Physical Science International Journal
11(2): 1-5, 2016, Article no.PSIJ.28109
ISSN: 2348-0130

SCIENCEDOMAIN *international*
www.sciencedomain.org

Series Expansion Method for Exploring Critical Behavior in Diluted Magnetic Semiconductors

Habte Dulla Berry[1*]

[1]*Department of Physics, College Natural and Computational Sciences, Dilla University, P.O.Box 419, Dilla, Ethiopia.*

Author's contribution

The sole author designed, analyzed and interpreted and prepared the manuscript.

Article Information

DOI: 10.9734/PSIJ/2016/28109
Editor(s):
(1) B. Boyacioglu, Vocational School of Health, Ankara University, Kecioren, Ankara, Turkey.
(2) Christian Brosseau, Distinguished Professor, Department of Physics, Université de Bretagne Occidentale, France.
Reviewers:
(1) P. N. Palanisamy, Kongu Engineering College, Perundurai, Tamilnadu, India.
(2) Yong Gan, California State Polytechnic University Pomona, California, USA.
Complete Peer review History: http://www.sciencedomain.org/review-history/15605

Original Research Article

Received 2nd July 2016
Accepted 19th July 2016
Published 31st July 2016

ABSTRACT

In this study the author focuses on thermal and magnetic properties of diluted magnetic semiconductors at critical point. Such properties are discontinuous at some point in the critical region so that it is very important to study their critical behavior in these regions. In order to study these critical behaviors the author uses series expansion technique and quantum lattice model with help of computer program.

Keywords: Critical behavior; diluted magnetic semiconductors; series expansion; quantum lattice model.

1. INTRODUCTION

The role of disorder in magnetism is important property in condensed matter physics and materials science. Widely accepted recent research activities [1-3] in diluted magnetic semiconductors (DMS) i.e. cationic substitution doping (by a few percent) of a semiconductor with magnetic impurities (e.g. $Ga_{1-x}Mn_xAs$ with $x \approx 0.01 - 0.1$) seemingly leads to an intrinsic ferromagnetic. The intrinsic mechanism of ferromagnetism is a big research topic recently, both from understanding the competition between disorder and magnetic interactions as well as for technological advancement i.e. the subject of 'spintronics'

**Corresponding author: E-mail: habtix07@gmail.com, habtedul@yahoo.com;*

(or spin electronics) [4]. In this article, the author deals with theoretically the competition of thermal and magnetic correlations in DMS materials using analytical arguments on a disordered Ising spin model [5].

In some cases, it is very difficult to get exact solutions, for such cases; there is a branching set of approaches which can be used. Among these techniques, the most popular one is series expansion method. This paper will be considered the so called series expansion methods, of which there are again a number of different kinds. The common feature of all of these techniques is that, they can compute a number of coefficients in a power series expansion for some quantity.

2. MODEL

After the investigation of quantum mechanics, the two known scientists (Heisenberg and Dirac) independently proposed that the magnetic order in solids might be understood on the basis of a model of exchange coupled quantum angular momenta ('spins'), with a Hamiltonian of the form [5].

$$E = -J\sum_{\langle ij\rangle}\sigma_i\,\sigma_j, \tag{2.1}$$

where σ_i is Ising spin variable at site *i*, and its values are ± 1, and *J* is constant interaction coupling parameter with dimension of energy. In this case we can assume a regular lattice of *N* sites, with nearest-neighbor interactions. The thermodynamic and magnetic properties can be derived from the partition function [6-7].

$$\mathrm{Z(K)} = \sum_{\{\sigma_i\}} e^{-\beta E} = \sum_{\{\sigma_i\}} exp\big(K\sum_{\langle ij\rangle}\sigma_i\,\sigma_j\big). \tag{2.2}$$

Where the first sum is over all spin configurations, and $\mathrm{K} = \beta\mathrm{J}$ is a temperature dependent coupling constant, and $\beta = 1/\mathrm{K_B\,T}$ as usual. We note that at high temperatures K is small.

