Relevant spontaneous magnetization relations for the triangular and the cubic lattice Ising model

Tuncer Kaya∗

Department of Physics, Yıldız Technical University, 34220 Davutpaşa, Istanbul, Turkey

The spontaneous magnetization relations for the 2D triangular and the 3D cubic lattices of the Ising model are derived by a new tractable easily calculable mathematical method. The result obtained for the triangular lattice is compared with the already available result to test and investigate the relevance the new mathematical method. From this comparison, it is seen that the agreement of our result is almost the same or almost equivalent to the previously obtained exact result. The new approach is, then, applied to the long-standing 3D cubic lattice, and the corresponding expression for the spontaneous magnetism is derived. The relation obtained is compared with the already existing numerical results for the 3D lattice. The essence of the method going to be used in this paper is based on exploiting the main characteristic of the order parameter of a second order phase transition which provides a more direct physical insight into the calculation of the spontaneous magnetization of the Ising model.

I. INTRODUCTION

The Ising model is an approximate mathematical model system to describe and investigate the physically very cumbersome problem of phase transition phenomena. It was originated with Lenz [1] in 1920 and was subsequently investigated by his student Ising [2]. Over a long period of time, it is seen that the model unifies the study phase transitions in systems as diverse as ferromagnet, gas-liquid, binary alloys, and so on. It may be the simplest mathematical model to analyze and investigate phase transitions theoretically. Its application to realistic systems such as the 3D lattices is, however, still too cumbersome to work with the conventional mathematical approaches used for the 2D lattices. Therefore, there is no exact result obtained from this mode for the 3D lattices. In other words, the 3D model has withstood challenges and remains, to this date, an outstanding unsolved problem. Even the application of the usual method to 2D lattices is very formidable and very daunting. I think, therefore, that a new mathematically more tractable and easily calculable method for the treatment of these lattices may be interesting. Before starting to introduce our mathematical approach to calculate the order parameter or the spontaneous magnetization of the triangular and the cubic lattices, it might be appropriate to introduce some important steps in the mathematical treatment of these problems.

The existence of the critical point, meaning the existence of second order phase transition, was first proven by Kramers and Wannier [3] using the method of a dual transformation. The qualitative calculation of Kramers and Wannier was verified by Onsager [4] and [5]. The existence of criticality led to investigate and calculate the average magnetization. Although, the spontaneous magnetization of the Ising model on rectangular lattice was first calculated by Onsager [6], he never bothered to publish his derivation [7]. Yang was the first person who published his derivation of the average magnetization of the square lattice Ising model [8]. His result is $< \sigma > = [1 - \sinh(2K)^{-1}]$. Since the method used in Yang’s derivation is too cumbersome, he recalled it as the longest calculation in his career [9]. Later, less complicated methods, but which are still too hard to recover, have been developed to obtain the partition function of the 2D Ising model [10–15]. For works in which other 2D Ising lattices are considered, one can give the relevant articles where average magnetization relations were obtained by Naya for the Ising model on honeycomb lattice [16] and for the triangular lattice by [17]. Of course, there are other important contributions done on this subject, but it is impossible to mention all of them in this paper. In other words, it goes well beyond the scope of the study.

