

# Effects of magnetic clusters on the helicity modulus and the BKT transition in a two dimensional diluted-magnetic system

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We develop a program to generate a two dimensional square lattice of which the number of magnetic sites and the size of magnetic clusters are adjustable. We adopt the lattice-generating program to study effects of magnetic clusters on the Berezinskii-Kosterlitz-Thouless transition and the helicity modulus in a two dimensional XY model of a diluted magnetic system via hybrid Monte Carlo simulations. We further show that the next nearest neighbor interaction is necessary near a clusterless lattice configuration.

## I. INTRODUCTION

Recently, a diluted magnetic material, such as Mn-doped GaAs<sup>1</sup>, Mn-doped GaP<sup>2</sup>, and Cr-doped ZnTe<sup>3</sup>, has been a focus of modern material research. Normally, in a presence of nonmagnetic impurities, magnetic properties and phase transition of a diluted magnetic system are different from those of a pure magnetic system. A powerful tool for analyzing thermodynamic properties of diluted magnetic materials is a Monte Carlo simulation. Wysin and Pereira *et al.* apply hybrid Monte Carlo simulations to study the Berezinskii-Kosterlitz-Thouless transition (BKT transition) in a two dimensional XY model when magnetic atoms randomly occupy a square lattice<sup>4</sup>. However, many works suggest that magnetic atoms tend to form clusters rather than randomly distribute over a lattice; for example, see ref 5-6. In this paper, we attempt to expand the work by Wysin and Pereira *et al.* by examining effects of magnetic clusters on a BKT transition temperature and on a helicity modulus of a two dimensional XY model on a square lattice.

A brief outline of the paper is as follow: In section 1, we develop a program to generate a square lattice that allows us to control both the number of magnetic sites and the size of magnetic clusters. In section 2, we review the XY model in two dimensions, provide the meaning of the helicity modulus and its relationship to the BKT transition temperature in a diluted magnetic system, and review the work of Wysin and Pereira. Then we examine the effect of magnetic clusters on the helicity modulus and the BKT transition temperature from a lattice generated in section 1. In section 3, the next nearest neighbor correction to the Hamiltonian is added and its effect on the helicity modulus in a highly diluted system is investigated.

## II. LATTICE GENERATION AND ANALYSIS

In this section, we develop a lattice model with an adjustable size of cluster and adjustable number of magnetic sites which will later be adopted in the next following sections.

### A. The Metropolis algorithm for lattice generation

To generate a square lattice with adjustable size of magnetic cluster, we convert an Ising model with fixed magnetization into a percolation problem with a fixed number of occupied sites where (un)occupied sites are understood as (non-)magnetic sites. For an Ising model with fixed magnetization, the Hamiltonian of the system is written as

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + M, \quad (1)$$

where the magnetization is given by

$$M = \sum_i \sigma_i. \quad (2)$$

The mapping into a percolation problem with a fixed number of occupied sites can be done by interpreting a site with an up spin as an occupied site, a site with a down spin as a vacant site, and assigning the value of an occupied site with  $\sigma_i = +1$  whereas  $\sigma_i = 0$  for a vacant site. The assignment of  $\sigma_i$  is distinct from an Ising model in which  $\sigma_i$  is either +1 or -1. At an equilibrium, a fixed magnetization is then interpreted as a fixed number of occupied sites by the mapping

$$M = \sum_i \frac{\sigma_i}{N} N \equiv pN, \quad (3)$$

where  $N$  is the number of sites, and  $p$ , the ratio of the number of occupied sites to the total number of sites, is an occupation probability of a percolation problem. We note on a few points on the Ising to percolation mapping. First, in this modified percolation problem, a magnetization  $M$  in (3) is equivalent to the number of occupied sites as opposed to a magnetization in an Ising model which can take either positive or negative value. Second, unlike a typical percolation problem in which the likelihood of a site to be occupied solely depends on an occupation probability  $p$ , a *cluster parameter*  $J$  also plays an important role in inducing the nearest neighbor site to form an occupied cluster or an anti-cluster. For a positive  $J$ , the probability that an occupied cluster will form

is enhanced, while the probability that any cluster will form is reduced (enhanced anti-cluster) when  $J$  is negative. We expect that as  $J$  increase, occupied sites will form larger clusters.

