \pm \varepsilon v_i) = \pm u_i$. We can define symmetry for the core boundary around each point p_i and consider functions satisfying the n boundary conditions of equation (16). In real physical systems, this formulation of the topological classification of the spin configuration is complicated by the dynamical nature of the spins which can rotate, and of the frustrated bonds which can hop. Symmetry property (a) should hold as long as the density of the frustrated bond is sufficiently small, as in the case for La_2CuO_4 where the typical hole density range is below 0.3 [6]. The symmetry property (b) is modified to accommodate the bond orientation $\boldsymbol{v}_i$, but otherwise we expect it to hold as long as $K \gg J$. Problems arise in (c) and (d) because now the boundary $\mathcal{B}$ is no longer well defined. We expect, instead of a tiny core around the frustrated bonds, a string of site spins perturbed by the hopping holes that create the frustrated bonds. The typical size of the patch of spins perturbed by the hopping holes is determined by the hopping kinetic energy E_h and the magnetic exchange J. If $J \gg E_h$, then the site spins will quickly rotate so as to adjust to the local environment as soon as the hole hops to their neighbourhood, to create a frustrated bond. This is a quasi-static scenario which allows one to define a core boundary and apply the above notion of homotopy. On the other hand, when $J \ll E_h$, the site spins will take a typical time $\tau \simeq 1/J$ to rotate, but within this time the hole has hopped away, rendering the notion of a core of frustration obsolete. These results can equally apply to the case of one or several ferromagnetic frustrated bonds of strength $K' = -K$ on an antiferromagnetic Heisenberg magnet of strength $J' = -J$—we just have to partition the square lattice into two sublattices. Indeed, the above remarks on La_2CuO_4 assume ferromagnetic frustrated bonds in an antiferromagnet.

These investigations into the ground state properties of Heisenberg magnets with frustrations indicate the relevance of the XY model in the study of classical spin systems. It is expected that these results should have relevance in the corresponding quantum systems as we replace the bare coupling J and K by the renormalised values [7].

Discussion with Dr T K Ng is appreciated. K Y Szeto acknowledges support via grant (Canada) NSERC-URF0035153.

References

[1] Belavin A A and Polyakov A M 1975 *JETP Lett.* **22** 245
[2] Aharony A *et al* 1988 *Phys. Rev. Lett.* **60** 1330
[3] Birgeneau R J *et al* 1988 *Z. Phys.* B **71** 57
[4] Endoh Y *et al* 1988 *Phys. Rev.* B **37** 7443
[5] Szeto K Y 1990 *Physica C* to appear; unpublished
[6] Torrance J D *et al* 1988 *Phys. Rev. Lett.* **61** 1127
[7] Chakravarty S *et al* 1988 *Phys. Rev. Lett.* **60** 1057