We are now ready to give the general features of the method going to be used in this paper. Our treatment starts with the recently obtained relation by Kaya [18], given as $< \sigma_{0, i} > = < \tanh[K(\sigma_{1, i} + \sigma_{2, i} + \ldots + \sigma_{z, i}) + H] >$. Here, $K$ is the coupling strength and $z$ is the number of nearest neighbors. $\sigma_{0, i}$ denotes the central spin at the $i$th site while $\sigma_{l, i}$, $l = 1, 2, \ldots, z$, are the nearest neighbor spins around the central spin. When this relation is applied to a particular lattice, it produces inevitably odd spin correlation functions such as the three spins and five spins correlation functions. At this point it is important to mention that its applications to the honeycomb and the square lattices are the simplest in that only three spins correlation function appear in the final equation [19], making the mathematical treatment of the honeycomb and the square lattices are less complicated. The spontaneous magnetization relations
have also been investigated and obtained \[19\]. In the derivations of the spontaneous magnetization relation of those lattices, we had to use a conjectured mathematical form for the corresponding three spin correlation functions, given as 
\[
<\sigma_1\sigma_2\sigma_3> = a <\sigma> + (1-a) <\sigma^3>.
\]
Here $\beta$ denotes the magnetic critical exponent. We think it is also important to point out that the three spin correlation function of the 2D Ising model was considered by Baxter \[20, 21\] for three spins surrounding a triangle. He used the Pfaffian method. Later, a simpler derivation was given by Enting \[22\], who also calculated the three spin correlation for the honeycomb lattice. There are also some other important studies on the subject of the three spin correlation functions \[23, 24\] by the cited authors. The important consequence that we get from almost all of them is the common physical properties of the three spin correlation function: the three spin correlation function manifestly possesses the same critical exponent as the order parameter. As we are going to see in the next section, these physical properties are quite relevant and also apparently necessary to describe the three spin correlation function. Therefore, we are going the need to use these properties safely to propose a mathematical functional form for the three spin correlation function. In this current work, we will need to make a similar conjecture for the five spin correlation functions which are going to be appear in our current investigation. Once again, we are going to use the same physical reasoning as we made for the three spin correlation function, to construct the conjectured functional form for the five spin correlation functions.

One might be anxious for the evidence of the power of the approach which is going to be used in this paper. As a first clue, we simply want to point out the essence of the method from the outset. We are always going to start to our treatment with the relation given for the $<\sigma>$ in the above paragraph. Exceptional valuable feature of the our approach comes when this relation is combined with the conjectured odd spins correlation functions. This combination also provides a more direct physical insight into making a conjecture about the mathematical form of the odd spin correlation functions. That is to say, in the language of our approach, this combination leads to derive the spontaneous magnetization expression by exploiting the critical behavior of the order parameter $<\sigma>$. As we are going to see, our approach turns out to be very useful and essential in determining the desired analytical spontaneous magnetization expression for the long-standing the 3D cubic lattice problem.

We are going to first consider to calculate an average magnetization expression for the triangular lattice. For the sake of confirmation of the validity and relevance of the new mathematical method, we are going to compare the obtained result of this paper with the exact spontaneous magnetization relation for triangular lattice \[27\]. The conventional mathematical method used to investigate the 2D lattices is so complicated that, when used to investigate the 3D lattices, any exact results are still unknown \[29–31, 35\]. However, the new approach used to investigate to the 2D lattices with a easily tractable mathematics can also be used in calculations and investigations of the 3D cubic lattice safely. Indeed, we are going to deal with the 3D lattices \[32, 33\] here in this paper. It is going to be our main objective to obtain an analytical spontaneous magnetization expression for the cubic lattice.

This paper is organized as follows. In the next section, the average magnetization of the the triangular lattice is going to be calculated with an alternative analytic method based on the previously derived average magnetization relation by us \[19\]. The obtained expression is also going to be compared by the already available exact result derived by Potts. In the third section, the average magnetization relation is going to be derived by the same method for the 3D cubic lattice. The obtained result is going to compared with the available numerical results. In the same section, some discussions and conclusions are also going to be presented.

