Vol 18 No 5, May 2009
1674-1056/2009/18(05)/2048-06

Chinese Physics B

© 2009 Chin. Phys. Soc.
and IOP Publishing Ltd

Monte Carlo study of the antiferromagnetical Ising model on a centred honeycomb lattice*

Wang Zhou-Fei(王宙斐)[a)†] and Chen Li(陈 莉)[b)]

[a)] *College of Science, South China Agriculture University, Guangzhou* 510642, *China*

[b)] *College of Physics, Northeast Normal University, Changchun* 130024, *China*

(Received 13 September 2008; revised manuscript received 5 February 2009)

We use the Monte Carlo method to study an antiferromagnetical Ising spin system on a centred honeycomb lattice, which is composed of two kinds of 1/2 spin particles A and B. There exist two different bond energies $J_{\mathrm{A-A}}$ and $J_{\mathrm{A-B}}$ in this lattice. Our study is focused on how the ratio of $J_{\mathrm{A-B}}$ to $J_{\mathrm{A-A}}$ influences the critical behaviour of this system by analysing the physical quantities, such as the energy, the order parameter, the specific heat, susceptibility, etc each as a function of temperature for a given ratio of $J_{\mathrm{A-B}}$ to $J_{\mathrm{A-A}}$. Using these results together with the finite-size scaling method, we obtain a phase diagram for the ratio $J_{\mathrm{A-B}}$ / $J_{\mathrm{A-A}}$. This work is helpful for studying the phase transition problem of crystals composed of compounds.

Keywords: centred honeycomb lattice, antiferromagnetical Ising model, phase transition, Monte Carlo method

PACC: 7450D

1. Introduction

The Ising model on two dimensional lattices has been interesting for a long time due to its concise and significant role in studying various systems in physics.[1−13] However, studies of this model have been mainly focused on the lattice with unitary exchange energies between near neighbour particles. In fact, there should be several different exchange energies on the crystal lattices built by compounds.[14−17] The difference in exchange energy may have an influence on the critical behaviour of the system. Study on this topic should be meaningful for obtaining more information about phase transitions in crystals composed of compounds. In the present paper we study an antiferromagnetical Ising spin system on a two-dimensional centred honeycomb lattice,[15] which is composed of two kinds of Ising spin particles A and B, and there exist two kinds of bonds, A–A and A–B, with bond energies $J_{\mathrm{A-A}}$ and $J_{\mathrm{A-B}}$ respectively. The A–A bonds construct the honeycomb lattice and the A–B bonds construct the diamond lattice as shown in Fig.1. In general, $J_{\mathrm{A-A}}$ is not equal to $J_{\mathrm{A-B}}$. The ratio $J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$ may have an influence on the physical property of the system.

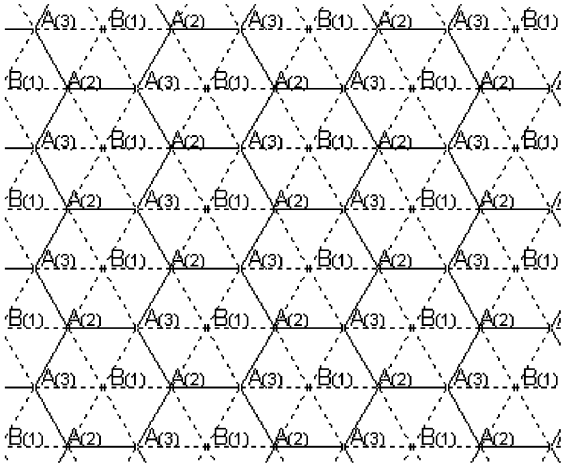


Fig.1. Centred Honeycomb Lattice, where A and B denote two kinds of parcels and (1), (2) and (3) represent the three sublattices with solid line and dashed line representing the A–A bond and A–B bond respectively.

Some studies have been done for spin models on this lattice. Zhang *et al* [16] studied the phase transition problem of the xy model on this lattice by

*Project supported by the National Natural Science Foundation of China (Grant No 10571091) and the National Science and Technology Supporting Program of China (Grant No 2006BAD11A07).

