Ising model with four-spin interaction on honeycomb lattice

Yuming Yang\textsuperscript{1,2,a} and Baohua Teng\textsuperscript{1,b}

\textsuperscript{1}Department of Applied Physics, University of Electronic Science and Technology of China, Chengdu, 610054, China
\textsuperscript{2}School of Mathematical Sciences, University of Electronic Science and Technology of China, Chengdu, 610054, China

\textsuperscript{a}yangym@uestc.edu.cn, \textsuperscript{b}phytbh@uestc.edu.cn

Abstract. The Ising model with the nearest-neighbor interaction $J_2$ and four-spin interaction $J_4$ on the honeycomb-lattice is investigated. The correlation relationships among two-spins and four-spins are calculated. The effects of spin-spin interactions on phase diagrams are investigated analytically and numerically. Evidence from our derivation indicates that the classification of the phase-transition depends on the ratio of $J_4$ to $J_2$.

1. Introduction
One of the most interesting phenomena in magnetic materials is ferromagnetism [1-4]. Ising model is a simplest and most popular model of a lattice system, and it can be used to simulate the structure of a ferromagnetic materials. The model and its various variants are extensively studied in statistical physics. Ising model on honeycomb lattice is such an extended application [2],[5-7], which can be used to mimic the material that has a geometry structure of honeycomb type, e.g., graphene[8], honeycomb type ZnO nanostructures [6], etc.

The influence of four-spin interactions on critical properties of Ising model has been studied [1-2],[5],[9-14], e.g. the results of effective-field theory, Monte Carlo simulations, Green’s function, and so on. The models with four-spin interactions have been used to describe the material properties of PbHPO\textsubscript{4}, H\textsubscript{2}C\textsubscript{2}O\textsubscript{4} and La\textsubscript{2}CuO\textsubscript{4}, etc. The phase diagram of ferroelectric thin films based on transverse Ising model with a four-spin interaction has been studied and the ferroelectric feature of the phase diagrams been discussed in Ref. [14].

For the honeycomb lattice Ising model, the thermal behaviours and susceptibility and other properties of the lattice system have been discussed in recent research papers [5],[15-17]. Some rigorous solutions have been obtained in the case of the special situation, e.g. the mixed spin transverse Ising model, a honeycomb lattice with interlayer coupling. However, there are few discussions of four-spin interactions on honeycomb lattice Ising model, though it is an important lattice structure.

The purpose of this work is to investigate the properties of the honeycomb lattice Ising model with the nearest-neighbour interaction $J_2$ and four-spin interaction $J_4$. It is to be hoped that one can obtain an
understanding of the basic qualitative and quantitative features for the effects of four-spin interactions on this lattice system.

2. The model and derivation
The system is an array of $N$ fixed lattice sites that forms a two-dimensional periodic lattice. The geometrical structure of the lattice is honeycomb lattice. $s_i (i=1,\cdots,N)$ associated with lattice site $i$ is a spin variable and its value is a number that is either +1 or -1. The Hamiltonian of the model is given by

$$H = -J_2 \sum_{<ij>} s_is_j - J_4 \sum_{<ijkl>} s_is_js_ks_l$$

where $<ij>$ denotes a nearest neighbor (NN) pair of spins, $<ijkl>$ a quartet of spins (four-spin), i.e., a spin and its three nearest neighbors (see figure 1). The strengths of interaction $J_2, J_4$ are all positive.

![Figure 1. Site $i$ and its neighbors. $<ij>, <il>$ and $<ik>$ are nearest neighbors. $<ijkl>$ is a quartet of spins and its central spin is site $i$.](image)

To solve this model, let $N_u$ be total numbers of up spins and $N_d$ for total number of down spins. The subscripts of a variable stands for the state of the spin, $u$ for spin-up state and $d$ is just the opposite. $N_{uu}, N_{ud}, N_{dd}$ are introduced for numbers of NN pair $(1,1)$, $(1,-1)$, and $(-1,-1)$ respectively, where $(1,-1)$ is not distinguished from $(-1,1)$. The variables $N_{uuuu}, N_{uudu}, N_{udud}, N_{duuu}, N_{duud}, N_{dudu}$ and $N_{ddud}$ are introduced for numbers of quartet of spins $(1,1,1,1)$, $(1,1,1,-1)$, $(1,1,-1,1)$, $(1,-1,-1,1)$, $(-1,1,1,1)$, $(-1,1,1,-1)$, $(-1,1,-1,1)$ and $(-1,-1,-1,1)$ respectively. There are eight types of quartet of spins $(1,1,1,1), (1,1,1,-1), (1,1,-1,1), (1,-1,-1,1), (-1,1,1,1), (-1,1,1,-1), (-1,1,-1,1)$ and $(-1,-1,-1,1)$, The first item of a four-spin stands for the state of the central spin. Therefore, a state of a four-spin depends on the state of its central spin together with the up-spin or down-spin number of the states of the rest three spins, e.g. $(1,1,1,1)$ is not distinguished from $(1,1,-1,1)$ or $(1,-1,1,1)$ . However, $(1,1,1,-1)$ is distinguished from $(-1,1,1,1)$.
Suppose that the spatial distribution of spin is uniformly at random in a honeycomb lattice system, but the values of \( N_{uu}, N_{dd}, N_{ud}, N_{du}, N_{uuu}, N_{uuud}, N_{uudd}, N_{uuuu}, N_{uuud}, N_{uudd}, N_{uddd}, N_{duuu}, N_{duud}, N_{dudd}, N_{dddd} \) are given numbers. So, a spins pair \((1,1)\) appears with probability \(2N_{uu}/(3N)\), which approximates to \((N_u/N)^2\). Using similar ideas, one can get a set of correlation functions of spins pair as follows