## II. THE SPONTANEOUS MAGNETIZATION CALCULATION OF THE TRIANGULAR LATTICE

To investigate and test the validity and relevance of the method which is going to be used in this paper, we start by considering its application on the triangular Ising lattice. The treatment is going to be very similar to the procedure applied in the calculation of to the honeycomb and the square lattice cases studied in \[19\]. To start the calculation, we need to rewrite the equation introduced in the above introduction once more as,
\[
<\sigma_{0,i}> = <\tanh[K(\sigma_{1,i} + \sigma_{2,i} + \cdots + \sigma_{5,i}) + H]>
\]  
\[1\]
For the case of the triangular lattice shown in Fig.1, this equation can expressed quite readily in the absence of external field as,
\[
<\sigma> = <\tanh[\kappa(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 + \sigma_6)]>,
\]  
\[2\]
where we keep only numerical indices for notational simplicity. Apparently, this final equation is very similar to the previously used ones \[19\] except for extra more spin terms which create eventually some mathematical complication as expected. But, the treatment is going to be the same. That means, we need to write an equivalent relation which is equal to the hyperbolic tangent function appearing in the last equation. Thus, recalling the odd functional properties
Now considering different orientations of the spin variables \( \sigma_i = \pm 1 \), the unknown functions can be obtained after some algebra as,

\[
\begin{align*}
A_t &= \frac{1}{64} \tanh(6K) + \frac{1}{8} \tanh(4K) + \frac{13}{64} \tanh(2K) \\
B_t &= \frac{1}{32} \tanh(6K) - \frac{3}{32} \tanh(2K) \\
C_t &= \frac{3}{64} \tanh(6K) - \frac{1}{8} \tanh(4K) + \frac{7}{64} \tanh(2K).
\end{align*}
\]

If Eq. (3) is substituted into Eq. (2), after taking into account the equivalent odd spins correlations, it leads to,

\[
\begin{align*}
\langle \sigma \rangle &= 6A_t \langle \sigma \rangle + B_t \left[ 5 \langle \sigma_1 \sigma_2 \sigma_3 \rangle + 13 \langle \sigma_1 \sigma_3 \sigma_4 \rangle + 2 \langle \sigma_1 \sigma_3 \sigma_5 \rangle \right] + 6C_t \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 \rangle.
\end{align*}
\]

FIG. 1. The triangular lattice. The numbers from 1 to 6 indicate the spins around the central spin denoted with number zero. The black circles denote the central spins.
express the three and five spin correlation functions as,

\[
<\sigma_1\sigma_2\sigma_3> = a_{t,1} <\sigma> + (1 - a_{t,1}) <\sigma)^{1+\beta^{-1}}
\]
\[
<\sigma_1\sigma_3\sigma_5> = a_{t,2} <\sigma> + (1 - a_{t,2}) <\sigma)^{1+\beta^{-1}}
\]
\[
<\sigma_1\sigma_3\sigma_4\sigma_5> = a_{t,3} <\sigma> + (1 - a_{t,3}) <\sigma)^{1+\beta^{-1}}
\]
\[
<\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5> = a_{t,4} <\sigma> + (1 - a_{t,4}) <\sigma)^{1+\beta^{-1}}
\].

Substituting the last relations into Eq. (5), it can be written as,

\[
<\sigma> = [6A_h + (5a_{h,1} + 13a_{h,2} + 2a_{h,3})B_h + 6C_1a_{h,4}] <\sigma> + \\
[20B_h + 6C_h - (B_h + \frac{3}{10}z_1)] <\sigma)^{1+\beta^{-1}}
\].

In the last equation, there are four unknown parameters that need to be determined properly. To this end, it is relevant to consider the restrictions which these parameters need to satisfy. First, all of these parameters have to assume positive real values less than unity. Second, considering the distances between spins, it is easy to see that \(a_{t,1} > a_{t,2} > a_{t,3}\) and \(a_{t,4}\) must have the values less that the values of all the other three parameter because it is used in expressing five spins correlation function. From the obtained values for the parameters in the \([19]\), one can intuitively assume that all of the four parameters take values close to each other. Under these considerations, we introduce the following statements to present the last equation with a single parameter equation. Apparently, we need to define the new parameter in terms of the four parameters. Thus, if we name \(z_1 = 5a_{t,1} + 13a_{t,2} + 2a_{t,3}\) and \(z_2 = 6a_{t,4}\), one can easily see that \(z_2 \approx \frac{6}{20}z_1\) due to the assumption that the values of all of the four parameters are approximately equal to each other. Under this consideration the last equation can be expressed as,

\[
<\sigma> = [6A_h + (B_h + \frac{3}{10}C_h)z_1] <\sigma> + \\
[20B_h + 6C_h - (B_h + \frac{3}{10}z_1)] <\sigma)^{1+\beta^{-1}}
\].