Next, we write a program to generate a  $32 \times 32$  lattice with a periodic boundary condition using the Metropolis algorithm which is summarized as follow<sup>7,8</sup>:

1. Create a lattice with down spin on every site. Randomly pick  $pN$  sites and associate them with up spin.
2. Calculate and define the energy of the system as  $E_{old}$ .
3. Randomly choose one site with up spin and one site with down spin, then interchange their spins. Calculate and define the energy of the system as  $E_{new}$ .
4. Define  $\Delta E = E_{new} - E_{old}$ . If  $\Delta E < 0$ , do nothing. Otherwise, interchange spins of the two sites back to the original configuration with probability  $1 - e^{-\beta\Delta E}$ .
5. Repeat step 2 to 4 until the equilibrium is met, i.e. the average cluster size of the lattice is unchanged.

### B. Properties of a lattice at various $p$ and $J$

Some analysis on generated lattices are given in this subsection as a sanity check of our model. Examples of lattices generated by this algorithm are demonstrated in figure 1 to 5. Figure 6 demonstrates the average cluster size in a  $32 \times 32$  lattice for some values of  $J$  and  $p$ . As expected, the occupied sites tend to form larger clusters as  $J$  and  $p$  increase. Figure 7 shows the phase transition of the system from no-percolation to percolation as we vary  $p$ . The result suggests that larger  $J$  enhances the percolation probability of the occupied sites. Table 1 lists the percolation critical probability,  $p_c$ , for some values of  $J$  where we define  $p_c$  to be an occupation probability when the probability to percolate reaches 0.5. The reason for defining  $p_c$  is due to a finite size effect which slowly increases the probability to percolate from 0 to 1 as a function of  $p$  instead of switching instantaneously from 0 to 1 around some  $p$  as in an infinite lattice system. For a typical percolation problem ( $J = 0.0$ ), we obtain  $p_c = 0.58$  which agrees within 3% with  $p_c \approx 0.5931$  which is the result from the precision Monte Carlo simulation on a large lattice.<sup>9</sup>

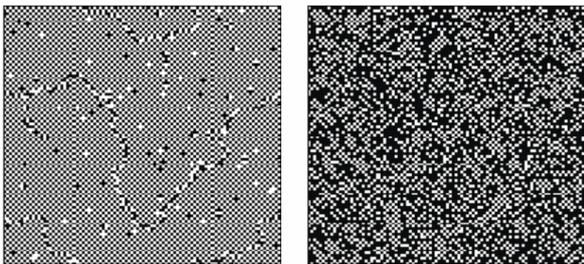


Figure 1: a lattice generated at  $J = -0.6, p = 0.5$ (left) and  $p = 0.7$ (right)

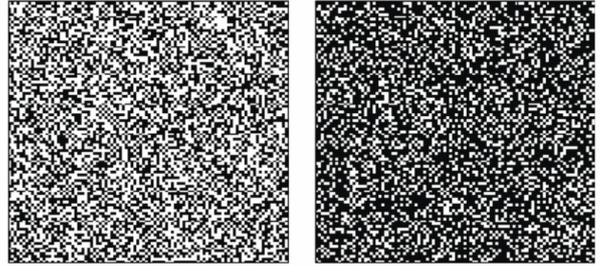


Figure 2: a lattice generated at  $J = -0.2, p = 0.5$ (left) and  $p = 0.7$ (right)



Figure 3: a lattice generated at  $J = 0.0, p = 0.5$ (left) and  $p = 0.7$ (right)

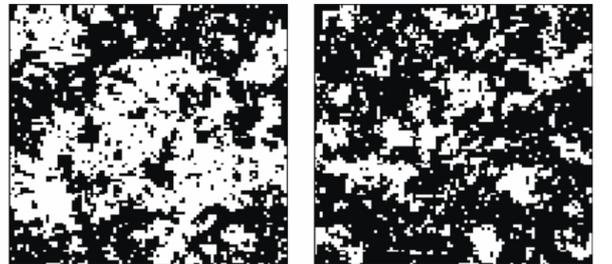


Figure 4: a lattice generated at  $J = 0.4, p = 0.5$ (left) and  $p = 0.7$ (right)