†Corresponding author. E-mail: wangzhoufei@scau.edu.cn

using the mean-field theory. Diep *et al* [17] studied the anisotropic Ising model by using an exact solution method for this lattice, in which reentrance and partial disorder problems were discussed. Using the Monte Carlo method, we investigate the influence of the ratio $J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$, which varies in a large range, on the critical behaviour of the antiferromagnetical Ising spin system of this lattice. For this purpose we examine the pattern where the physical quantities such as energy, order parameter, specific heat, etc change with temperature for various values of $J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$ of the system for several different sizes, and use the finite-size scaling method[18] to obtain information in the case of the thermodynamic limit. The remainder of the present paper is organized as follows. We present the system in Section 2. We study the cases where $J_{\mathrm{A-B}} < J_{\mathrm{A-A}}$ in Section 3 and $J_{\mathrm{A-B}} > J_{\mathrm{A-A}}$ in Section 4. In Section 5, we present phase diagrams for $J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$ and summarize this study.

2. System

The Hamiltonian of the antiferromagnetical Ising spin system on a two-dimensional centred honeycomb lattice is written as

$$H = J_{\mathrm{A-A}} \sum_{i,j\in \mathrm{A-A}} \sigma_i\sigma_j + J_{\mathrm{A-B}} \sum_{i,j\in \mathrm{A-B}} \sigma_i\sigma_j,$$

where $\sigma_i = \pm 1$ is an Ising spin of particles A or B occupying the lattice site i. $J_{\mathrm{A-A}}$ is the exchange energy between near neighbour A–A particles, $J_{\mathrm{A-B}}$ is the exchange energy between near neighbour A–B particles. We separate this lattice into three sublattices, (1), (2) and (3) as shown in Fig.1. For the antiferromagnetical case, $J_{\mathrm{A-A}} \geq 0$, and $J_{\mathrm{A-B}} \geq 0$. Let $r = J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$. When $J_{\mathrm{A-A}} = J_{\mathrm{A-B}}$, namely $r = 1$, this system is an antiferromagnetical Ising model on a normal triangular lattice with uniform near neighbour bonds, for which there exists very severe frustration.[19] So there is no phase transition at finite temperatures. When $J_{\mathrm{A-B}} = 0$, that is $r = 0$, the energy of the system is fully determined by the honeycomb lattice constructed by A–A bonds. There are two long range ordered ground states for this honeycomb lattice. So there exists phase transition at finite temperatures in this system. Baxter[20] obtained the transition temperature $T/\left|J_{\mathrm{A-A}}\right| = 1.52$ by using an exact solution method while we obtained the same result by using the Monte Carlo method. When $J_{\mathrm{A-A}} = 0$, which means $r \to \infty$, the energy of the system is fully determined by the A–B bonds that are composed of a diamond lattice as shown in Fig.2.

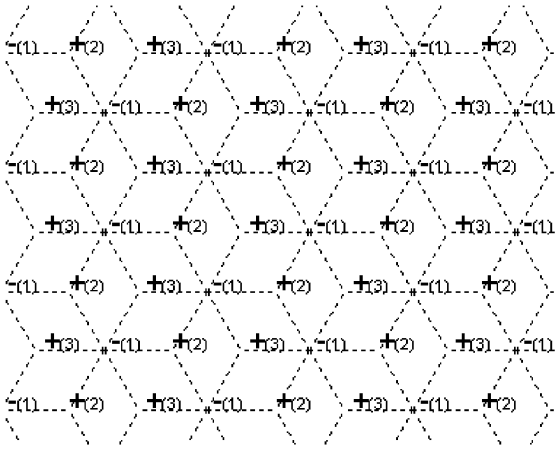


Fig.2. Arrangement of spin and interacting bonds on the lattice, where $J_{\mathrm{A-A}} = 0$, and signs '+' and '–' denote 'up' spin state and 'down' spin state, respectively.