The power series expansions of the partition function in terms of *K* [8-9]. We obtain

$$Z(K) = \sum_{\{\sigma_i\}}\prod_{\langle ij\rangle} e^{-\beta\sigma_i\sigma_j} = \sum_{\{\sigma_i\}}\prod_{\langle ij\rangle}\sum_{l=0}^{\infty}\frac{K^l}{l!}(\sigma_i\sigma_j)^l \tag{2.3}$$

The term $(\sigma_i\sigma_j)^l$ is related with an *l*-fold line joining sites *i* and *j* on the lattice. The equation (2.3) can be represented by a diagram of the entire lattice with each bond $\langle ij\rangle$ and multiplicity l_{ij}. At each site *i* there will be a factor σ^p, where *p* is the sum of multiplicities of all bonds connecting to site *i*. We refer to this as the degree of site *i*. The simple result [9].

$$\sum_{\sigma=\pm 1}\sigma^{\mathrm{p}} = \begin{cases} 2, & \mathrm{p\ even} \\ 0, & \mathrm{p\ odd}\end{cases} \tag{2.4}$$

immediately shows that the only non-zero terms come from graphs in which every vertex is of even degree (including zero). Therefore, the partition function will be

$$\mathrm{Z_N(K)} = 2^{\mathrm{N}}\sum_{\{\mathrm{g_0}\}}\frac{\mathrm{C(g)}}{\mathrm{w(g)}}\mathrm{K}^{\mathrm{l_g}} \tag{2.5}$$

where the sum is over all possible graphs with all even vertices, $\mathrm{l_g}$ is the number of lines, including multiplicities, *w*(*g*) is a combinatorial factor for multiple lines, and $\mathrm{C(g)}$ is the number of ways in which the graph can be located on the lattice of *N* sites (the embedding factor) [10-13].

In the case of the Ising model, an immediate simplification is possible by use of the identity [9]

$$e^{-\beta\sigma_i\sigma_j} = coshK(1 + v\sigma_i\sigma_j) \tag{2.6}$$

which is valid for $\sigma_i, \sigma_j = \pm 1$, with $v = tanhK$. The zero-field partition function can then be written as

$$\begin{aligned}\mathrm{Z_N(K)} &= (\mathrm{coshK})^{\mathrm{Nq/2}}\sum_{\{\sigma\}}\prod_{\langle ij\rangle}\big(1 + v\sigma_i\sigma_j\big) \\ &= 2^N(\mathrm{coshK})^{\mathrm{Nq/2}}\sum_{\{\mathrm{g_0}\}}\mathrm{C(g)}\,\mathrm{v}^{\mathrm{l_g}}\end{aligned} \tag{2.7}$$

In equ. (2.7) q is the coordination number of the lattice, i.e. the number of neighbors of any site ($\mathrm{Nq/2}$ is the number of nearest-neighbor pairs), and the sum is again over a set of even-vertex graphs. However, only single-bonded graphs occur.

Taking the embedding constant data [13] and the logarithm as before, yields

$$\frac{1}{N}ln\mathrm{Z_N} = \ln 2 + 3\ln\cosh\mathrm{K} + 2\upsilon^2 + 3\upsilon^4 + 6\upsilon^5 + 11\upsilon^6 + \cdots \tag{2.8}$$

There is usually no need to do this, as υ can itself serve as a high-temperature expansion variable. We note that the number of graphs (to sixth order) has been reduced from 25 to 6. This is a simple example of renormalization, which is an idea that will recur later.

Let us now return to the full Hamiltonian, with the field term, and derive a high temperature series [14-19] for the zero-field magnetic susceptibility from the corresponding thermodynamic potential, or the logarithm of the partition function, one obtains the usual thermodynamic and magnetic quantities, per site.

Internal energy:

$$U = -\frac{\partial}{\partial\beta}\left(\frac{1}{N}\ln Z\right) \quad (2.9)$$

Specific heat:

$$C = \frac{dU}{dT} = -k_B\beta^2\frac{dU}{d\beta}. \quad (2.10)$$

Magnetization or order parameter:

$$m = -\frac{1}{\beta}\frac{\partial}{\partial h}\left(\frac{1}{N}\ln Z\right) \quad (2.11)$$

(*h* is an appropriate field which couples to the order parameter operator in the Hamiltonian).

