The ground state of the classical Heisenberg model on the triangular lattice

Shigetoshi Katsura and Tsugio Ide

Department of Applied Physics. Tohoku University. Sendai

Recently magnetic properties of magnetic materials on the triangular lattice have attracted much attention. Most of them, however, are based on the Ising model. In this paper, the ground state of the classical Heisenberg model with first and second neighbor interaction on the triangular lattice are obtained by the method of Yoshimori[1] and Nagamiya[2], and the conditions for the 120° structure and the screw spin structure are classified. The Hamiltonian is given by

$$H = -\frac{1}{2}\sum_{\ell}\sum_{r} I(r) S_{\ell}\cdot S_{\ell+r}$$

$$= -\frac{1}{2}\sum_{q} J(q)\sigma_{q}\cdot\sigma_{-q} \qquad (1)$$

where

$$S_{\ell}\cdot S_{\ell} = 1 \qquad (2)$$

$$J(q) = \sum_{r} I(r)\exp(-iq\cdot r) \qquad (3)$$

$$\sigma_{q} = \frac{1}{N}\sum_{\ell} S_{\ell}\exp(-iq\cdot\ell) \qquad (4)$$

$$\sum_{q} \sigma_{q}\cdot\sigma_{-q} = 1 \qquad (5)$$

$$\sum_{q} \sigma_{q}\cdot\sigma_{q'-q} = 0 \qquad (6)$$

Assuming that the single Q (and -Q) satisfying (5) makes (1) the maximum we have

$$H = -\frac{1}{2}J(Q) \qquad (7)$$

$$S_{\ell} = i\cos(Q\cdot\ell+\alpha) + j\sin(Q\cdot\ell+\alpha) \qquad (8)$$

where i and j are a set of orthogonal unit vectors in the spin space (the axis is independent of that in the configuration space).

The coordinate of the triangular lattice is shown Fig.1. The J(Q) of the classical Heisenberg model for the triangular lattice with first (J_1) and second (J_2) neighbor interaction is given by

$$J(Q)=2J_1[\cos Q_x + \cos Q_y + \cos(Q_x-Q_y)]$$

$$+2J_2[\cos(Q_x+Q_y) + \cos(2Q_x-Q_y) + \cos(Q_x-2Q_y)] \quad (9)$$

$$=2J_1(2XY+2Y^2-1) + 2J_2[2X^2-1+2XY(4Y^2-3)] \quad (10)$$

where

$$X = \cos\frac{Q_x+Q_y}{2} \qquad Y = \cos\frac{Q_x-Q_y}{2} \quad (11)$$

The condition $\partial J(Q)/\partial Q_x=\partial J(Q)/\partial Q_y=0$ gives

$$[J_1Y+J_2(2X+4Y^3-3Y)](1-X^2)^{1/2} = 0 \quad (12)$$

$$[J_1(X+2Y)+J_2(12XY^2-3X)](1-Y^2)^{1/2} = 0 \quad (13)$$

The solution of (12) and (13) are classified in Table 1 and shown in Fig.2 in the first Brillouin zone. The domain in J_1-J_2 plane of the appearances of each configurations are shown in Fig.3. The spin configulations are classified in 4 patterns. They are shown in Fig.4 A-D . Pattern in type D is a screw configlation and the period depends on $\xi\equiv J_1/J_2$.

The ground state in the hexagonal lattice is now under investigation.

[1] A. Yoshimori, J. Phys. Soc. Japan 14 807 (1959)

[2] T. Nagamiya, Solid State Phys. 20 305 (1967)

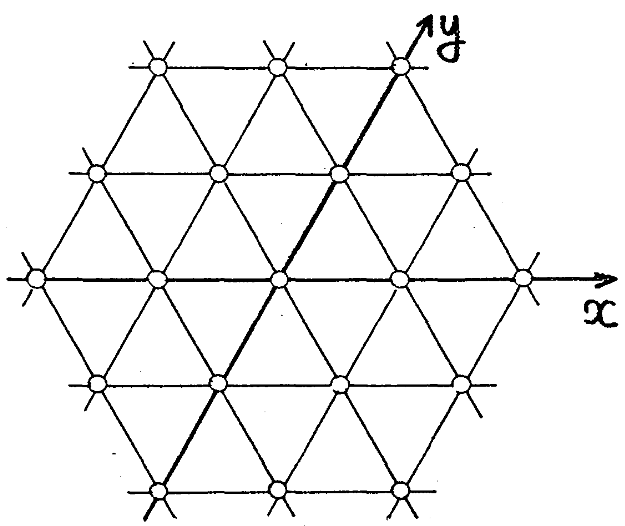

Fig. 1 Triangular lattice and the oblique coordinate used in the present paper.

