

A Study of Oguchi Approximation (OA) for Ising-Spin Magnetic Model

Raied Abbass Saleh

Thi-Qar University – College Of Science – Department of Physics

Abstract

An isospin magnetic system with spin values $S=\pm 1$ is studied for square and simple cubic lattice, the curie temperature has been calculated for these lattices based on the usual Oguchi approximation (OA). Within this scheme considered here, four atoms are considered where the three nearest-neighbor spin correlation are taken into account when the Hamiltonian is derived. The results for the critical temperature are remarkably accurate comparing to the effective field ones.

1 - Introduction

There have been extensive studies of isospin Ising model investigated both theoretically and experimentally [1]. Many of approximations have been existed to solve the Ising model of an Isospin system with spin values ($S_i = \pm 1$) and derived general expression of the magnetic moment of the system as a function of the temperature. A mathematical approximation for Ising model of an isospin system has been existed by Oguchi, within this approximation a crystal lattice of N magnetic atoms and a pair of atoms are considered where the first nearest-neighbor spin interaction is taken into account when the Hamiltonian is derived in this approximation [2]. The mean-field approximation (MFA) describes cooperative phenomena in which the effect of ordering interaction represented by a mean field proportional to the average net magnetic moment of magnetic system [3]. Bobak presents a development on the effective field theory (EFT) to obtain an approximation-or exact solution to the two-spin cluster Ising model [4]. It is worth mentioned that this methods is based on an exact thermal average for the pair of neighboring spins and utilizes the difference in operator technique [5]. Here, our procedure is based on the finite spin cluster of small size. We have used the simplest assumption of finite cluster with two block spins of three nearest-neighbor interactions. The two clusters are assumed to be independent on each other. Since the number of correlated nearest-neighbor spin pairs depends on the cluster size and the lattice structure [6]. Thus, the correlation of the nearest-neighbor spins in each cluster have been taken into consideration provide that one neglects only correlations between the two clusters considered [4].

Within this work, we try to extend the Oguchi approximation (OA) scheme to a new one to get more exact results of the critical temperature comparing to the previous works.

2. Theory

Very few statistical mechanical models have been solved exactly; the Ising model is one of best developed models in statistical physics. It has been solved in one-dimensional and certain two-dimensional lattice. In three-dimension not even the nearest neighbour spin-1/2 Ising model is tractable, therefore it is necessary to resort to approximation methods [7]. Abubrig *et. Al.* potentially presented a new and helpful scheme for improving the

values of the critical temperature for a number of lattices in Ising spin system, these methods use rigorous and complicated solutions which represent substantial improvements of the standard MFA [3]. Another formwork has been presented by Bobak et. Al. and is based on the introduction of differential operator technique, taking into account the effects of many-body static spin correlations [5] . It is conventional and convenient to use magnetic language and write the model Hamiltonians of an isospin system in term of spin variables. The Hamiltonian for the spin-1/2 Ising system in zero field is defined by [7]:

$$H = -\sum_{i,j} J_{ij} S_i S_j , \quad S_i = \pm 1 \dots\dots\dots (1)$$

where the sum runs N identical spins, and J_{ij} is the exchange interaction between spins sites i and j . Our work considers four lattices (i, j, k and ℓ) whose spin states denoted by (S_i) , (S_j) , (S_k) and (S_ℓ) respectively , together with their nearest neighbors as shown in Fig.(1), and

according to our scheme considered, we can decompose the Hamiltonian in equ.(1) as follows :

$$H = -J_{ij} S_i S_j - J_{k\ell} S_k S_\ell - h_m S_i - h_n S_j - h_o S_k - h_p S_\ell \dots\dots\dots(2)$$

where

$$\begin{aligned} h_m &= \sum_m^{z-2} J_{im} S_m & ; & \quad h_n = \sum_n^{z-2} J_{jn} S_n \\ h_o &= \sum_o^{z-2} J_{ko} S_o & ; & \quad h_p = \sum_p^{z-2} J_{\ell p} S_p \end{aligned} \dots\dots\dots (3)$$

Where z is the coordination number ($z=4, 6$ for square and simple cubic lattices, respectively). And since the system under study is an isospin system ($S_i \equiv S_j \equiv S_k \equiv S_\ell = \pm 1$) we can say that:

$$J_{ij} \equiv J_{k\ell} \equiv J_{im} \equiv J_{jn} \equiv J_{ko} \equiv J_{\ell p} = J \dots\dots\dots (4)$$

$$\sum_m S_m \equiv \sum_n S_n \equiv \sum_o S_o \equiv \sum_p S_p = m \dots\dots\dots (5)$$

Where m is the average magnetic moment of the system, Now the Hamiltonian of the system in equ.(2) can be written as:

$$H = -JS_i S_j - JS_k S_\ell - (z - 2)Jm(S_i + S_j + S_k + S_\ell) \dots\dots\dots (6)$$

Now, we can calculate the average magnetic moment, of the magnetic system, as a function of the temperature from Maxwell Boltzman distribution state that [8]:

$$m = \frac{\sum_{S_i} \sum_{S_j} \sum_{S_k} \sum_{S_\ell} \frac{1}{4}(S_i + S_j + S_k + S_\ell) e^{-\beta H}}{Z} \dots\dots\dots (7)$$

Where $\beta=1/K_B T$ and T represent the temperature of the system, Z is the partition function of the system which is defined as:

$$Z = \sum_{S_i=\pm 1} \sum_{S_j} \sum_{S_k} \sum_{S_\ell} e^{-\beta H} \dots\dots\dots (8)$$

Substituting equ. (8) in equ.(7) and expanding the summations over each of the spin value of $(S_i, S_j, S_k \text{ and } S_\ell)$ with ± 1 we get :

$$m = \frac{1}{2} \frac{2 \sinh(2h) + e^{2t} \sinh(4h)}{4 \cosh(2h) + e^{2t} \cosh(4h)} \dots\dots\dots (9)$$

We have just derived the general expression for evaluation the magnetization of the spin-1/2 Ising model, when $h=t(z-2)m$ and $t=J/K_B T$. Consequently, at this moment, we can determine the critical temperature $K_B T$.