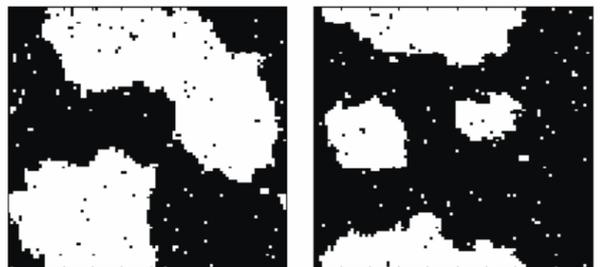


Figure 5: a lattice generated at  $J = 0.6, p = 0.5$ (left) and  $p = 0.7$ (right)

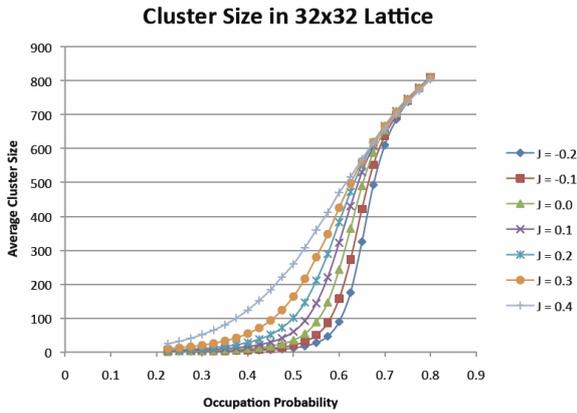


Figure 6: graphs of an average cluster size on a  $32 \times 32$  lattice as a function of occupation probability  $p$  for some values of  $J$

$J$	$p_c$
-0.2	0.62
-0.1	0.60
0.0	0.58
0.1	0.56
0.2	0.54

Table 1: critical occupation probability  $p_c$  at some values of cluster parameter  $J$

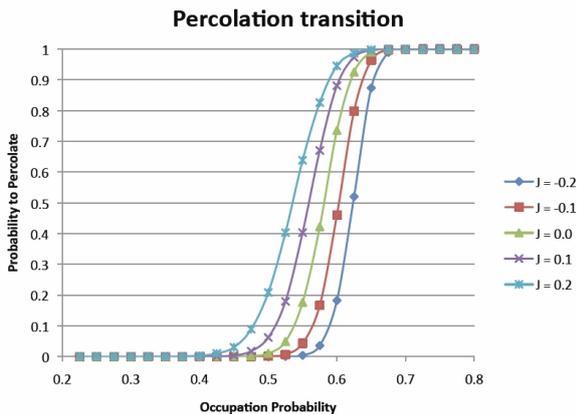


Figure 7: graphs of percolation probability as a function of occupation probability  $p$  at some values of cluster parameter  $J$

### III. EFFECTS OF MAGNETIC CLUSTERS

#### A. The BKT transition, the helicity modulus and all that

The Hamiltonian of a two dimensional XY model on a square lattice is given by

$$H = -K \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \quad (4)$$

This system exhibits the Berezinskii-Kosterlitz-Thouless phase transition (BKT phase transition). The magneti-

zations at a zero external magnetic field of both ordered and disordered phase vanishes. However, in the ordered phase ( $T < T_c^{BKT}$ ), the correlation function decays algebraically as opposed to decaying exponentially in the disordered phase ( $T > T_c^{BKT}$ ). One can imagine the disordered phase as spins pointing in completely random directions, while in the ordered phase spins gradually twist from one site to the nearest neighbor sites. But still, there is no special direction in the ordered phase. The different behaviors of correlation function at the two phases can be understood by pairing and screening mechanism of vortices and anti-vortices.

