Analytic average magnetization expression for the body-centered cubic Ising lattice

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Abstract The average magnetization of the body-centered cubic Ising lattice is investigated by the use of the interrelation developed recently by us. We apply the same conjectures made for the odd spins correlation functions as in our previous works. The mathematical forms of the odd spin correlation functions are eventually elucidated by some physical discussions. We have seen that the obtained average magnetization expression is in good agreement with the numerical data for the body-centered cubic lattice Ising model.

1 Introduction

The Ising model was proposed for a mathematical model of ferromagnetism in statistical mechanics by Lenz in 1920. Lenz’s student Ising investigated the model in one dimension in his 1924 [1] thesis. The model consists of discrete variables that represent magnetic dipole moment at each lattice site that can be in one of two states (+1 or −1). The model allows the identification of phase transitions as diverse as gas–liquids, ferromagnets, binary alloys, and so on [2–6]. The model has an exact solution in one-dimension (1D) with the prediction of the absence of phase transition at finite temperature [7–11]. The model has been studied using several theoretical approaches, such as high and low-temperature series expansions, Monte Carlo simulations, renormalization group methods, and perturbative field theoretical methods [12–18].

A more extensive list of methods and references can be found in the exhaustive review article by Pelissetto and Vicari [19]. Almost seventy years have passed since Onsager’s [20] celebrated the solution of the Ising model free energy in 1944, followed by Yang’s [21] proof of Onsager’s result for the spontaneous magnetization in 1952, there is, however, no known solution for the 3D model [22–24]. Therefore, Onsager and Yang’s works of the square lattice Ising model is still one of the very few exactly solved models [25–27], it now serves as a proving ground for new theories, approximations, and numerical algorithms [28–31].

It is impossible to mention all of the important steps in the investigation of the Ising model, but we still think that it is relevant to mention shortly the important achievements of the subject. The proof of the existence of the critical point by Kramers and Wannier [32] with the method of a dual transformation was an important development in the investigation of phase transition. Later, the qualitative calculation of Kramers and Wannier was proven analytically by Onsager and [33, 34]. The spontaneous magnetization of the Ising model on rectangular lattice was first calculated by Onsager, he has not, however, published his derivation [35].

The average magnetization expression of the square lattice Ising model, \( \langle \sigma \rangle = 1 - \sinh(2K)^{-1} \) was first published by Yang [36]. The method used in Yang’s derivation is too cumbersome, he recalls it as the longest calculation in his career [37]. Later, a less complicated method, but is still too hard to recover, has been proposed to study the 2D Ising model [38–43]. In addition, the average magnetization relations were obtained for the Ising model on the honeycomb lattice [44] by Naya and by [45] for the triangular lattice.

Now let us introduce the main steps that will be used in the calculation of the average magnetization of the body-centered cubic lattice. For the sake of confirmation of the validity and relevance of the method that will be used in this paper, we first want to mention some important features of the odd spins correlation function since they will be one important part of the calculation of the average magnetization of body-centered cubic Ising lattice in his paper. Unfortunately, there is no large available literature except for some papers on three-spin correlation functions.

The three-spin correlation function of the 2D Ising model [46, 47] was first considered by Baxter for three spins surrounding a triangle by using the Pfaffian method. A simpler derivation of the three-spin correlation of the honeycomb lattice was also given by Enting [48].

We think that it is important to mention that there were some other important studies on the subject of the three-spin correlation functions [49–52]. The common physical properties of the three-spin correlation function obtained in these works are that: the three-spin correlation function manifestly assumes the same critical coupling strength and the same critical exponent as the order
parameter. As we will see in the next section, these physical properties are relevant as well as necessary to describe the three-spin correlation functions.

We can, therefore, use these physical properties to propose a relevant mathematical functional form for the odd spin correlation functions. These points will be elucidated more through this paper.

In the next section, we will try to obtain the desired average magnetization expression for the body-centered cubic lattice with the same analytic method used in our previous paper [53, 54] and the previously derived average magnetization interrelation by us [55]. The obtained expression will be compared to the already available simulation result [56]. In the same section, we will discuss the relevance of the obtained average magnetization relation and we will also present some concluding remarks about the obtained relation.

2 The average magnetization calculation of body-centered cubic Ising lattice

The previously derived formula [55] can be arranged in the absence of an external magnetic field for the body-centered cubic lattice as,

$$\langle \sigma_{0,i} \rangle = \langle \tanh[K(\sigma_{1,i} + \sigma_{2,i} + \cdots + \sigma_{8,i})]\rangle.$$

(1)

Here $\sigma_{0,i}$ denotes the central spin at the $i^{th}$ site while $\sigma_{l,i}$, $l = 1, 2, \cdots, 8$, are the nearest neighbor spins around its central spin and $K$ is the coupling strength.

