Magnetic susceptibility of the square lattice Ising model

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Abstract In this work, we obtained an analytical relation for the susceptibility of the square lattice Ising model. Our investigation is based on an average magnetization interrelation which was recently obtained by us. To proceed further, we have to make a mathematical conjecture about the three-site correlation function appearing in the average magnetization interrelation. We presented the conjectured mathematical form of the three spin correlation function with the relation, $\langle \sigma_i \sigma_j \sigma_l \rangle = a(K,H)\langle \sigma \rangle + [1-a(K,H)]\langle \sigma \rangle^{1+\beta^{-1}}$. Here, $\beta$ denotes the critical exponent for the average magnetization and $a(K,H)$ is a function whose behavior will be described around the critical point with an arbitrary constant. To elucidate the relevance of the method, we have first calculated the susceptibility of the 1D chain as an example, and the obtained susceptibility expression for the 1D chain is equivalent to the result of the susceptibility obtained by the conventional method. Applying the same method, we obtained the values of the magnetic critical exponent $\gamma$ of the square lattice Ising model. The values of $\gamma$ are obtained as $\gamma = 1.72$ for $T > T_c$, and $\gamma = 0.91$ for $T < T_c$.

1 Introduction

The square lattice Ising model is probably the most important statistical mechanical model ever proposed in terms of its applications. Since Onsager’s [1] celebrated the solution of the Ising model free energy in 1944, followed by [2] the proof of Onsager’s result for the spontaneous magnetization in 1952, physicists have devoted themselves to the study of the problem of elucidating the susceptibility of the square lattice Ising model. As is well known, the Onsager’s solution in 1944 was publicly presented without a proof [3]. Although there is no known closed-form expression for the susceptibility $\chi$, a large body of knowledge about the susceptibility is available. Attempting to list all these contributions is impossible in this paper.

We will, however, only mention some of the research to indicate the main mathematical approaches in the investigation of the square lattice Ising model. We refer the reader to McCoy’s book [4] and the review article [5] for a review of these developments. We crave the forgiveness of the researchers whose papers are not cited in this paper. In 1976 Wu, McCoy, Tracy, and Barouch [6] showed that the susceptibility could be expressed as an infinite sum of $n$-dimensional integrals. The main result of their analysis can be given as the statement: for the low-temperature susceptibility ($T < T_c$), only even powers of $n$ contribute, starting at $n = 2$, while for the high-temperature susceptibility ($T > T_c$), only odd powers contribute. In 1999, Nickel [7, 8] showed that the susceptibility has a natural boundary in the complex plane and that such functions cannot be $D$-finite or holonomic functions. Later it was proved that each of these integrals $\chi(n)$ is $D$-finite but argued that their infinite sum, that is, the full susceptibility $\chi$ itself, is not [9, 10].

In a series of papers, Maillard and co-workers [11–16] found the linear ordinary differential equations satisfied by $\chi(3), \ldots, \chi(6)$. In 2011, Chan and his coworkers [17] extended the work in Ref. [7] to other two-dimensional lattices and gave an expansion of the scaled form of the susceptibility to unprecedented accuracy. Almost half a century has passed since the formal expression for the magnetic susceptibility of square lattice Ising model [5] is obtained. There is still, however, so much discussion and uncertainty in the investigation of the magnetic susceptibility of the square lattice Ising model.

Therefore, it is natural to ask the question: why is it so hard to obtain a closed expression for the susceptibility in this model. To answer this question, it is proper to recall the basic definition of magnetic susceptibility, which is given by the relation $\chi(T) = \frac{d\langle \sigma \rangle}{dH} |_{h=0}$. Here, $\langle \sigma \rangle$ is the average magnetization, $T$ denotes the temperature, and $h$ is the external field. Since the average magnetization is known only in zero magnetic fields ($h=0$), it is impossible to take the derivative appearing in the definition of magnetic susceptibility. Therefore, the susceptibility is usually studied through its relation with the zero-field spin–spin correlation function:

$$\chi(T) = \frac{1}{k_B N T} \sum_{i,j,k,l} \left[ \langle \sigma_{i,k,j} \sigma_{i,l,j} \rangle - \langle \sigma \rangle^2 \right].$$

Here, $i, j$ and $k, l$ denote lattice positions and run all over the system and $k_B$ is the Boltzmann’s constant.