Susceptibility:

$$\chi = \frac{\partial m}{\partial h} = -\frac{1}{\beta}\frac{\partial^2}{\partial h^2}\left(\frac{1}{N}\ln Z\right) \quad (2.12)$$

Using the identity (2.6), and a similar one for the field term, yields

$$Z_N(K) = (\cosh K)^{Nq/2}(\cosh\beta h)^N \sum_{\{\sigma\}}\prod_{\langle ij\rangle}\big(1 + v\sigma i\sigma jk(1+\tau\sigma k)$$

$$= (\cosh K)^{Nq/2}(\cosh\beta h)^N\Lambda_N \quad (\tau = \tanh\beta h) \quad (2.13)$$

where

$$\Lambda_N = \sum_{\{\sigma\}}\prod_{\langle ij\rangle}\left(1 + v\sigma_i\sigma_j\right)\prod_k(1 + \tau\sigma_k)$$

and hence

$$\frac{1}{N}\ln Z = \frac{q}{2}\ln\cosh K + \ln\cosh\beta h + \frac{1}{N}\ln\Lambda_N \quad (2.14)$$

The quantity $\ln\Lambda_N$ can be expanded graphically, as before. In every bond in the graph there is a term $v\sigma_i\sigma_j$ and, in addition, each site carries a factor either 1 or $\tau\sigma_k$. Only those graphs with precisely two τ factors contribute to (2.12). According to equ. (2.4) the graphs which contribute are those which have with precisely two vertices of odd degree, those to be compensated by the two $\tau\sigma_k$ factors. Based on the above calculations we obtain the following expression for susceptibility:

$$\beta^{-1}\chi(v) \equiv \bar{\chi}(v) = 1 + 2\sum_{\{g_2\}} c(g)v^{l_g}. \quad (2.15)$$

In this equ. the sum is over the set of graphs $\{g_2\}$, and $c(g)$ denotes the coefficient of N in the embedding factor (the lattice constant of the graph).

Therefore, expression for internal energy will be:

$$U = -\frac{\partial}{\partial\beta}\left(\frac{q}{2}\ln\cosh K + \ln\cosh\beta h + \frac{1}{N}\ln\Lambda_N\right) \quad (2.16)$$

and based on equ.(2.16) we will find thermal specific heat and magnetization respectively as:

$$C = k_B\beta^2\frac{d}{d\beta}\frac{\partial}{\partial\beta}\left(\frac{q}{2}\ln\cosh K + \ln\cosh\beta h + \frac{1}{N}\ln\Lambda_N\right) \quad (2.17)$$

and

$$m = -\frac{1}{\beta}\frac{\partial}{\partial h}\left(\frac{q}{2}\ln\cosh K + \ln\cosh\beta h + \frac{1}{N}\ln\Lambda_N\right) \quad (2.18)$$

The author will be concerned with models which exhibit finite-temperature phase transitions, particularly critical points, where the free energy develops a mathematical singularity at some temperature T_c (for this the thermodynamic limit is crucial). Not only is the determination of T_c important but, even more so, the asymptotic behavior of thermodynamic quantities in the vicinity of T_c.

3. RESULTS AND DISCUSSION

Finding exact finite-temperature properties of such quantum lattice models can be very difficult but in order to get approximate values, one has to devise series expansions techniques for the lattice model in the thermodynamic limit. A very popular approach of these series expansions are high-temperature expansions (HTEs), in which the partition function Z and other extensive properties of the system are expanded in powers of the inverse temperature $\beta = (k_BT)^{-1}$. Based on these techniques the author identified critical properties of diluted magnetic semiconductors.

According to the mathematical derivation above the internal energy of the system strongly depends on temperature. As the Fig. 1 indicated when the temperature increases, internal energy also increases. This is in line with the theoretical explanations i.e internal energy (kinetic energy) of the system directly related to the temperature. In general, this series expansion technique is suitable technique in order to determine magnetic and thermodynamic properties at critical region.