Apparently from now on, carrying the index $i$ is not necessary. Expressing the tangent hyperbolic function with the following equivalent mathematical form with the help of Fig. 1 as

$$\tanh[K(\sigma_1 + \sigma_2 + \cdots + \sigma_8)] = A_1[\sigma_1 + \sigma_2 + \cdots + \sigma_8]$$

+ $A_2[\sigma_1\sigma_2\sigma_3 + \cdots] + A_3[\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5 + \cdots]$

+ $A_4[\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6 + \cdots].$

It is worthwhile to mention that in the parentheses of this equation indicated as [$\cdots$] coming after $A_1, A_2, A_3,$ and $A_4$, there are 8, 56, 56, 8 terms respectively. Writing the relation $\tanh[K(\sigma_1 + \sigma_2 + \cdots + \sigma_8)]$ for different orientations of the eight spin degrees of freedom, one can only obtain four linearly independent equations as

$$\tanh(8K) = 8A_1 + 56A_2 + 56A_3 + 8A_4,$$

$$\tanh(6K) = 6A_1 + 14A_2 - 14A_3 - 6A_4,$$

$$\tanh(4K) = 4A_1 - 4A_2 - 4A_3 + 4A_4,$$

$$\tanh(2K) = 2A_1 - 6A_2 + 6A_3 - 2A_4.$$

The solution of this system of linear equations, after some algebra the solution for $A_1, A_2, A_3,$ and $A_4$, can be obtained readily,

$$A_1(K) = \frac{1}{128}[14\tanh(2K) + 14\tanh(4K) + 6\tanh(6K) + \tanh(8K)],$$

$$A_2(K) = \frac{1}{128}[-6\tanh(2K) - 2\tanh(4K) + 2\tanh(6K) + \tanh(8K)],$$

$$A_3(K) = \frac{1}{128}[6\tanh(2K) - 2\tanh(4K) - 2\tanh(6K) + \tanh(8K)],$$

$$A_4(K) = \frac{1}{128}[-14\tanh(2K) + 14\tanh(4K) - 6\tanh(6K) + \tanh(8K)].$$

by these expressions. Now, substituting the equivalent mathematical form of tangent hyperbolic function into Eq. (1) and followingly taking the average of both sides, Eq. (1) turns out to be

$$\langle \sigma \rangle = 8A_1\langle \sigma \rangle + A_2[24(\sigma_1\sigma_2\sigma_3) + 24(\sigma_1\sigma_2\sigma_7) + 8(\sigma_1\sigma_3\sigma_6)]$$

+ $A_3[24(\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5) + 24(\sigma_1\sigma_2\sigma_3\sigma_7) + 8(\sigma_1\sigma_3\sigma_5\sigma_7)]$

+ $A_4[\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7].$

(2)

Now let us introduce some physical interpretations of the odd spins correlation functions appearing in this equation. To this end, taking into account the critical behavior of the order parameter $\langle \sigma \rangle$ might be helpful. Recalling the singularity of the order parameter at the critical point, one can easily see that the odd spins correlation function can be expressed as a function of the order parameter.

On the other hand, it is not easy or not even possible to propose an exact relation for the odd spins correlations, but taking into account the general behavior of the critical properties of the order parameter, one can conjecture or propose heuristic functional forms for the odd spins correlation functions with the following relations as,
The body-centered cubic lattice structure, the eight spins surrounding the central spin $\sigma_0$.

The plot of $A_1, A_2, A_3,$ and $A_4$ with respect to $K$.

\[
\langle \sigma_1 \sigma_2 \sigma_3 \rangle = a_{2,1} \langle \sigma \rangle + (1 - a_{2,1}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_2 \sigma_7 \rangle = a_{2,2} \langle \sigma \rangle + (1 - a_{2,2}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_3 \sigma_6 \rangle = a_{2,3} \langle \sigma \rangle + (1 - a_{2,3}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \rangle = a_{3,1} \langle \sigma \rangle + (1 - a_{3,1}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_2 \sigma_3 \sigma_7 \sigma_8 \rangle = a_{3,2} \langle \sigma \rangle + (1 - a_{3,2}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_2 \sigma_3 \sigma_5 \sigma_7 \rangle = a_{3,3} \langle \sigma \rangle + (1 - a_{3,3}) \langle \sigma \rangle^{1/3},
\]
\[
\langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \sigma_6 \sigma_7 \rangle = a_{4,1} \langle \sigma \rangle + (1 - a_{4,1}) \langle \sigma \rangle^{1/3}.
\]

Substituting these conjectured odd spins correlation functions into Eq. (2), leads to

\[
\langle \sigma \rangle = \left[ 8A_1 + 24A_2 \left( a_{2,1} + a_{2,2} + \frac{a_{2,3}}{3} \right) \right] + 24A_3 \left( a_{3,1} + a_{3,2} + \frac{a_{3,3}}{3} \right) + 8A_4a_{4,1} \langle \sigma \rangle^{1/3},
\]
\[
+ \left[ 24A_2 \left( \frac{7}{3} - \left( a_{2,1} + a_{2,2} + \frac{a_{2,3}}{3} \right) \right) \right] + 24A_3 \left( \frac{7}{3} - \left( a_{3,1} + a_{3,2} + \frac{a_{3,3}}{3} \right) \right)
\]
\[
+ 8A_4(1 - a_{4,1}) \langle \sigma \rangle^{1/3}.
\]

In the above equation, there are seven unknown parameters which are needed to be obtained.