From this equation, one can easily obtain in a self-consistent manner, the value of \(z_1\) at critical point as,

\[
1 - [6A_h + (B_h + \frac{3}{10}C_h)z_1]|_{K=K_c} = 0.
\]

Substituting the critical coupling strength value for triangular lattice \(K_c = 0.2747\) into the last relation, the value of \(z_1\) is calculated as \(z_1 = 16.13\). Finally, from Eq. (7), one can easily obtain the following expression for the spontaneous magnetization of the triangular lattice as,

\[
<\sigma> = \left[1 - [6A_h + (B_h + \frac{3}{10}C_h)z_1] \right]^{\beta}
\]

In Fig. 2, the spontaneous magnetization expression given in Eq. (10) and the exact result \([17, 27]\), given as

\[
<\sigma> = \frac{(3 - e^{4K})(1 + e^{4K})^3}{(3 + e^{4K})(1 - e^{4K})^3}
\]

are plotted. As seen from the figure, they are almost equivalent. This means that an almost exact result is obtained by avoiding the very daunting and cumbersome conventional method used previously to calculate the 2D lattice spontaneous magnetization. In addition, the relevance of the conjectured odd spins correlation functions are testified and confirmed by this excellent agreement. Hence, the conjectured functional form can be used safely regardless of the lattice types for the 2D lattice Ising model. At this point, it is important to mention once more that the mathematical and physical approaches used in this paper are a lot more easier than the calculation with the conventional calculation methods. We think, therefore, that it may help us in the calculation of the spontaneous magnetization for the 3D lattices. If we recall that all attempts have been unsuccessful since now for the analytical treatment of the 3D lattices. We are now in a position to deal with the long-standing unsolved problem. Due to the relevance and tractability of the method used in this paper, we are really hopeful that one can obtain the analytic expression for the spontaneous magnetization for the 3D lattices with almost in the same manner as used for the 2D lattices. To this end, we are going to consider the cubic lattice Ising model in the following section.
The following equation can be easily written from the Eq. (12) as,

$$<\sigma> = \tanh[\kappa(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 + \sigma_6)]$$  \hspace{1cm} (12)

As used above, our next step is to write an equivalent function for the hyperbolic tangent appearing in this equation to relate the spontaneous magnetization with the other correlation functions. To this end, we find that the following relation is convenient to satisfy the desired equivalence,

$$\tanh[\kappa(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 + \sigma_6)] = A_c[\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4 + \sigma_5 + \sigma_6] + B_c[\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_4 \sigma_1 + \sigma_4 \sigma_2 + \sigma_1 \sigma_3 \sigma_4 + \sigma_2 \sigma_3 \sigma_4 + \sigma_2 \sigma_3 \sigma_5 + \sigma_3 \sigma_4 \sigma_5 + \sigma_3 \sigma_4 \sigma_6 + \sigma_2 \sigma_4 \sigma_5 + \sigma_1 \sigma_2 \sigma_3 + \sigma_4 \sigma_5 + \sigma_1 \sigma_2 \sigma_6 + \sigma_1 \sigma_3 \sigma_6 + \sigma_1 \sigma_3 \sigma_5 + \sigma_2 \sigma_4 \sigma_6 + \sigma_5 \sigma_6 \sigma_1 + \sigma_5 \sigma_6 \sigma_2 + \sigma_5 \sigma_6 \sigma_3 + \sigma_5 \sigma_6 \sigma_4] + C_c[\sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 + \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_6 + \sigma_1 \sigma_2 \sigma_3 \sigma_5 \sigma_6 + \sigma_1 \sigma_2 \sigma_4 \sigma_5 \sigma_6 + \sigma_1 \sigma_2 \sigma_4 \sigma_5 \sigma_6 + \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 + \sigma_1 \sigma_2 \sigma_4 \sigma_5 \sigma_6 + \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5].$$  \hspace{1cm} (13)