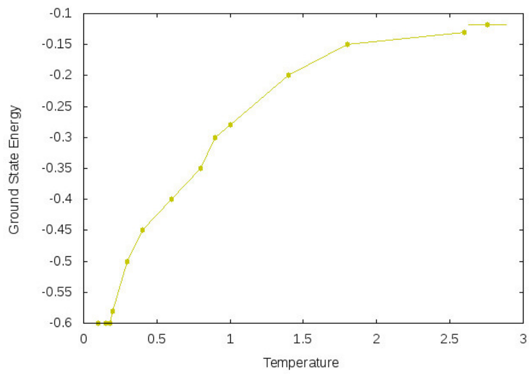

Fig. 1. The dependence of internal energy on temperature

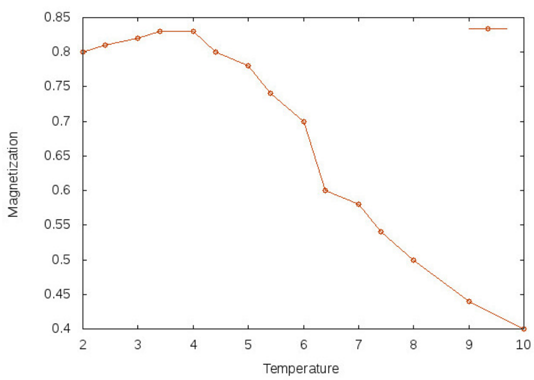

Fig. 2. Explains the relationship between magnetization and temperature

Usually, magnetization is the order parameter that distinguish the phase transition in magnetic materials. Therefore magnetization is strongly related with temperature i.e. at high temperature the magnetization approaching to zero and there is no magnetic alignment in the system (see Fig. 2). According to the figure the value of magnetization (order parameter) is high at low temperature and its magnitude decreases with increasing temperature.

4. CONCLUSION

In conclusion, the series expansion technique that we have used here is very important to identify the critical behavior of materials. In this study we have mainly used high temperature series expansion with the concept of quantum lattice model in order to determine the magnetic and thermodynamic property of materials at critical region. Specifically the properties that we have identified (Energy, heat capacity and magnetization) are in line with results from other mathematical and computational methods.

COMPETING INTERESTS

Author has declared that no competing interests exist.

REFERENCES

1. Das Sarma S, Hwang EH, Kaminski A. How to make semiconductors ferromagnetic: A first course on spintronics. Solid State Comm. 2003;127: 99
2. Timm C. Disorder effects in diluted magnetic semiconductors (topical review). J. Phys. Condens. Matter. 2003;15:R1865.
3. MacDonald AH, Schiffer P, Samarth N. Ferromagnetic semiconductors: Moving beyond (Ga, Mn)As. Nature Materials. 2005;4:195.
4. Ohno H. Properties of ferromagnetic III-V semiconductors. J. Magn. Magn. Mater. 1999;200:110.
5. Oitmaa J, Zheng WH. Series expansion for the $J1–J2$ heisenberg antiferromagnet on a square lattice. Physical Review B. 1996;54(5):3022.
6. Oitmaa J, Hamer CJ, Weihong Z. Low-temperature series expansions for the (2+1)-dimensional Ising-model. Journal of Physics A Mathematical and General. 1991;24:2863.
7. Nickel BG, Rehr JJ. High-temperature series for scalar- field lattice models – generation and analysis. Journal of Statistical Physics. 1990;61:1.
8. Domb C, Green MS. Phase Transitions and Critical Phenomena, Academic Press, London; 1974.
9. Oitmaa HC, Zhang JW. Series Expansion Methods for Strongly Interacting Lattice Models, Cambridge University Press, Cambridge, England; 2006.
10. Sykes MF, Essam JW, Heap BR, Hiley BJ. Lattice constant systems and graph theory. Journal of Mathematical Physics. 1966;7: 91557.
11. Rigol M, Bryant T, Singh RRP. Numerical linked-cluster approach to quantum lattice models. Phys. Rev. Lett. 2006;97:187202.
12. Rigol M, Bryant T, Singh RRP. Numerical linked-cluster algorithms. I. Spin systems on square, triangular, and kagom´e lattices. Phys. Rev. E. 2007;75:061118.

13. Rigol M, Bryant T, Singh RRP. Numerical linked-cluster algorithms. II. $t - J$ models on the square lattice. Phys. Rev. E. 2007;75:061119.
14. Singh RRP, Oitmaa J, High-temperature series expansion study of the Heisenberg antiferromagnet on the hyperkagome lattice: Comparison with Na4Ir3O8. Phys. Rev. B. 2012;85:104406.
15. Singh RRP, Oitmaa J. Corrections to pauling residual entropy and single tetrahedron based approximations for the pyrochlore lattice Ising antiferromagnet. Phys. Rev. B. 2012;85:144414.
16. Oitmaa J. High-temperature multigraph expansions for general Ising systems. Canadian Journal of Physics. 1981;59:15.
17. Rajan VT, Riseborough PS. High-temperature series expansion for random Ising magnets. Physical Review B. 1983;27:532.
18. Singh RRP, Chakravarty S. Critical behavior of an Ising spin-glass. Physical Review Letters. 1986;57: 245.
19. Zheng WH, Hamer CJ, Singh RRP, Trebst S, Monien H. Linked cluster series expansions for two-particle bound states. Physical Review B. 2001b;63: 144410.

Peer-review history:
The peer review history for this paper can be accessed here:
http://sciencedomain.org/review-history/15605