In that lattice, there are six nearest neighbour bonds for sublattice (1), and there are three nearest neighbour bonds for sublattices (2) and (3). For the antiferromagnetical Ising model there is no frustration on this lattice. The ground state is long range ordered. The degenerate degree of this ground state is 2. The average ground state energy for one lattice site is $-2J_{\mathrm{A-B}}$. Figure 2 shows one of the ground states we obtained by using the Monte Carlo method. The sign '+' denotes the 'up' spin state and the sign '–' denotes the 'down' spin state. There exists a finite phase transition temperature for this system, which is $T/\left|J_{\mathrm{A-B}}\right| = 2.3$ obtained by our Monte Carlo simulation. When neither $J_{\mathrm{A-A}}$ nor $J_{\mathrm{A-B}}$ equals zero, there still exists a phase transition in general for this system, and the critical behaviour changes with $r = J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$. We examine the critical behaviour of the system for r varying from 0.1 to 0.99 and then from 1.01 to 90 by using the Monte Carlo method, with keeping $J_{\mathrm{A-A}} + 2J_{\mathrm{A-B}} = 3$. Then by analysing the information obtained and using the finite-size scaling method we achieve the pattern where the critical behaviour of this system changes with r. In the Monte Carlo simulation the total number of lattices, $N = L^2$, where L ranges from 42 to 168 with periodic boundary condition. We assume the system to reach equilibrium after 10^5 Monte Carlo sweeps at each temperature, and then we obtain an average value. The number of Monte Carlo steps used for averaging varies from 8×10^4 to 4×10^5.

3. Critical behaviour for $r < 1$

From $r = J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$ and $J_{\mathrm{A-A}} + 2J_{\mathrm{A-B}} = 3$, one can obtain $J_{\mathrm{A-A}} = 3/(2r+1)$ and $J_{\mathrm{A-B}} = 3r/(2r+1)$. When $0 < r < 1$, the spin arrangement of the ground state for this system is shown in Fig.3. The spins on sublattices (2) and (3)

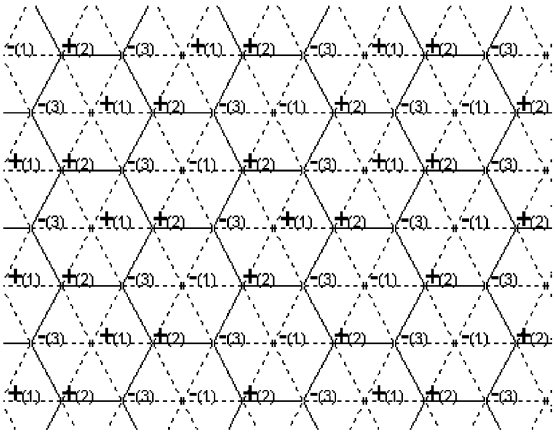


Fig.3. One kind of ground state when $r = 0.6$, where spins are randomly arranged on sublattice (1) and long range ordered on sublattices (2) and (3), and solid lines and dashed lines denote the A–A bond and A–B bond respectively.

are ordered, while those on sublattice (1) are randomly arranged; thus the system is partially disordered. We denote this ground state by AFP. When the temperature $T \to 0$, $|m_1| = 0$, $|m_2| = 1$, and $|m_3| = 1$, where m_α ($\alpha = 1, 2, 3$) are average single lattice site magnetizations for sublattices (1), (2) and (3) respectively. We choose the order parameter as $m = \dfrac{1}{2}(|m_1| + |m_2| + |m_3|)$. At low temperatures $m = 1$, and for high temperatures $m \to 0$ apart from finite-size effects. Our calculation shows that there is a critical temperature for both the energy and the order parameter when $0 \leq r \leq 0.90$, where the system undergoes a phase transition; and there exists a peak of the specific heat of the system near this critical temperature. Figures 4 and 5 show the energy and the order parameter each as a function of temperature respectively, for $r = 0$, 0.1, 0.2, ..., 0.9 and 1. The triangles and the crosses denote the curves for $r = 0$ and $r = 1$ respectively. Between the two curves the critical temperature decreases as r increases. Figure 6 shows the curves for specific heat versus temperature for $r = 0$, 0.1, 0.2, 0.9 and 1.

