Classical Ring-exchange Processes on the Triangular Lattice

June Seo Kim, Jung Hoon Han

Department of Physics and Institute for Basic Science Research, Sungkyunkwan University, Suwon 440-746, Korea
CSCMR, Seoul National University, Seoul 151-747, Korea

Abstract

The effects of the ring-exchange Hamiltonian $H_3 = J_3 \sum_{(ijk)} (S_i \cdot S_j)(S_i \cdot S_k)$ on the triangular lattice are studied using classical Monte Carlo simulations. Each spin $S_i$ is treated as a classical XY spin taking on $Q$ equally spaced angles ($Q$-states clock model). For $Q = 6$, a first-order transition into a stripe-ordered phase preempts the macroscopic classical degeneracy. For $Q > 6$, a finite window of critical phase exists, intervening between the low-temperature stripe phase and the high-temperature paramagnetic phase.

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The importance of higher-order ring-exchange processes in low-dimensional magnets and its potential role in stabilizing liquid-like exotic ground states has recently been under intense investigation[1,2]. Generically the Hamiltonian is of the type

$$H = \sum_{n \geq 2} H_n$$

with $H_n$ for $n = 2, 3, 4$ given by

$$H_2 = J_2 \sum_{(ij)} S_i \cdot S_j$$
$$H_3 = J_3 \sum_{(ijk)} (S_i \cdot S_j)(S_i \cdot S_k)$$
$$H_4 = J_4 \sum_{(ijkl)} (S_i \cdot S_j)(S_k \cdot S_l).$$

(2)

Each $S_i$ is a Heisenberg spin, and $(ij)$, $(ijk)$ and $(ijkl)$ refer to nearest-neighbor pair, triplet, and quartet of sites, respectively.

In particular the possibility to realize a stable spin-liquid ground state due to $H_3$ in a two-dimensional triangular lattice has been suggested in the variational Monte Carlo study of Motrunich[2]. It may be inferred that the three-site exchange process has the “frustrating” effect which renders the liquid ground state energetically more stable over a $\sqrt{3} \times \sqrt{3}$ magnetically ordered structure.

In this paper, we report the first results of isolating the effects of the three-site exchange process by studying the following model. First, we consider the classical counterpart of the Hamiltonian (1) where $S_i$ is treated as a unimodular vector. Secondly, only $H = H_3$ is considered in this paper while leaving the study of the compound models such as $H = H_2 + H_3$ or $H = H_2 + H_3 + H_4$ for the future. Thirdly, we consider the planar spin $S_i = (\cos \theta_i, \sin \theta_i)$. The angle $\theta_i$ is divided up into $Q$ equally spaced segments. The same strategy had been applied for $H = H_2$ as a way to asymptotically approach the behavior of the XY model ($Q = \infty$) and is known as the $Q$-states clock model[3,4].

Antiferromagnetic $Q$-states models on a triangular lattice have double transitions of XY- and Ising-types with extremely close critical temperatures[5]. The same subtlety might pervade the $H = H_3$ model too, but here we choose to focus on the broader issue: What is the nature of the low-temperature phase exhibited by $H = H_3$? The results for $Q = 2$ and $Q = 6$ are discussed in detail in this paper. Some preliminary specific heat data for larger $Q$ are presented.

$Q=2$: It turns out that $Q = 2$ model maps onto the antiferromagnetic Ising model on the triangular net, first
studied by Wannier[8]. In the Ising case spins take on \( S_i = \pm 1 \), and the Hamiltonian \( H_3 \) reduces to

\[
(S_i \cdot S_j)(S_i \cdot S_k) \rightarrow S_j S_k, \quad H_3 \rightarrow 2J_3 \sum_{ij} S_i S_j, \tag{3}
\]

which is the antiferromagnetic Ising model. This model possesses macroscopic degeneracy[8,9] which is also revealed as the residual entropy \( S_0 \). Our Monte Carlo (MC) calculation gives \( S_0 \approx 0.323k_B \), in excellent agreement with the value predicted earlier[8,9]. There is no long-range order down to zero temperature in this model.

With \( Q \geq 3 \) \( H_2 \) and \( H_3 \) are no longer equivalent. The lowest-energy configurations for \( H_3 \) consist of two-up and one-down (or vice versa) spins for each elementary triangle. Thus, macroscopic degeneracy is a general feature of \( H = H_3 \) for an arbitrary even integer \( Q \). It is also well known that the magnetic ordering for \( H = H_2 \) is obtained for angles of 120° between nearest-neighbor spins. Such situations are possible if \( Q \) is a multiple of 3. To allow the realization of both, we consider the case \( Q = 6 \).

\( Q=6 \): With \( Q = 6 \) we observed a first-order transition at \( T_c/J_3 \approx 1.05 \). Hysteresis in the average energy and the order parameter (defined below) in our MC runs vindicate the first-order nature, as shown in Fig. 1.

The nature of the low-temperature, ordered phase is clearly demonstrated in Fig. 1. We find the spontaneous emergence of stripe-like domains of up and down spins below \( T_c \). The ground state degeneracy is lifted through the order-from-disorder mechanism[6,7]. While a conventional order-from-disorder idea predicts the gradual separation of the free energies of different classical ground state configurations with rising temperatures and no phase transition, our model exhibits a first-order transition which pre-empts the classical macroscopic degeneracy. The difference is due to the discrete nature of our model. The order parameter appropriate for this stripe-like configuration is

\[
m = \frac{1}{N} \left| \sum_i (-1)^{i_1} S_i \right|, \tag{4}
\]

where each lattice site is given the coordinate \( i = i_1 \hat{e}_1 + i_2 \hat{e}_2, \hat{e}_1 = \hat{x}, \hat{e}_2 = -\hat{x}/2 + \sqrt{3} \hat{y}/2 \), and \( N \) is the number of sites.

\( Q>6 \): For a finer spin segmentation we still obtain the low-temperature stripe-like phase. A single first-order phase transition observed for \( Q = 6 \) is split into two transitions, at temperatures \( T_1 \) and \( T_2 \) with \( T < T_1 \) being the stripe-ordered phase. The intermediate phase \( T_1 \leq T \leq T_2 \) appears to be critical[4,10].

![Fig. 1. Low-temperature configuration for the \( Q = 6 \) model, \( H = H_3 \). Ferromagnetic ordering within a diagonal stripe and antiferromagnetic ordering between adjacent stripes are apparent in (a). Both the average energy (b) and the average magnetization (c) data are consistent with the first-order phase transition to the low-temperature phase.](image)

![Fig. 2. Specific heat \( C(T)/T \) for \( Q = 12, H = H_3 \), for \( 48 \times 48 \) and \( 72 \times 72 \) lattices. The two peaks are indicative of the presence of two phase transitions. The low temperature phase is given by the stripe configuration shown in Fig. 1.](image)

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