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The correlation terms appearing in the above general relation are approximated by replacing the correlation function with \( \langle \sigma_{0,0}\sigma_{i,j} \rangle \) or even with \( \langle \sigma_{0,0}\sigma_{i,i} \rangle \).

We recall that for the isotropic square lattice Ising model, horizontal and vertical interaction constants have the same value \( J \). Then, the spontaneous magnetization is given for \( T < T_c \) by \( \langle \sigma \rangle = (1 - k_1^2)^{1/8} \). Here, \( k_1 = \sinh(2J/k_B T)^{-1/2} \) and \( \langle \sigma \rangle \) is zero for \( T > T_c \). \( T_c \) denotes the critical temperature. The correlation function appearing in the susceptibility relation has been studied by many authors \([18-20]\) and by various methods. However, a compactly closed expression of any \( \langle \sigma_{0,0}\sigma_{i,j} \rangle \) has not been yet found \([21]\), which indicates that the calculation of the square lattice susceptibility is still an open problem.

Of course, applying daunting mathematical treatments, the above-cited studies have made substantial advances in elucidating the properties of the susceptibility of the square lattice Ising model. On the other hand, the mathematics used in these research papers gets so complicated that it is impossible to follow up on the physical reasoning and even the mathematical approximations used. Therefore, it might be relevant and important to investigate the susceptibility of the square lattice Ising model from a different perspective.

To this end, we are going to exploit the recently obtained interrelation \([22]\) for the average magnetization, which is given by the following expression as

\[
\langle \sigma \rangle = \langle \tanh[K(\sigma_1 \cdots \sigma_z) + H] \rangle.
\] (1)

Here, \( \sigma_1, \cdots, \sigma_z \) are the nearest neighbors spins around its central spin. By applying this relationship together with a physically plausible assumption for odd spins correlation functions, we have obtained almost exact average magnetization expressions for the 2D lattices \([23]\) and 3D cubic lattice \([24]\) in the absence of external magnetic field.

We think it is worthwhile to mention that, in our recent papers, we have given the details of the calculations (with some useful tricks and tools) allowing one to obtain average magnetization expressions for other 3D Ising lattices. The obtain average magnetization expressions are almost equivalent to the exactly obtained results and simulation data. In addition, in the calculation of the average magnetization relations, applied mathematics is quite tractable and manageable.

Our primary goal in this paper is to calculate the susceptibility of the square lattice Ising model with the same tractable and manageable mathematical procedures. In doing so, we would also like to gain some more insight into the additional relevance of the conjectured assumption in our previous work. Here, the susceptibility of the square lattice is going to be investigated by the same average magnetization interrelation and we will use the same mathematical form of odd spins correlation function used in our previous studies. Of course, the odd spins correlation function is going to be modified slightly to take into account the external magnetic field dependence.

To elucidate the mathematical procedure, we first calculate the susceptibility of the 1D Ising model as an example, so that we can compare our result with the well-known exact susceptibility expression of the 1D Ising chain.

In doing so, we hope to provide adequate confirmation for the relevance of the method which will be used in the investigation of the susceptibility of the square lattice Ising model.

This paper is organized as follows. In the next section, we are going to calculate the susceptibility of the 1D Ising chain to elucidate and test the validity of the mathematical procedure which is going to be used in the calculation of the susceptibility of the square Ising lattice. In the last section, the susceptibility of the square Ising lattice is going to be calculated with the method developed for the treatment of the 1D chain.

In doing so, we are going to try to present our calculations and the necessary assumption as clearly as possible. In the same section, we are going to discuss both the used method and some useful indications of possible future research problems which can be treated with the method of this paper.