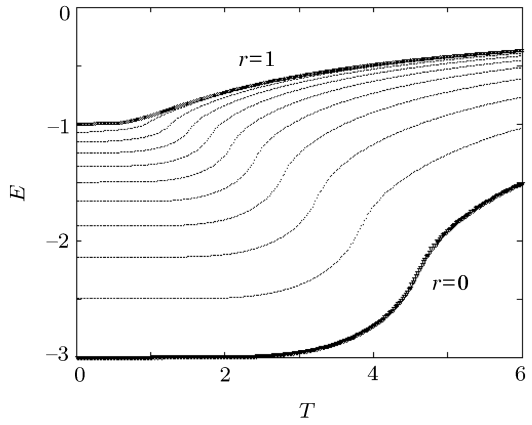


Fig.4. Temperature dependences of energy for r=0, 0.1, 0.2..., 0.9, 1, where curves are arranged upwards as r increases and triangles and the crosses are for $r = 0$ and $r = 1$ respectively.

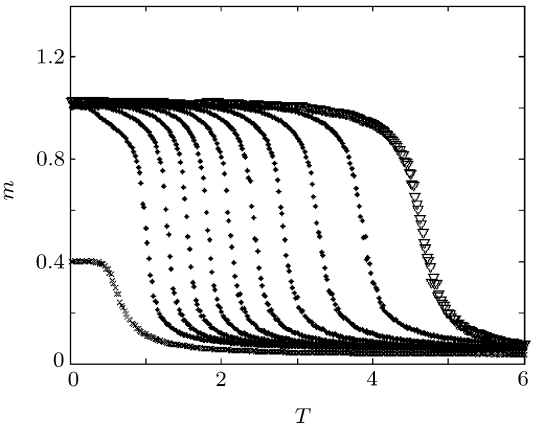


Fig.5. Temperature dependences of order parameter for $r = 0$, 0.1, 0.2, ..., 0.9, 1, where curves are arranged from right to left as r increases and triangles and crosses are for $r = 0$ and $r = 1$ respectively.

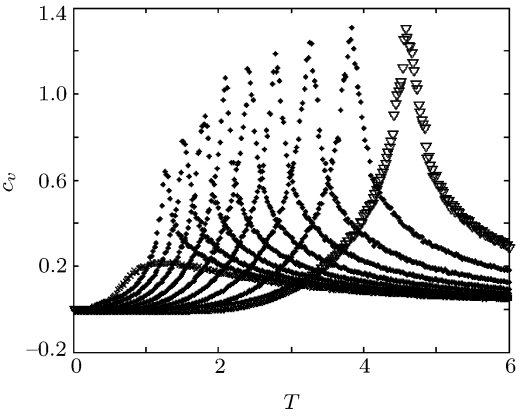


Fig.6. Fig.6. Temperature dependences of specific heat for $r = 0$, 0.1, 0.2, ..., 0.9, 1, where curves are arranged from right to left as increases and triangles and crosses are for $r = 0$ and $r = 1$ respectively.

We can find that the peaks of the curves shift evenly toward low temperatures as r increases. Using

the finite-size scaling method, such as the histogram method, the analysing of the Binder cumulant of energy, etc, which we used in Ref.[21], we find that there are no two peaks appearing in the histograms of the energy and the order parameter, and there is a crossing point of the Binder cumulants versus temperature for different sizes of the lattice for each r. So, the transition is continuous. The phase transition temperature is at the crossing point of the Binder cumulants of different sizes for each r. (We will show these transition temperatures in Section 5.) When $0.9 < r < 1$, the curves such as energy–T, $m - T$ and $c_v - T$ are distorted apparently. Figures 7 and 8 show the order parameter and the specific heat each as a function of temperature when $r = 0.94$, respectively. The order parameter of ground state for this case is still 1 and of the AFP type. We can see two small peaks to appear on the specific curve.