\[
\begin{align*}
N_{uu} &\approx 1.5N_u^2/N \\
N_{ud} &\approx 3N_u(1-N_u/N) \\
N_{dd} &\approx 1.5N(1-N_u/N)^2 \\
N_{uuu} &\approx N_u^4/N^3 \\
N_{uuud} &\approx 3(1-N_u/N)N_u^3N^{-2} \\
N_{uudd} &\approx 3N_u^2(1-N_u/N)^2N^{-1} \\
N_{uuuu} &\approx N_u(1-N_u/N)^3 \\
N_{uudd} &\approx N_u^3(1-N_u/N)N^{-2} \\
N_{uudd} &\approx 3N_u^2(1-N_u/N)^2N^{-1} \\
N_{uddd} &\approx 3N_u(1-N_u/N)^3 \\
N_{duuu} &\approx (1-N_u/N)^4N \\
\end{align*}
\]

(2)

![Figure 2. Various correlation functions of spins. The points are obtained from MC simulations for a randomly arranged lattice system on honeycomb with size \(N=48^2\) and the solid lines are corresponding to the theoretical calculations. Every group of data is normalized by the total number of itself. There exists one solid line for the same two formulas in the right hand side of Eq. (2).](image)
Meanwhile the Monte Carlo (MC) simulations for the spin correlation functions are also carried out, and the MC simulation and theory results based on Eq. (2) are shown in Fig. 2. It is easy to see that the theoretically calculated results are in very good accordance with the MC numerical simulation results. And these results are independent of the size of the lattice system, which indicates that even in the thermodynamic limit these correlation functions work very well.

Noticing that

\[ \sum_{i=1}^{N} s_i = N_u - N_d = 2N_u - N \]

\[ \sum_{<ij>} s_i s_j = N_{uu} + N_{dd} - N_{ud} \]

\[ \sum_{<ijkl>} s_i s_j s_k s_l = N_{uuuu} - N_{uudd} + N_{duuu} - N_{duud} - N_{uuud} + N_{dudd} - N_{duda} + N_{dddd} \] (3)

and substituting Eq. (2) into Eq. (3), it becomes

\[ \sum_{<ij>} s_i s_j \approx (N - 2N_u)^2 / 2N \]

\[ \sum_{<ijkl>} s_i s_j s_k s_l \approx (N - 2N_u)^4 / N^3 \] (4)

Let \( L = 2N_u / N - 1 \), using Eqs. (2) and (4), the Hamiltonian (1) can be rewritten as

\[ H = (-1.5 J_2 L^2 - J_4 L^4)N \] (5)

Hence, the partition function of the system becomes

\[ Q(T) = \sum_{\{s_i\}} \exp[\beta N(1.5 J_2 L^2 + J_4 L^4)] \] (6)

where \( \beta = 1/kT \) and the sum is over all configurations. Noticing that the number of ways to choose \( N_u \) out of \( N \) is \( N! / N_u! (N-N_u)! \), the partition function can be rewritten as

\[ Q(T) = \sum_{L=-1}^{1} \frac{N!}{[N(1+L)/2][N(1-L)/2]} \exp[\beta N(1.5 J_2 L^2 + J_4 L^4)] \] (7)

In order to obtain the thermodynamic functions, Helmholtz free energy should be considered and calculated, i.e., \(-kT \log Q(T)\). Firstly, by taking the limit approximation, the \( \log Q(T) \) is replaced by the logarithm of the largest term in the summand when \( N \) goes to infinity. Using Stirling’s approximation, one can find that

\[ \frac{1}{N} \log Q(T) \approx \beta(1.5 J_2 L^2 + J_4 L^4) - \frac{1+L}{2} \log_e - \frac{1-L}{2} \log_e = \frac{1-L}{2} \frac{1+L}{2} \] (8)

where \( \hat{L} \) is the value of \( L \) that maximizes the summand of Eq. (7) and \( \hat{L} \) is the root of the following equation

\[ \log_e \frac{1+L}{1-L} = 2\beta(3J_2 \hat{L}^2 + 4J_4 \hat{L}^4) \] (9)
Thus one can deduce the phase transition properties of the system from the solution of Eq. (9). Series expansion technique and numerical methods are employed to solve it.