One way to find  $T_c^{BKT}$  is to analyze the helicity modulus or the magnetic stiffness of the system. The helicity modulus measures a free energy changed caused by an infinitesimal twisting of spins across the system along one direction<sup>10</sup>,

$$\gamma = \frac{\partial^2 f}{\partial \Delta^2} \quad (5)$$

where  $\gamma$  is the helicity modulus,  $f$  is the free energy per site,  $\Delta$  is a small twisted angle across the system along one direction. The value of  $\gamma$  is finite in the ordered phase and vanishes in the disordered phase. The Kosterlitz-Thouless renormalization group equation<sup>11</sup> implies a universal jump in the value of  $\gamma$  from  $\frac{2}{\pi} T_c^{BKT}$  to 0 at the critical temperature,  $\lim_{T \rightarrow T_c^{BKT}} \frac{\gamma}{k_b T} = \frac{2}{\pi}$ . Equivalently,

$$\gamma_c = \frac{2}{\pi} k_b T_c^{BKT} \quad (6)$$

Although the renormalization group equation leading to (6) assumes a pure magnetic system to begin with, an argument is made by Castro, Pires, and Plascak that the helicity modulus at the transition temperature is independent of nonmagnetic impurities concentration<sup>12</sup>. In other words, (6) is still applicable in a diluted magnetic system.

#### B. Randomly occupied lattice and the BKT transition

We first give a review of the work by Wysin and Pereira *et al.* on BKT transition in a 2-d XY model of a diluted magnetic system<sup>4</sup>. When sites can be occupied by either magnetic atoms or non-magnetic atoms, the Hamiltonian of the system is modified to

$$H = -K \sum_{\langle i,j \rangle} \sigma_i \sigma_j \cos(\theta_i - \theta_j) \quad (7)$$

where  $\sigma_i = 1$  for an occupied site (magnetic site) and 0 otherwise. The interaction of an unoccupied site with its nearest neighbors contributes zero magnetic energy, independent of a nearest neighbor configuration. From (5), the Helicity modulus can be rewritten as

$$N\gamma = \left\langle \frac{\partial^2 H}{\partial \Delta^2} \right\rangle - \beta \left\{ \left\langle \left( \frac{\partial H}{\partial \Delta} \right)^2 \right\rangle - \left\langle \frac{\partial H}{\partial \Delta} \right\rangle^2 \right\} \quad (8)$$

Following ref. 4, the first and second partial derivative of the Hamiltonian with respect to an infinitesimal twisted can be expressed as

$$\frac{\partial H}{\partial \Delta} = \sum_{\langle i,j \rangle} \sigma_i \sigma_j (\hat{e}_{i,j} \cdot \hat{x}) \sin(\theta_i - \theta_j) \equiv G_s \quad (9)$$

$$\frac{\partial^2 H}{\partial^2 \Delta} = \frac{1}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j \cos(\theta_i - \theta_j) \equiv G_c \quad (10)$$

where  $K$  is chosen to be unity,  $\hat{e}_{i,j}$  denotes a unit vector pointing from the site  $i$  to the site  $j$ , and  $\hat{x}$  denotes a unit vector pointing in the x-direction. By utilizing hybrid Monte Carlo simulations<sup>4,13,14</sup> which incorporate over-relaxation, cluster spin flip, and simple Monte Carlo to obtain a helicity modulus as a function temperature, the critical temperature can then be estimated from the intersection between the curve  $\gamma(T)$  and the straight line  $\gamma = \frac{2}{\pi} k_b T$ , which has the same functional form of the helicity modulus at the critical temperature as in (6).

The result is that the BKT transition is not manifested ( $T_c^{BKT} \rightarrow 0$ , meaning that it is impossible to further reduce a temperature to reach the ordered phase, dominated by spin waves.) when the occupation probability  $p$  decreases to 0.59 which is the same value as the critical probability of percolation in 2-d lattice. The conclusion is that when the vacancy reaches the percolation threshold, the long-ranged correlation between spins is disrupted, and the ordered phase does not exist.

### C. Effects of $J$ on $\gamma$ and $T_c^{BKT}$

We now explore effects of clustering of magnetic atoms on the Helicity modulus and the BKT transition, generalizing the analysis of a randomly occupied lattice above. Adopting lattice generated in section 2, we run hybrid Monte Carlo simulations for different values of cluster parameter  $J$  to find the helicity modulus  $\gamma$  as a function of temperature. The algorithm is outlined below:

1. Create a lattice with fixed occupation probability  $p$  and cluster parameter  $J$  from a metropolis algorithm described in section 2.
2. Apply an over-relaxation method to all spins in the lattice, and follow by a few simple Monte Carlo steps. In an over-relaxation step, we create a new spin configuration by evolving each spin on the original lattice by the Metropolis algorithm. This step of evolving each spin by a small rotation is an approximate method that greatly reduces a run time to reach an equilibrium result. In simple Monte Carlo steps, a site is randomly picked to evolve following the Metropolis algorithm.
3. Calculate  $G_s$ ,  $G_s^2$ , and  $G_c$ .
4. Repeat step 2 and 3 for  $2 \times 10^4$  times, then perform

thermal average to calculate  $\gamma$ . We note that during steps 2 to 4, we calculate  $\gamma$  as a function of temperature. The annealing method that reduces run time of reaching equilibrium at low temperature is to begin the computation at high temperature, then reduce the temperature of the same configuration down and continue the process until reaching the desired temperature.

5. Repeat steps 1 to 4 and average the results. The number of repetition to obtain a reasonable average depends on a lattice size. The smaller the lattice size, the more repetition is required due to large relative fluctuation of the results. For a lattice size of  $32 \times 32$ , we limit our calculation to 50 repetitions (50 lattice configurations), due to large time consumption of the program, and obtain sensible results though 100 repetition yields much improved precision.

We run simulations for  $J = 0$  at some  $p > 0.6$  and found that the results agree with ref. 4 within 15% error. However, as  $p$  decreases down below 0.6, the error grows significantly. Near the percolation probability  $p_c = 0.59$  at which the transition temperature is expected to be in the vicinity of zero, an error in the transition temperature is relatively large. Also, the transition temperature does not converge to zero as we reduce  $p$  down below 0.59. Unfortunately, our program alone is not sufficient to estimate a critical occupation probability  $p_c$  below which the BKT transition is extinguished. We suspect the main source of error comes from our lattice size of  $32 \times 32$  which is too small to obtain accurate transition temperature. A precision of transition temperature can be improved by a finite-size scaling and by extending the lattice size. We hope to make an accuracy improvement in a future work in order to predict as a function of  $J$  a critical probability under which there is no BKT transition and we doubt that the relationship roughly follows table 1 as is the case of  $J = 0$ . Nevertheless, without too much concern about the precision of the transition temperature, we manage to observe broad effects of clusterness on BKT transition quantitatively at large occupation probability. From figure 9, at  $p = 0.7$ , both the transition temperature and the helicity modulus near zero temperature increase monotonically with  $J$ . The explanation is that as  $J$  increases, the occupied sites tend to form larger clusters; as a result, it is more difficult for the vacancy to disrupt the long-ranged topological correlation of the system.

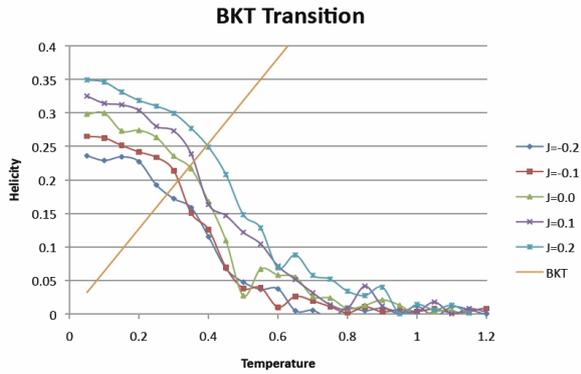


Figure 8: Graphs of helicity modulus as a function of temperature at a fixed occupation probability  $p = 0.7$  for some values of  $J$

#### IV. NECESSITY OF THE NEXT NEAREST NEIGHBOR INTERACTION IN A HIGHLY DILUTED REGIME

Let us first consider a diluted magnetic material with a fixed occupation probability  $p = 0.5$ , i.e. 50% magnetic atoms and 50% non-magnetic atoms on a lattice. In the limit  $J \rightarrow -\infty$ , the magnetic atoms will occupy every other site as in figure 10. When we run simulations in section 3 to find the helicity modulus, it turns out that the helicity modulus vanishes. This is not surprising because a lattice in a highly negative  $J$  limit has no nearest neighbor magnetic interaction regardless of spin configurations of the occupied sites; therefore, the free energy is independent of a spin configuration.