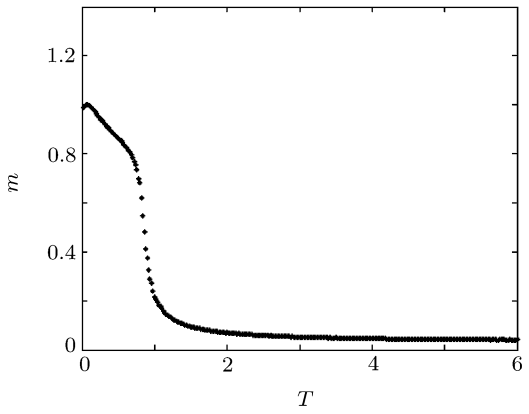


Fig.7. Order parameter versus temperature when $r = 0.94$.

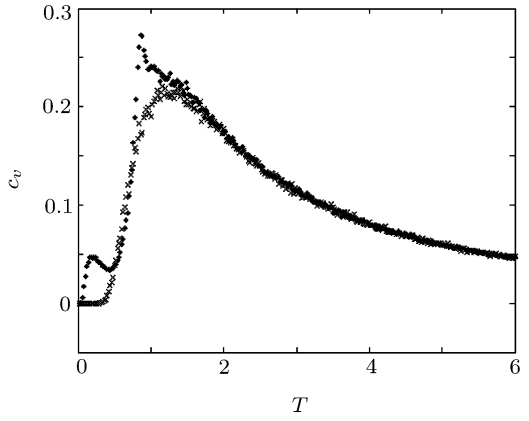


Fig.8. Curves for specific heat versus temperature, where solid dots are for $r = 0.94$ and crosses are for $r = 1$.

The results obtained by using the finite-scaling method show that no phase transition point is found, which means that the system will go to the ground state in multisteps when cooling down. In Figs.4–8 the value of L is 42, i.e. $L = 42$.

4. Critical behaviour for $r > 1$

When $J_{\mathrm{A-A}} \neq 0$ and $J_{\mathrm{A-B}} > J_{\mathrm{A-A}}$, that is, $r > 1$, the arrangements of the spins on sublattices (1), (2) and (3) for the ground state are still the same as those shown in Fig.2. We denote this ground state by AF. When $T \to 0$, $|m_1| = |m_2| = |m_3| = 1$. We choose the order parameter as $m = \dfrac{1}{3}(|m_1| + |m_2| + |m_3|)$, then when $T \to 0$, $m = 1$ and $m \to 0$ for high temperatures. We calculate energies, order parameters, specific heats, etc each as a function of temperature for $r = 1.01$, 1.03, 1.05, 1.07 and $r = 1.1$, 1.2, ... , 1.9 together with $r = 2$, 3, ... , 90 by using the Monte Carlo method. The results show that when $r \geq 1.1$, the system undergoes phase transition at finite temperatures, and the phase transition temperature increases with r, but it increases more and more slowly. When $r > 10$, it increases with r very slowly. Figures 9 and 10 show the energy and the order parameter each as a function of temperature respectively, with $r = 1$, 2, 3, ... , 10. The triangles and the crosses denote the curves for $J_{\mathrm{A-A}} = 0$ ($r \to \infty$) and $r = 1$ respectively. Between the two curves the critical temperature increases as r increases. Figure 11 indicates the specific heats each as a function of temperature. Using the finite-size scaling method, we obtain the same result as those in Section 3. So the phase transition is also continuous, and the critical temperatures we obtained for different values of r are shown below