Table 1

Type		(X,Y)	(Q_x, Q_y)	Energy per spin
A	1	(1 , 1)	(0 , 0)	$-3J_1(1 + \frac{1}{\xi})$
	2	(-1 , -1)	(2π , 0)	
B	3	(1 , $-\frac{1}{2}$)	($\frac{2}{3}\pi$, $-\frac{2}{3}\pi$)	$-3J_1(-\frac{1}{2} + \frac{1}{\xi})$
	4	(-1 , $\frac{1}{2}$)	($\frac{4}{3}\pi$, $\frac{2}{3}\pi$)	
C	5	(1 , -1)	(π , $-\pi$)	$J_1(1 + \frac{1}{\xi})$
	6	(-1 , 1)	(π , π)	
	7	(0 , 0)	(π , 0)	
D	8	$(-\frac{1}{2}(\xi + 1), 1)$	$(\cos^{-1}X, \cos^{-1}X)$	$\frac{J_1}{2}(\xi + \frac{3}{\xi})$
	9	$(\frac{1}{2}(\xi + 1), -1)$	$(\cos^{-1}X + \pi, \cos^{-1}X - \pi)$	
	10	$(\frac{1}{2}(1-\xi)^{\frac{1}{2}}, \frac{1}{2}(1-\xi)^{\frac{1}{2}})$	$(\cos^{-1}X+\cos^{-1}Y, \cos^{-1}X-\cos^{-1}Y)$	
	11	$(-\frac{1}{2}(1-\xi)^2, -\frac{1}{2}(1-\xi)^2)$	$(\cos^{-1}X+\cos^{-1}Y, \cos^{-1}X-\cos^{-1}Y)$	
E	12	$(1, -\frac{1}{6}\xi + \frac{1}{2})$	$(\cos^{-1}Y, -\cos^{-1}Y)$	$-J_1(\frac{\xi^2}{54} - \frac{\xi}{3} + \frac{1}{2} - \frac{1}{\xi})$
	13	$(-1, \frac{1}{6}\xi - \frac{1}{2})$	$(\pi+\cos^{-1}Y, \pi-\cos^{-1}Y)$	
	14	$(\frac{\xi}{6}(3-\frac{\xi}{3})^{\frac{1}{2}}, -\frac{1}{2}(3-\frac{\xi}{3})^{\frac{1}{2}})$	$(\cos^{-1}X+\cos^{-1}Y, \cos^{-1}X-\cos^{-1}Y)$	
	15	$(-\frac{\xi}{6}(3-\frac{\xi}{3})^{\frac{1}{2}}, \frac{1}{2}(3-\frac{\xi}{3})^{\frac{1}{2}})$	$(\cos^{-1}X+\cos^{-1}Y, \cos^{-1}X-\cos^{-1}Y)$	

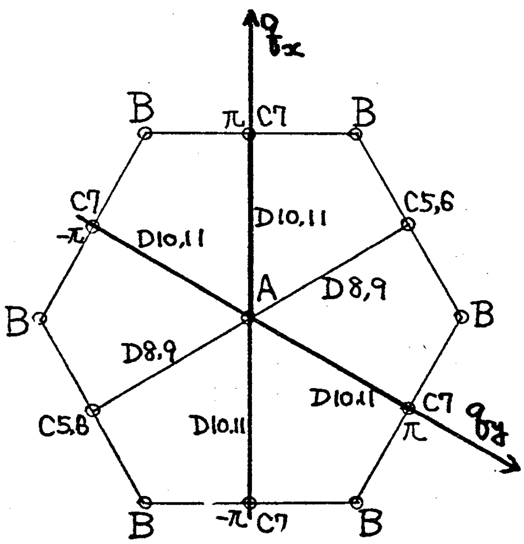

Fig. 2 First Brillouin zone of the triangular lattice. A,B,C,D and the number shows the spin pattern of the ground states.

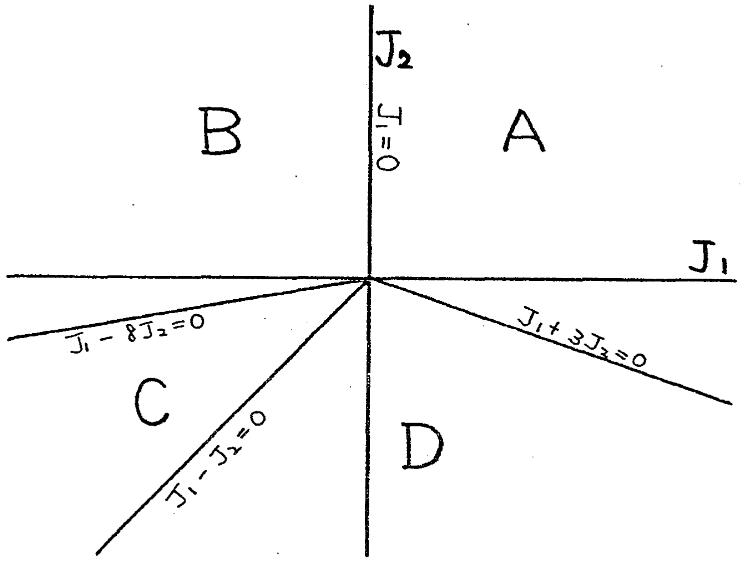

Fig. 3 Phase diagram of the triangular lattice in J_1-J_2 plane.