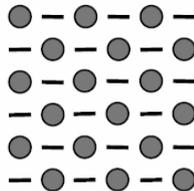


Figure 9: A portion of sites from a lattice in the limit  $J \rightarrow -\infty$  at a fixed  $p = 0.5$

However, adding the next nearest neighbor interaction generates a free energy that depends on a spin configuration on a lattice in figure 10 which might yield a non-vanishing helicity modulus. The Hamiltonian then becomes

$$H = -K_1 \sum_{\langle i,j \rangle_1} \sigma_i \sigma_j \cos(\theta_i - \theta_j) - K_2 \sum_{\langle i,j \rangle_2} \sigma_i \sigma_j \cos(\theta_i - \theta_j) \quad (11)$$

where  $K_1 > K_2 > 0$ ;  $\langle i,j \rangle_1$  and  $\langle i,j \rangle_2$  denote the first and second nearest neighbor pair.

Again, we study this system from hybrid Monte Carlo simulations. The method is analogous to the one outlined in section 3 part c. For  $K_1 = 1$  and  $K_2 = 0$ , results agree with section 3. We then run the simulation at  $K_1 = 1$  and  $K_2 = 0.37$ . The result is shown in figure 10.

From the graph, we obtain the helicity modulus for  $T$  near 0 ( $\gamma_0$ ), specifically at  $T = 0.2$ , and for  $T = T_c^{BKT}$  ( $\gamma_c$ ). For  $J \leq 0$ , both  $\gamma_0$  and  $\gamma_c$  increase for decreasing  $J$ . This behavior is not observed in section 3 where the helicity modulus near zero temperature decreases as  $J$  decreases as seen in figure 8. We next compute and graph the ratio  $\frac{\gamma_0}{\gamma_c}$  which is plotted in figure 11. In a highly negative  $J$  regime, the system is rather uniform with an occupied site surrounded by vacant sites and vice versa; hence, the behavior of the system in this regime is expected to be similar to a pure magnetic system with the interaction strength of the second nearest neighbor interaction  $K_2$  as an effective nearest neighbor interaction. Consequently, the ratio  $\frac{\gamma_0}{\gamma_c}$  should converge to a large saturation value as  $J$  decreases which is roughly shown in figure 11. We thus observe that the second nearest neighbor interaction is not negligible in a highly diluted system as it significantly modifies the behavior of the helicity modulus, and possibly other thermodynamic quantities as well, in a nearly clusterless lattice configuration.

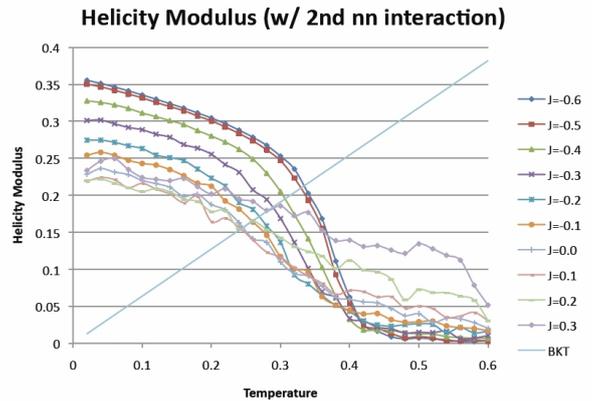


Figure 10: Graphs of helicity modulus as a function of temperature at a fixed  $p = 0.5$  when the 2<sup>nd</sup> nearest neighbor interaction is included. Specifically,  $K_1 = 1$  and  $K_2 = 0.37$ .

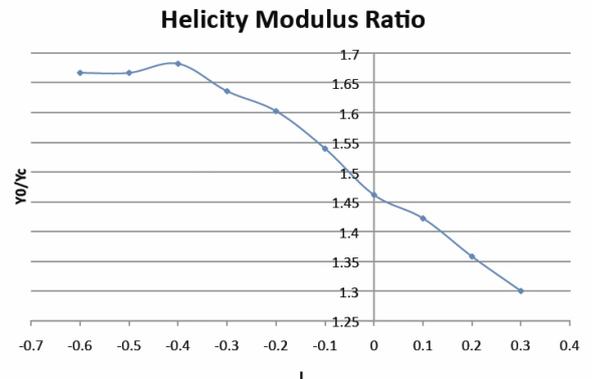


Figure 11: A graph of the helicity modulus ratio  $\frac{\gamma_0}{\gamma_c}$  as a function of  $J$