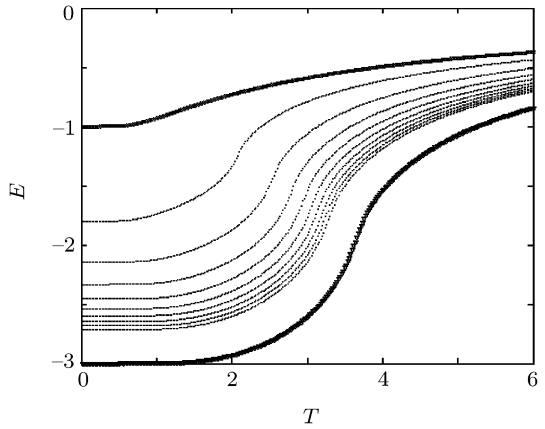


Fig.9. Temperature dependences of energy for $r = 1$, 2, 3, ... , 10 and $J_{\mathrm{A-A}} = 0$, where curves are arranged downwards as r increases and triangles and crosses are for $J_{\mathrm{A-A}} = 0$ ($r \to \infty$) and $r = 1$ respectively.

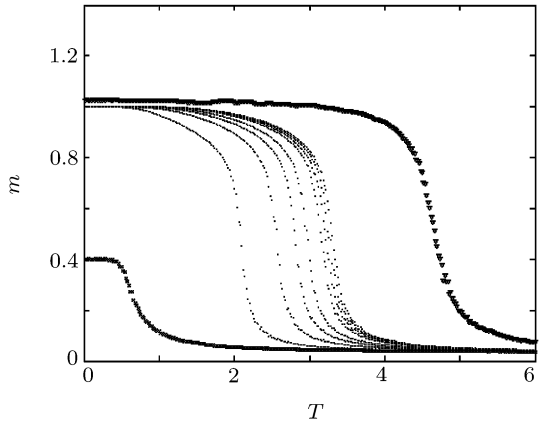


Fig.10. Temperature dependences of order parameter for $r = 1, 2, 3, \ldots, 10$ with $J_{\mathrm{A-A}} = 0$, where curves are arranged from left to right as r increases and triangles and crosses are for $J_{\mathrm{A-A}} = 0$ ($r \to \infty$) and $r = 1$ respectively.

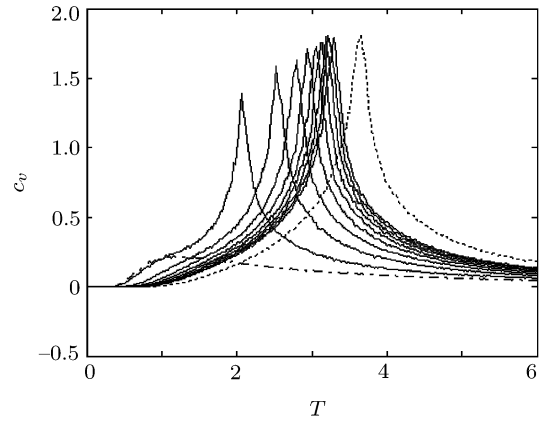


Fig.11. Temperature dependences of specific heat for $r = 1, 2, 3, \ldots, 10$ and $J_{\mathrm{A-A}} = 0$, where curves are arranged from left to right as r increases and dotted line and dash dotted lines are for $J_{\mathrm{A-A}} = 0$ ($r \to \infty$) and $r = 1$ respectively.

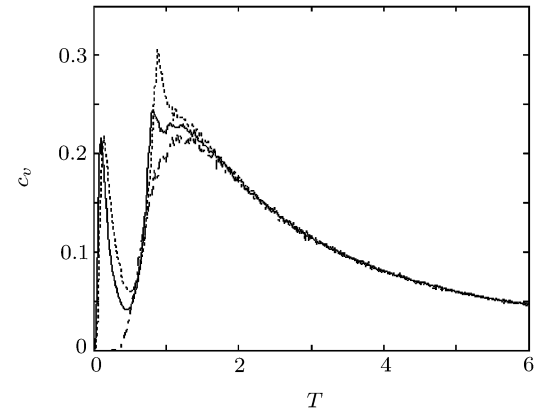


Fig.12. Specific heats versus temperature when r is very close to 1, where dash dotted, solid and dotted lines are for $r = 1$, 1.05 and 1.07 respectively.

in Fig.14 of Section 5. When $r < 1.1$, the curves are distorted by the frustration effect. The $c_v - T$ curve is very close to that in the case of $r = 1$ in a low temperature area, and two peaks appear on the $c_v - T$ curves, which do not change apparently as the size of the lattice increases. Figure 12 shows the $c_v - T$ curves when $r = 1$ (dash dotted line), 1.05 (solid line) and 1.07 (doted line) respectively. In Figs.9–12, the value of L is 42, i.e. $L = 42$.