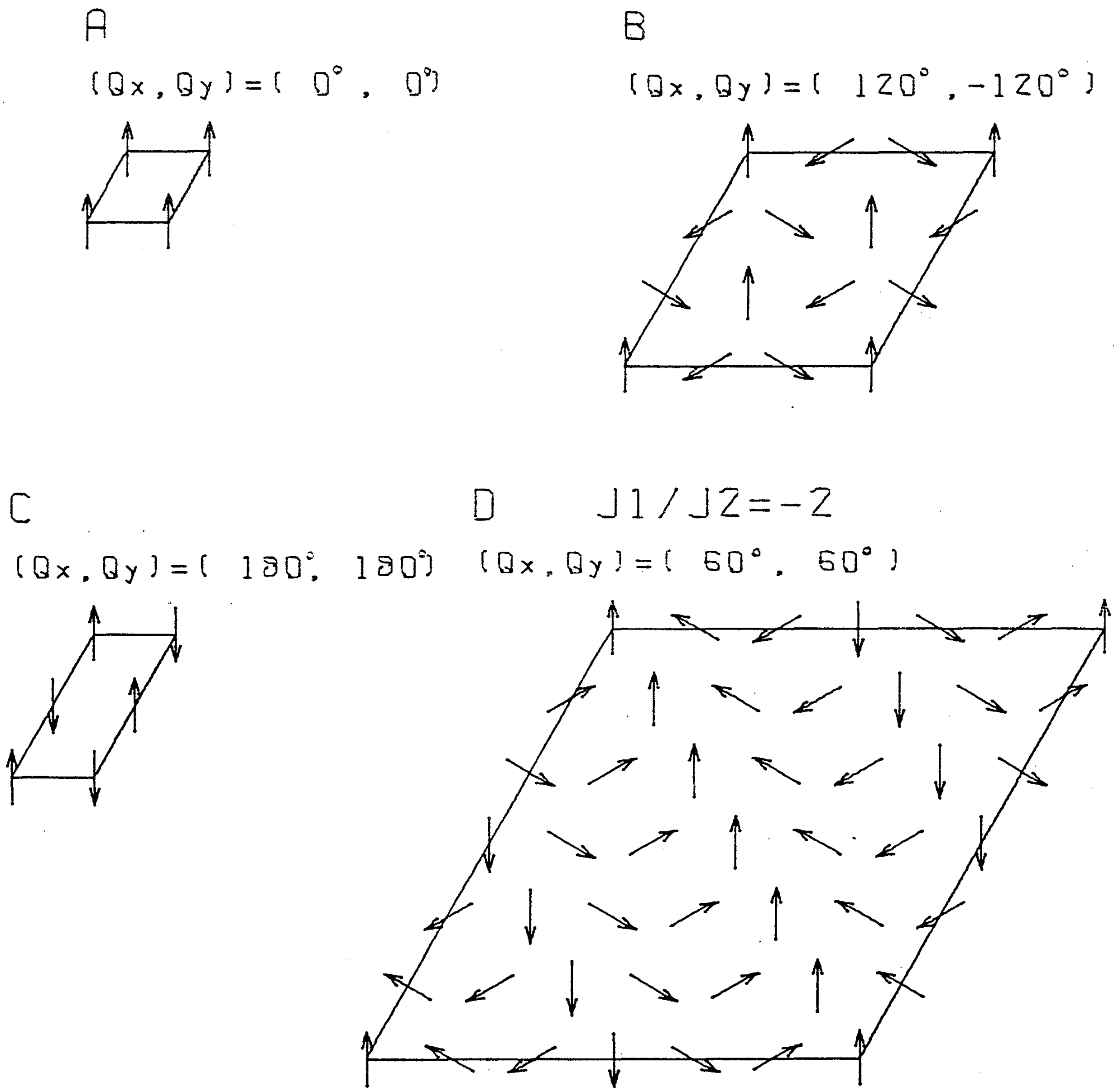

Fig. 4 Spin pattern in the ground state of the triangular lattice.