## V. CONCLUSION AND DISCUSSION

From an Ising to percolation mapping and from a program utilizing the Metropolis algorithm, we are able to generate a two dimensional square lattice and can control both the number of magnetic sites and the size of magnetic clusters via input parameters  $p$  and  $J$ , respectively. The lattice-generating program provides a way to model diluted magnetic materials whose magnetic atoms tend to form clusters. Adopting generated lattices, we found that increasing the size of the magnetic clusters increases both the helicity modulus and the BKT transition temperature. Because the long-range topological correlation in the ordered phase is enhanced when cluster forms, it is more difficult to destroy the correlation and advance into a disordered phase. As a result, the transition temperature is increased. However, in the limit of highly negative cluster parameter  $J$  where the lattice configuration is almost clusterless provided the system is sufficiently diluted, the helicity modulus vanishes. This result suggests that the free energy of the system is independent of spin configurations which is counter intuitive. By adding the second nearest neighbor interaction into our Hamiltonian, the helicity modulus now takes a finite and non-zero value in an almost clusterless lattice

configuration. In a low temperature regime, the helicity modulus increases as  $J$  decreases to a highly negative value (clusterless configuration). This behavior is not observed in the Hamiltonian with only the nearest neighbor interaction. Hence, longer range spin-spin interaction becomes essential in a diluted magnetic system.

We attempt to analyze the effect of cluster parameter  $J$  on the critical occupation probability  $p_c$  below which the BKT transition is not manifested, i.e. the BKT transition temperature approaches zero as  $p_c$  is approached from above. But due to insufficient precision of our method, we are unable to obtain a transition temperature near zero value so the dependence of  $p_c$  on  $J$  can not be extracted. By including a method of finite-size scaling, by increasing the number of repetition in the program to obtain a more accurate average of many quantities, and by expanding the lattice size, we hope to improve the precision of our program in a future work and analyze the dependence of  $p_c$  on  $J$ . A longer range spin-spin interaction, e.g. the third nearest neighbor interaction, can also be added to improve the precision of the helicity modulus when the system is highly diluted. Above all, we need to develop a theoretical understanding of the dependence of thermodynamic properties of diluted magnetic system on both an occupation probability  $p$  and a cluster parameter  $J$ .

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- [1] H. Ohno, *Science* **281**, 951 (1998)
  - [2] N. Theodoropoulou et al., *Phys. Rev. Lett.* **89**, 107203 (2002).
  - [3] H. Saito, V. Zayets, S. Yamagata, and K. Ando, *Phys. Rev. Lett.* **90**, 207202 (2003).
  - [4] G.M. Wysin and A.R. Pereira al., *Phys. Rev. B.* **72**, 094418(2005)
  - [5] D. J. Priour, Jr. and S. Das Sarma, *Phys. Rev. B.* **73** 165203 (2006).
  - [6] S. Wei et al., *Phys. Rev. B.* **77** 245208 (2008)
  - [7] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller, *J. Chem. Phys.* **21**, 1087(1953)
  - [8] K. Binder, *Monte Carlo Methods in Statistical Physics* (Springer, New York, 1979)
  - [9] P.J. Reynolds, H. E. Stanley, and W. Klein, *Phys. Rev. B.* **21** 1223-1245(1980)
  - [10] M.E. Fisher, M.N. Barber and D. Jasnow, *Phys. Rev. A.* **8** 1111-1124(1973)
  - [11] J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6**, 1181 (1973)
  - [12] L.M. Castro, A.S.T. Pires, and J.A. Plascak, *J. Magn. Mater.* **248**, 62(2002)
  - [13] H. G. Evertz and D. P. Landau, *Phys. Rev. B* **54**, 12302(1996)
  - [14] U. Wolff, *Phys. Rev. Lett.* **62**, 361 (1989).
  - [15] S. A. Leonel, P. Zimmermann Coura, A. R. Pereira, L. A. S. Ml, and B. V. Costa, *Phys. Rev. B* **67**, 104426 (2003)
  - [16] M. Kardar, *Statistical Physics of Fields* (Cambridge University Press, 2007)