3. Numerical results and discussion
The main features of the solutions are illustrated in this section. Some special results will be presented here.

First, consider a simple situation, $J_2 > 0$, $J_4 = 0$, by treating Eq. (9) with series expansion technique, one can get critical temperature given by

$$kT_c = 3J_2$$

such that

$$\bar{L} = \begin{cases} 
0 & (T > T_c) \\
\pm L_0 & (T < T_c) 
\end{cases}$$

Here, the results are the same as those of the Bragg-Williams approximation. The phase transition of the system is always continuous whatever the value $J_2$ taken.

Second, in the case of $J_2 > 0$, $J_4 > 0$, the things are very different from those stated in the first case. For small value of $J_4$, The phase transition is always continuous as in before case. However, a discontinuous transition is found for sufficiently high values of $J_4$. The crossover happens at value $J_4 = J_2/4$.

In the latter case, one can search carefully the roots of Eq. (9) by numerical method and series expansion technique. It will be found that its roots go to zero continuously if the temperature increases to the critical point in the case of $J_4 < J_2/4$. The phase transition is continuous. If they jump to zero, one has a discontinuous phase transition. In the situation of $J_4$ less than $J_2/4$, critical temperature is the same as indicated in Eq. (10). The critical exponent is the same as that obtained by traditional mean field method. In the situation of $J_4$ bigger than $J_2/4$, the lower critical temperature is the same as Eq. (10) but the upper critical temperature $T_{uc}$ is given by the transcendental Eq. (12).

$$\begin{align*}
tanh(\frac{3J_2\bar{L} + 4J_4\bar{L}^3}{kT_{uc}}) &= \bar{L} \\
\frac{3J_2 + 12J_4\bar{L}^2}{kT_{uc}} &= \frac{1}{1 - \bar{L}}
\end{align*}$$

4. Conclusions
In summary, the properties of the phase transition for Ising model on two dimensional honeycomb lattice system have been investigated. And the correlation functions of two-spin pairs and four-spin have been obtained, theoretical results are in good accordance with numerical simulation results. The results have shown that the strength of four-spin interaction has deep affection on transition properties. It exhibits a crossover behaviour, namely when $J_4$ becomes greater than $J_2/4$, the phase transition is discontinuous. It is believed that the theory presented in this work can also be applied to more complex geometrical situations, such as face-centred cubic lattice, body-centred cubic lattice, and so on. It can also be
applied to more complex practical systems, such as Ising model in a uniform magnetic field, and can provide quantitative and qualitative results.

5. References
[1] N. De La Espriella, A.J. Arenas, M.S. Páez Meza 2016 J. Magn. Magn. Mater. 417 434-441.
[2] B. Deviren, O. Canko, M. Keskin 2008 J. Magn. Magn. Mater. 320(18) 2291-2299.
[3] N. Şarlı, S. Akbudak, Y. Polat, M.R. Ellialtıoğlu 2015 Physica A 434 194-200.
[4] U. Yu 2015 Physica A. 419 75-79.
[5] D. F. de Albuquerque, I.P. Fittipaldi, J.R. de Sousa, N.O. Moreno, 2006 Physica B. 384(1) 230-232.
[6] C. S. Prajapati, D. Visser, S. Anand, N. Bhat 2017 Sens. Actuators, B 252 764-772.
[7] X. Shi, Y. Qi 2015 J. Magn. Magn. Mater. 393 204-208.
[8] M. Wierzbicki 2017 Physica E 87 220-227.
[9] Ü. Akıncı and G. Karakoyun 2017 Physica B. 521 365-370.
[10] N. De La Espriella, C.A. Mercado, G.M. Buendía 2016 J. Magn. Magn. Mater. 417 30-36.
[11] B. Teng, Y. Chen, H. Fu, Y. Tang, M. Tu, Y. Chen, J. Tang, 2002 Solid State Commun. 124(9) 347-351.
[12] J. P. Santos, F.C. Sá Barreto 2017 J. Magn. Magn. Mater. 439 114-119.
[13] Y. Yang, B. Teng, H. Yang, H. Cui 2017 Physica. A 483 243-249.
[14] B. H. Teng, H.K. Sy 2006 Europhys. Lett. 73(4) 601-606.
[15] Y. Yüksel, Ü. Akıncı, H. Polat 2012 Physica A. 391(3) 415-422.
[16] Q. Zhang, G. Wei, Z. Xin, Y. Liang 2004 J. Magn. Magn. Mater. 280(1) 14-22.
[17] B. Teng, H.K. Sy, 2004 Solid State Commun. 130(3) 193-197.