To this end, if we define more proper parameters in terms of the coefficients as, $z_1 = a_{2,1} + a_{2,2} + \frac{a_{2,3}}{3}$ and $z_2 = a_{3,1} + a_{3,2} + \frac{a_{3,3}}{3}$.

And assuming intuitively that $z_1$ and $z_2$ have approximately equal values, one can define $a_{4,1}$ in terms of $z_1$ and $z_2$ as $a_{4,1} = \frac{3}{7} \frac{z_1 + z_2}{2}$.
Fig. 3 The plot of the average magnetization of the body-centered cubic Ising lattice with respect to $K$

This final approximation can be elucidated if we consider Fig. 2. From this figure one can see that $A_1$ assumes values a lot larger than all the others, $A_2$, $A_3$ and $A_4$. Meaning that any rough approximate values of $a_{4,1}$ can only change the final result very slightly (or even the effect of it is unnoticeable).

Thus the number of unknown parameters is reduced to two unknown, $z_1$ and $z_2$. To obtain these two unknowns, one can exploit the physical properties of the average magnetization. For example, if $K$ goes to infinity, $\langle \sigma \rangle$ must go to one. Unfortunately, this property of average magnetization cannot produce a relation between $z_1$ and $z_2$. Using the critical behavior of the average magnetization, one can use the property of $\langle \sigma \rangle$ at the critical point: it assumes the value of zero if $K < K_c$, and it assumes values different from zero if $K > K_c$. Using this final remark and assuming $z_1 \simeq z_2$, and denoting both of them with $z$, one can obtain the value of $z$ as $z = 0.8238$ if the critical value of $K$ for body-centered cubic lattice $K_c = 0.1573$ is considered.

After this short analysis, we obtain the following relation for the average magnetization of body-centered cubic Ising lattice as,$$
\langle \sigma \rangle = \left[ \frac{1 - 8A_1 - 24(A_2 + A_3 + \frac{1}{7}A_4)}{24(A_2 + A_3)(\frac{7}{5} - z) + 8A_4(1 - \frac{7}{5}z)} \right]^\beta,
$$
where the value of $\beta$ can be taken as equal to 0.325 for all the 3D Ising lattice.

We have plotted Fig. 3 for the obtained average magnetization expression presented with Eq. (3). In this figure, the red data points indicate the simulation results of [56] and the blue curve shows the result of Eq. (3). As seen in Fig. 3, the agreement of the obtained expression for average magnetization of body-centered cubic lattice in this paper and the simulation data is almost perfect. Even, it is almost impossible to see the differences in this figure. Therefore, we can claim that the heuristically obtained average magnetization relation given by Eq. (3) is almost exact. This means that the conjectures used here in this paper have been previously applied to the square, honeycomb, triangular, and simple cubic lattices in references [53, 54] for the odd spins correlation functions are relevant and also valuable.

Before closing this section we would like to point out some possible applications of the theoretical approach used in this paper to the mix-spin system, particularly to the ferrimagnetic system. Since the mixed ferrimagnetic Ising system has been a subject of intensive investigation [57–62].

In contrast to ferromagnets and antiferromagnets, in ferrimagnets there is an important possibility of the existence, under certain conditions, of a compensation temperature $T_{comp}$, at which the resultant magnetization vanishes below the transition temperature $T_c$. In a ferrimagnet the different temperature dependences of the sublattice magnetizations raise the possibility of the existence of compensation temperatures. It has been found that the coercivity diverges at the compensation point.

We believe that the method used in this paper can overcome some of the calculation difficulties appearing in the mix-spin system in two dimensions if only the nearest neighbor interactions are taken into account. However, to obtain the known properties of the ferrimagnetic material, the next nearest neighbor interactions need to be taken into account in the theory [63, 64].

Of course, the inclusion of the next nearest neighbor interaction can create some difficulties in the application of the approach used in this paper. Therefore, the application of the used in this paper to the ferrimagnetic system will be our research interest in the future.

3 Conclusion and discussion

In this paper, the calculation of the average magnetization of the body-centered cubic Ising lattice was considered by the method which was developed previously in a series of papers of us. Indeed, we have obtained an average magnetization relation for this lattice structure, and we observed that the obtained expression is in good agreement with the simulation data.
Recalling, the almost exact agreement of the previously obtained result for honeycomb, square, triangular, and simple cubic structure average magnetization relation and the average magnetization relation obtained in this current paper for the body-centered cubic lattice.

We can claim that the conjectured mathematical forms for the odd spins correlation functions are relevant and also important since they lead to an analytical calculation of the average magnetization of Ising lattices. Of course, the method is inevitably heuristic. However, we think that any relevant analytical calculation method developed for the calculation of the average magnetization expressions of Ising lattices can be considered valuable and helpful.

In other words, in this paper, we obtain the average magnetization relation of the body-centered cubic Ising lattice with very simple and tractable mathematical and physical approaches. We think that this point is also important if we recall the mathematical procedure applied to obtain the square lattice average magnetization by Yang.

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Data Availability Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

Declarations

Conflict of interest The author declares that he has no conflict of interest.

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