Now considering different orientations of the spin variables $\sigma_i = \pm 1$, the unknown functions can be obtained after some algebra as,

$$A_t = \frac{1}{64} \tanh(6K) + \frac{1}{8} \tanh(4K) + \frac{13}{64} \tanh(2K)$$
$$B_t = \frac{3}{32} \tanh(6K) - \frac{9}{32} \tanh(2K)$$
$$C_t = \frac{3}{64} \tanh(6K) - \frac{1}{8} \tanh(4K) + \frac{7}{64} \tanh(2K).$$  \hspace{1cm} (14)

Now, taking into account the equivalent spin orientations which apparently produce the same correlation functions, the following equation can be easily written from the Eq. (12) as,

$$<\sigma> = 6A_c <\sigma> + B_c[4 <\sigma_1 \sigma_2 \sigma_3 > + 8 <\sigma_1 \sigma_2 \sigma_6 > + 4 <\sigma_1 \sigma_3 \sigma_6 > + 4 <\sigma_1 \sigma_5 \sigma_6 >] + C_c[2 <\sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 > + 4 <\sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 >].$$  \hspace{1cm} (15)
We now find it convenient to define $z_i$. Substituting these functions into Eq. (15) leads to

$$
\text{Eq. (18) as,}
$$

From this equation it is clear that the critical behavior of the three spins correlation functions and the five spins correlation functions must have the same critical feature as the order parameter. Hence, for all practical purposes the conjectured form for the correlation functions for the 2D lattices can be also have the same functional form for the cubic lattice. This means that the following relations for those correlation functions appearing in the last equation can be relevant and safe functional forms. Thus,

$$
\begin{align*}
< \sigma_1 \sigma_2 \sigma_3 >& = a_{c,1} < \sigma > + (1 - a_{c,1}) < \sigma > ^{1+\beta} - 1
\end{align*}
$$

Substituting these functions into Eq. (15) leads to

$$
<\sigma>= [6A_c + (B_c + \frac{3}{10} C_c)z_1] < \sigma > + [B_c (4(1 - a_{c,1}) + 8(1 - a_{c,2}) + 4(1 - a_{c,3}) + 4(1 - a_{c,4})) + C_c ((1 - a_{c,5})4(1 - a_{c,6}))] < \sigma > ^{1+\beta} - 1.
$$

We now find it convenient to define $z_1 = 4a_{c,1} + 8a_{c,2} + 4a_{c,3} + 4a_{c,4}$ and $z_2 = 2a_{c,5} + 4a_{c,6}$. If we assume the values of $a_{c,j}$ are close to each others as assumed for the triangular lattice case, $z_2$ can be approximated as $z_2 \approx \frac{9}{20}z_1$. Taking into account these final remarks, the last equation may be written as

$$
<\sigma>= [6A_c + (B_c + \frac{3}{10} C_c)z_1] < \sigma > + [20B_c + 6C_c - (B_c + \frac{3}{10} C_c)z_1] < \sigma > ^{1+\beta} - 1.
$$

From this equation the value of $z_1$ can be obtained self-consistently, by considering the criticality of the spontaneous magnetization at the critical point $K_c = 0.226$ as

$$
1 - [6A_c + (B_c + \frac{3}{10} C_c)z_1]|_{K=K_c} = 0.
$$

This equation produces $z_1 = 9.6105$. Now, it is straightforward to obtain the spontaneous magnetization relation for the cubic lattice from the Eq. (18) as,

$$
<\sigma> = \left( \frac{1 - [6A_c + (B_c + \frac{3}{10} C_c)z_1]}{20B_c + 6C_c - (B_c + \frac{3}{10} C_c)z_1} \right)^{\beta}.
$$
FIG. 4. The plot of the spontaneous magnetization for the cubic lattice given by Eq. (16). The symbol □ indicates the numerical data calculated in Tapalov paper.