5. Summary

We have studied the phase transition of an antiferromegnetical Ising spin system on a two-dimensional centred honeycomb lattice with two different values of exchange energies $J_{\mathrm{A-A}}$ and $J_{\mathrm{A-B}}$ by using the Monte Carlo method. Our study is focused on the effect of $r = J_{\mathrm{A-B}}/J_{\mathrm{A-A}}$ on the critical behaviour of the system. The patterns where the quantities such as energy, order parameter and specific heat change each are a function of temperature for different values of r in large ranges are obtained. Using the finite-size scaling method, we find that there are no two peaks appearing in the histograms for the energy and the order parameter and there is a crossing point of Binder cumulants of the order parameter each as a function of T for different sizes, i.e. $0 \leq r \leq 0.9$ and $r \geq 1.1$. Figure 13 is for $r = 0.5$ case, as an example, from which it follows that the transition is continuous and the critical temperature $T_{\mathrm{c}} = 2.02 \pm 0.02$. Using this method we obtain the phase diagram as shown in Fig.14. The errors come from the determination of the crossing points. We find from the phase diagram that there is no typical phase transition in the dash line area. In this area, the system will lose its crystal property, and the cooling process to the ground state will become multistep and gradual.

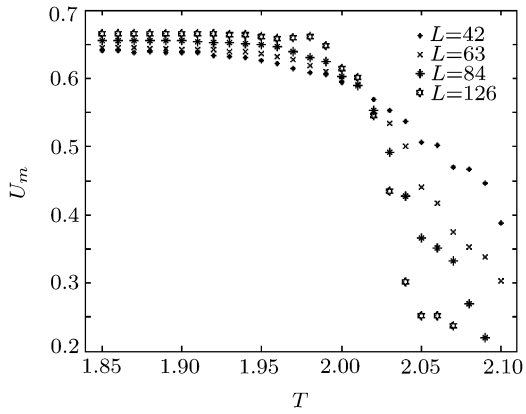


Fig.13. Binder cumulants each as a function of T for size $L = 42$, 63, 84, and 126 in the case $r = 0.5$, where curves cross at $T_{\mathrm{c}} = 2.02$.

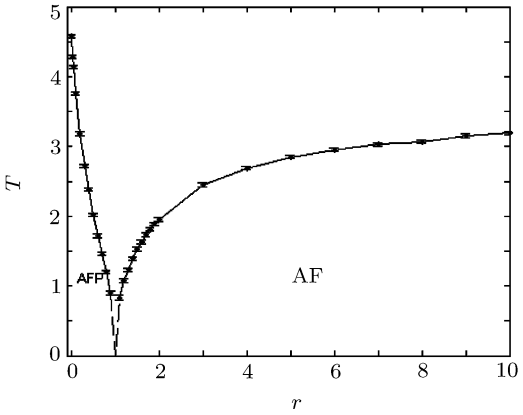


Fig.14. The phase diagram $T-r$, where no typical phase transition occurs in the dashed line area.