### 2 The susceptibility of 1D Ising chain

We start this section with the previously derived formula in reference \([22]\), which is given by Eq. (1) in the introduction. To find the critical coupling strength, we need to consider \( H = 0 \) case. So, taking into account Eq. (1) for 1D Ising chain in the absence of external field and if the hyperbolic tangent function is expressed as

\[
\tanh[K(\sigma_1 + \sigma_2)] = \frac{1}{2}(\sigma_1 + \sigma_2) \tanh(2K).
\] (2)

The critical coupling strength, \( K \), can be readily obtained as follows. Substituting this relation into Eq. (1) leads to \( \langle \sigma \rangle = \langle \sigma \rangle \tanh(2K) \). From this equation, it is obvious that the non-zero values for average magnetization \( \langle \sigma \rangle \) are only possible at zero temperature. Here, \( K \) is defined as \( K = J/(k_B T) \), where \( J \) is the nearest neighbor coupling constant. Thus, the critical temperature \( T_c \) for a 1D chain is equal to zero. Since the susceptibility is defined as the derivative of the average magnetization with respect to the external magnetic field \( h \), which is defined as \( H = h/(k_B T) \), we need to obtain the average magnetization of the 1D chain as a function of \( H \). To this end, we write the hyperbolic tangent function appearing in Eq. (1) as

\[
\tanh[K(\sigma_1 + \sigma_2) + H] = C_1(\sigma_1 + \sigma_2) + C_2\sigma_1\sigma_2 + C_3.
\] (3)
Under the consideration of different orientations of $\sigma_1$ and $\sigma_2$, the coefficients $C_1$, $C_2$ and $C_3$ can be obtained as,

\[
C_1(K, H) = \frac{1}{4}\{\tanh(2K + H) - \tanh(-2K + H)\},
\]
\[
C_2(K, H) = \frac{1}{4}\{\tanh(2K + H) + \tanh(-2K + H) + 2\tanh(H)\} - \tanh(H),
\]
\[
C_3(K, H) = \frac{1}{4}\{\tanh(2K + H) + \tanh(-2K + H) + 2\tanh(H)\}.
\]

Substituting these final relations into Eq. (3) and then taking the average of the both side of the equation leads to

\[
\langle \sigma \rangle = 2C_1\langle \sigma \rangle + C_2\langle \sigma_1\sigma_2 \rangle + C_3.
\] (4)

Thus, $\langle \sigma \rangle$ can be expressed as

\[
\langle \sigma \rangle = \frac{C_2\langle \sigma_1\sigma_2 \rangle + C_3}{1 - 2C_1}.
\] (5)

The susceptibility is defined as

\[
\chi(K, 0) = \frac{d\langle \sigma \rangle}{dH} \big|_{h=0} = \frac{1}{k_B T} \left. \frac{d\langle \sigma \rangle}{dH} \right|_{h=0}.
\] (6)

After doing some algebra, $\chi(K, 0)$ can be expressed as

\[
\chi(K, 0) = \frac{1}{k_B T} \left(1 + \left[\frac{1}{2} + \langle \sigma_1\sigma_2 \rangle\right]\text{sech}^2(2K)\right).
\] (7)

For large values of $K$ or small values of $T$, this equation can be expressed as

\[
\chi(K, 0) = \frac{1}{k_B T} e^{J/K_B T}.
\] (8)

This final susceptibility relation is equivalent to the susceptibility relation obtained in [25]. At this point, it is important to point out that we have obtained the susceptibility relation without using the well-known 1D chain average magnetization relation, which is given by the following relation as

\[
\langle \sigma \rangle = \frac{\sinh(H)}{[e^{-4K} + \sinh^2(H)]^{\frac{1}{2}}}.
\] (9)

In the next section, our primary goal will be to calculate the susceptibility of the square lattice Ising model in the same manner used in this section. Exploiting these advantages of mathematical simplicity and tractability, we will make use of the available average magnetization relation for the square lattice. We will work with almost the same mathematical form for the three spins correlation function conjectured previously in Ref. [23]. Focusing on the transition region, we can calculate the susceptibility relation for the square lattice and we are also able to extract the values of the magnetic critical exponent $\nu$ for $K < K_c$ and $K > K_c$ for the square lattice.