It is now quite natural to ask about the relevance of the obtained spontaneous magnetization relation for the cubic lattice. There is, of course, no immediate answer for this question since there is no previously obtained analytic expression for the spontaneous magnetization for the cubic lattice. On the other hand, there are some numerical calculation results for the 3D cubic lattice [36]. So it is convenient to plot the graphics of the Eq. (20) together with the numerical data. Indeed, Fig. 4 is plotted to compare Eq. (20) with the numeric data obtained by Tapalov and Blöte [36]. As seen from the figure, the numeric data points are totally in agreement with the curve of Eq. (20). Furthermore, in the paper of Tapalov, an empirical or numerical relation is introduced which is valid in the interval 0.0005 < t < 0.26. The relation expressed by the Eq. (10) of Tapalov paper is given as,

\[ < \sigma > = t^{0.32694}[1.691904 - 0.343577t^{0.5084} - 0.42572t] \]

where \( t = 1 - \frac{K}{K_c} \), \( K_c = 0.2216544 \) was used by Tapalov. The value of the critical exponent for \( \beta \) is obtained as 0.32694 in the same paper. These critical values are also obtained with very high accuracy in [37, 38]. At this point it is also important to notice that Tapalov’s numerical relation is confirmed by the research paper [39], in which a new coarse grain tensor renormalization group method based on the higher order singular value decomposition method is used. Therefore, we think that the Eq. (10) of Tapalov paper is relevant enough to safely compare the spontaneous magnetization relation obtained in this paper. Fig. 5 is plotted for comparing Eq. (20) with the Eq. (10) of Tapalov.

As seen from the figure, these two relations are almost equivalent within the claimed range of the Eq. (10) of the Tapalov’s paper. We, therefore, think that the spontaneous magnetization relation expressed in Eq. (20) of this paper is quite relevant result to be safely used wherever it is necessary. In other words, we now have a relevant and almost exact analytical expression for the 3D cubic lattice. Therefore, Eq. (20) can be considered as a very important development for the analytic treatment of the 3D Ising model. In summary, we have achieved to derive an relevant and almost exact formula for the spontaneous magnetization of the cubic lattice almost 70 years after the the square lattice solution of Yang. In addition, from the obtained result of this paper, we can also claim that the conjectured
functional forms for the odd spins correlation functions around the central spin can possibly considered as the almost exact expression for those correlation functions. This means that one can safely use these conjectured forms wherever they are needed.

IV. CONCLUSION AND DISCUSSION

In this work we have derived the spontaneous magnetization relations for the triangular and for the cubic lattice Ising model by considering a novel mathematical approach. The new approach is based on the previously obtained general equation, which relates the spontaneous magnetization with the corresponding odd spin correlation functions \[18\]. Taking into account the criticality properties of the spontaneous magnetization, we are forced to assume that the odd spins correlation functions have to also obey the same criticality of the spontaneous magnetization. Exploiting these similarities, the mathematical functional forms for the odd spins correlation functions are conjectured. Using these conjectured functions, the spontaneous magnetization relations for those lattices are obtained. Comparing the obtained spontaneous magnetization expressions with the already available results, the physical relevance of the obtain magnetization expressions are tested. Since the agreement between our results and the previously obtained results are almost the same, we may claim that the method used in this paper is quite relevant and is a safe method to calculate the spontaneous magnetization of the Ising lattices in general. In other words, the approach used in this paper simplifies not only the mathematical work needed for the exact treatments, but also it retains almost exactly the same essential critical features of the problem. It is also important to mention once more that there has been no analytic spontaneous magnetization relation for the cubic lattice in 3D up to now. The analytic spontaneous magnetization expressed by Eq. (16) of this paper is, therefore, very important and valuable. In addition, we can also claim from the result of this paper that the conjectured mathematical form for the odd spins correlation functions can be considered as excellent approximations (or almost exact expressions). Furthermore, because of the simplicity and generality of the method, it can be also used the calculation of the spontaneous magnetization of the other 3D lattices. Maybe even under some restrictions, it can be used to calculate the spontaneous magnetization in the presence of the external field.

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