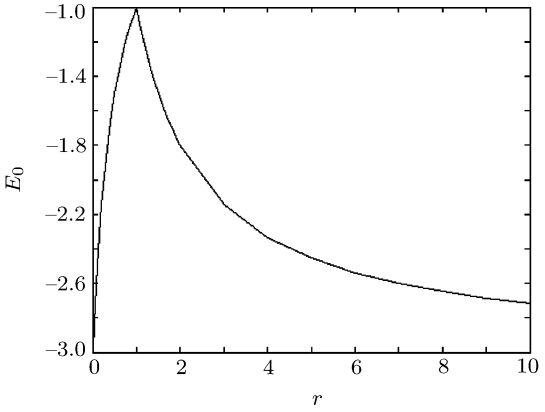


Fig.15. Average ground state energy of one lattice site versus r.

For the system under study, the average energy of the ground state of one lattice site, E_0, changes with r. The relationship is as follows: when $r \leq 1$, $E_0 = -3/(2r+1)$; when $r > 1$, $E_0 = -3(2r-1)/(2r+1)$ as shown in Fig.15. Using this relationship we can obtain the $T/E_0 - r$ phase diagram as shown in Fig.16. The results we obtained will be helpful for studying the phase transition problems of systems composed of compounds.

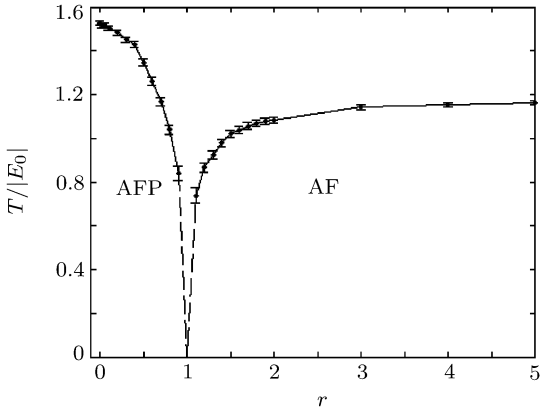


Fig.16. Phase diagram $T/|E_0|-r$, where no typical phase transition occurs in the dashed line area.

References

[1] Guo Z Z, Xuan Z G, Zhang Y S and An C H 2008 *Acta Phys. Sin.* **57** 6571 (in Chinese)

[2] Zhang Y, Liu D and Long G L 2007 *Chin. Phys.* **16** 324

[3] Shao Y Z, Zhong W R, Lin G M and Li J C 2005 *Chin. Phys.* **14** 2110

[4] Jiang Q and Tao Y M 2004 *Chin. Phys.* **13** 1149

[5] Liang Y Q, Wei G Z, Zhang Q, Qiu W and Zang S L 2004 *Chin. Phys.* **13** 2147

[6] Shao Y Z, Lai J K L, Shek C H, Lin G M and Lan T 2004 *Chin. Phys.* **13** 243

[7] Tao Y M and Jiang Q 2004 *Chin. Phys.* **13** 1149

[8] Jiang W, Wei G Z, Du A and Zhang Q 2002 *Chin. Phys.* **11** 823

[9] Ismail G and Hassan S 2002 *Chin. Phys.* **11** 948

[10] Yan S L 2002 *Chin. Phys.* **11** 1066

[11] Zhou Y S, Chen J C and Lin D L 2000 *Acta Phys. Sin.* **49** 2477 (in Chinese)

[12] Zhang L and Zhong W L 2000 *Acta Phys. Sin.* **49** 2296 (in Chinese)

[13] Laaboudi B, Saber M, Benaboud A and Kerouad M 1999 *Chin. Phys.* **8** 199

[14] Zhitomirsky M E and Zaliznyak I A 1996 *Phys. Rev.* B **53** 3428

[15] Plumer M L, Caille A and Kawamura H 1991 *Phys. Rev.* B **44** 4461

[16] Zhang W, Saswal W M and Gabay M 1991 *Phys. Rev.* B **44** 5129

[17] Diep H T, Debauche M and Giacomini H 1991 *Phys. Rev.* B **43** 8759

[18] Landau D P and Binder K 2000 *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge: Cambridge University Press) p77

[19] Kawamura H 1987 *J. Phys. Soc. Jpn.* **56** 474

[20] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic Press) p87

[21] Wang Z F and Southern B W 2003 *Phys. Rev.* B **68** 094419