In addition, we also give reasonable discussion for the modification of the conjectured form of the three spins correlation function in the presence of an external magnetic field. To better understand this connection between the three spins correlation function in the presence and the absence of an external magnetic field, we trust the relevance of the previously obtained average magnetization relations obtained in Refs. [23, 24] in which the same mathematical form of the three spin correlation function was used.

### 3 The susceptibility of the square Ising lattice

In this section, we apply the same method used in the previous section to calculate the susceptibility of the square Ising lattice. As it is done above, the procedure starts by writing Eq. (1) for square lattice as

\[
\langle \sigma \rangle = \langle \tanh[K(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) + H] \rangle,
\] (10)

where $K$ is the coupling strength, and $\sigma$ denotes the central spin, while $\sigma_i$, $i = 1, 2, 3, 4$ are the nearest neighbor spins around the central spin. In what follows the index $i$ is not used since it is not necessary in the treatment.

We express the hyperbolic tangent function with the following equivalent relation as

\[
\tanh[K(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) + H] = A_1\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4
\]
\[+ A_2\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 + \sigma_1\sigma_3 + \sigma_2\sigma_4],
\]
\[+ A_3\sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2] + A_4\sigma_1\sigma_2\sigma_3\sigma_4 + A_5,
\] (11)

$A_1$, $A_2$, $A_3$, $A_4$ and $A_5$ can be expressed easily with the following relations

\[A_1 = \frac{1}{16}\{\tanh(4K + H) - \tanh(-4K + H) + 2\tanh(2K + H) - 2\tanh(2K + H)\}, \]
Taking the derivative of both sides of Eq. (15) with respect to the external field \(I\), here,

\[
A_2 = \frac{1}{16} [\tanh(4K + H) + \tanh(-4K + H) - 2 \tanh(H)],
\]

\[
A_3 = \frac{1}{16} [\tanh(4K + H) - \tanh(-4K + H) - 2 \tanh(2K + H) + 2 \tanh(2K + H)],
\]

\[
A_4 = 2A_2 - A_3 + \tanh(H),
\]

\[
A_5 = A_2 + \frac{1}{4} [\tanh(2K + H) + \tanh(-2K + H) + 2 \tanh(H)].
\]

Now, Eq. (10) can be arranged as,

\[
\langle \sigma \rangle = 4A_1 \langle \sigma \rangle + A_2 [4\langle \sigma_1 \sigma_2 \rangle + 2\langle \sigma_1 \sigma_3 \rangle] + 4A_3 \langle \sigma_1 \sigma_2 \sigma_3 \rangle + A_4 \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle + A_5.
\]

The three spin correlation function is conjectured in Refs. [23, 24] as

\[
\langle \sigma_1 \sigma_2 \sigma_3 \rangle = a(K_c, 0) \langle \sigma \rangle + [1 - a(K_c, 0)] \frac{I_{\beta}}{\Tilde{\beta}}.
\]

In the absence of external magnetic field. It is important to notice that the value of \(a(K_c, 0)\) was obtained in our previous paper [23].

In this paper, we assume that the form of the three spin correlation function in the absence of external field can also be the relevant relation for the three spin correlation function in the presence of external magnetic field.

This can be expressed as,

\[
\langle \sigma_1 \sigma_2 \sigma_3 \rangle = a(K, H) \langle \sigma \rangle + [1 - a(K, H)] \frac{I_{\beta}}{\Tilde{\beta}}.
\]

Thus, substituting this relation into Eq. (12) leads to

\[
f_1(K, H) \langle \sigma \rangle + f_2(K, H) \langle \sigma \rangle \frac{I_{\beta}}{\Tilde{\beta}} = f_3(K, H).
\]

Taking the derivative of both sides of Eq. (15) with respect to the external field \(h\), the following expression for the susceptibility of square lattice obtained as,

\[
\lim_{H \to 0} \chi(K, H) = \frac{1}{k_BT} \lim_{H \to 0} \frac{I_1(K, H)}{I_2(K, H)}.
\]