3. Results and Discussions

In this section, let us show the results by solving equation (9) numerically using C++ programming language for square and simple cubic lattices ($z = 4, 6$ respectively). By way of comparison, we have listed the results of the MFA, OA and EFT. Table (1) shows clearly that the work represents here makes an improvement for the critical temperature comparing with other works mentioned above. As shown in table (1) the results of the Curie temperature for under study lattices (square and simple cubic lattice) which have been calculated within the current suggested approximation have been clearly approximate to it's exact values. The results also decreased the difference between practical and theoretical values computed according to the previous approximations (MFA, OA and EFT). Because of the fact that the present study concentrated on the effects of crystal system on a four adjacent atoms instead of one or two atoms as in MFA

or OA respectively [3,2]. Hence, the present approximation has added to the Hamiltonian of the system the exchange interaction term between each two spins in the cluster under consideration, and left the effect of the other atoms in the system on each atom in the two clusters within average net magnetic moment. While the current work have been distinguished from the EFT in approaching from the exact solution of the spin Ising system in obtaining approximate solution of Curie temperature, since that the EFT was limited because of mathematical and computing problems particularly when it deals with high spin systems or those atoms adjacent to a large number of neighboring atoms [4].

4. Conclusions:

In the present work, we use Ising spin system which is based on the usual Oguchi approximation, where we assume that the correlation among the first, second and third nearest-neighbour spins and mean-field approximation (MFA) are exist in the system. The results for the Curie temperature for each lattice are remarkably accurate comparing to the effective field.

Table (1) : Results for the critical temperature $K_B T_c$ of the square($z=4$) and simple cubic ($z=6$) lattices respectively

Method	Square $K_B T_c$	Simple Cubic $K_B T_c$
MFA ^[3]	4.0	6.0
OA ^[2]	3.7764	5.8469
EFT ^[4]	3.0250	5.0392
Present work	2.7070	4.8185
Exact ^[8]	2.2692	4.5108

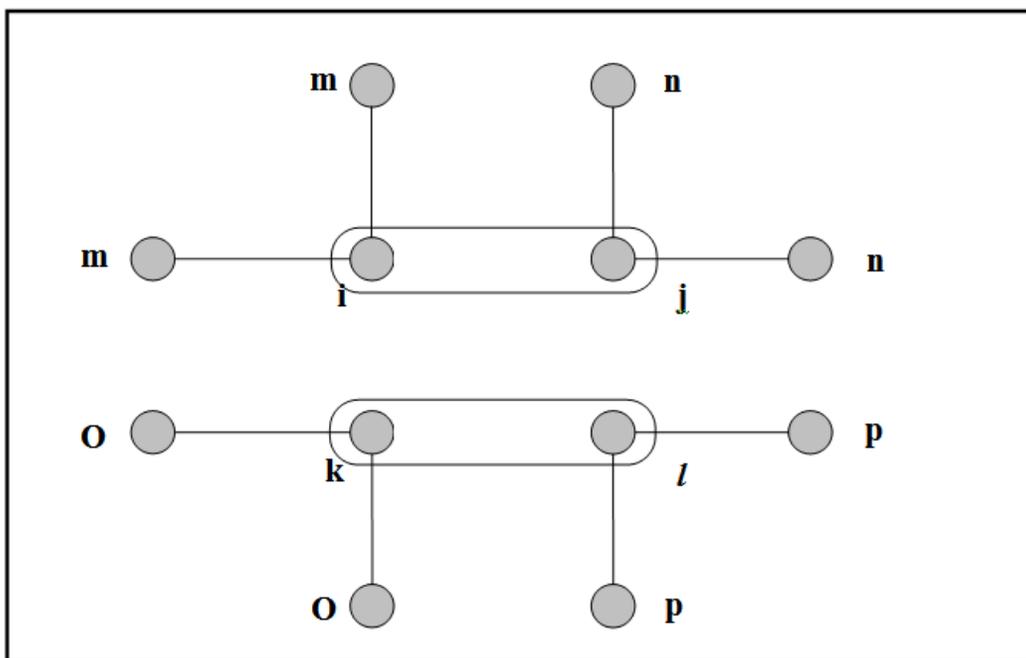


Fig.1: Two clusters of two-correlated pairs of spin (i, j) and (k, l) surrounded by the pairs of spin field in the case of a square lattice.

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دراسة في تقريب اكوشي لنموذج أيزنك للانظمة المغناطيسية

رائد عباس صالح

قسم الفيزياء - كلية العلوم - جامعة ذي قار

الخلاصة

تم دراسة نظام مغناطيسي متماثل الذرات قيم البرم لها $S=\pm 1$ من خلال حل موديل ايزنك لشبكة رباعية وشبيكة مكعب بسيط ، حيث تمثلت الدراسة بحساب درجة حرارة كوري لتلك الشبائك بواسطة موديل ايزنك بالاعتماد على توسيع اكوشي. وقد شمل التمثيل الجديد دراسة اربعة ذرات مركزية في النظام المذكور مع الاخذ بنظر الاعتبار دوال الارتباط بين اقرب الجارات الاولى والثانية والثالثة عند اشتقاق الهاملتوني لهذا النظام . النتائج المحصول عليها لدرجة حرارة كوري كانت مشجعة ومقاربة لنتائج نظرية المجال المؤثر لموديل ايزنك.