Here, \(I_1\) and \(I_2\) are given by the relations,

\[
I_1(K, H) = \frac{d f_3}{dH} - \langle \sigma \rangle \frac{d f_1}{dH} - \frac{I_{\beta}}{\Tilde{\beta}} \langle \sigma \rangle \frac{d f_2}{dH}
\]

\[
I_2(K, H) = f_1 + \frac{1 + \beta}{\beta} \langle \sigma \rangle f_2,
\]

\[
\lim_{H \to 0} \frac{d f_1}{dH} = - \frac{1}{4} [2 \tanh(4K) - 4 \tanh(2K)] \frac{a(K, H)}{dH} |_{H=0},
\]

\[
\lim_{H \to 0} \frac{d f_2}{dH} = \frac{1}{4} [2 \tanh(4K) - 4 \tanh(2K)] \frac{a(K, H)}{dH} |_{H=0},
\]

\[
\lim_{H \to 0} \frac{d f_3}{dH} = \frac{1}{8} \tanh(4K)^2 [4 \langle \sigma_1 \sigma_2 \rangle |_{H=0} + 2 \langle \sigma_1 \sigma_3 \rangle |_{H=0}]
\]

\[
+ \frac{1}{8} [3 - 4 \text{sech}(2K)^2 + \text{sech}(4K)^2] \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle |_{H=0},
\]

\[
f_1(K, 0) = 1 - \frac{1}{4} [4 \tanh(2K) + 2 \tanh(4K)]
\]

\[
f_2(K, 0) = - \frac{1}{4} [4 \tanh(2K) - 2 \tanh(4K)] [1 - a(K, 0)].
\]

For \(K < K_c\), using the above relations, the susceptibility can be expressed as

\[
\chi(K, 0) = \frac{1}{8} \tanh(4K)^2 C + \frac{1}{8} [3 - 4 \text{sech}(2K)^2 + \text{sech}(4K)^2] \langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle |_{H=0},
\]

\[
1 - [1 - a(K, 0)] \tanh(2K) - \frac{1}{2} [1 + a(K, 0)] \tanh(4K).
\]

Here, \(C\) is defined as \(C = [4 \langle \sigma_1 \sigma_2 \rangle |_{H=0} + 2 \langle \sigma_1 \sigma_3 \rangle |_{H=0}].\) Now, if we can figure out the form of the unknown function \(a(K, 0)\), then we can calculate the susceptibility for \(K < K_c\).
To this end, we are going to exploit $a(K_c, 0) = 0.75736$ which is obtained in Ref. [23]. Since our purpose is to obtain the susceptibility function for values near to $K_c$, we can expand $a(K, 0)$ around $K_c$ as

$$a(K, 0) = a(K_c, 0) + b(K - K_c) + \cdots,$$

where $b$ is equal to $\frac{\partial a(K, 0)}{\partial K} |_{K=K_c}$. After defining $a(K, 0)$, we are ready to investigate the expression for susceptibility. The first thing one may notice is that all of the terms in the numerator of $\chi(K, 0)$ are smooth functions and they all have finite values for any values of $K$, while the denominators go to zero (or they assume very small values) around the critical point.

This means that the behavior of $\chi$ strongly depends on the values of denominator and it is independent of the finite values of numerator. If the scaling form of susceptibility, which is defined as $\chi = (1 - \frac{K}{K_c})^{-\gamma}$, is recalled, the critical exponent $\gamma$ can be given by the following relation as

$$\gamma = \frac{\ln[1 - (1 - a(K, 0)\tanh(2K) - \frac{1}{2}[1 + a(K, 0)\tanh(4K)])]}{\ln(K_c - K)},$$

In Figs. 1 and 2, the critical exponent $\gamma$ is plotted for different values of the parameter $b$ introduced to describe $a(K, 0)$. From these figures, it is obvious that the values of $\gamma$ strongly depend on the values of $b$ and the values of $(K - K_c)$. It is clear from Fig. 1 that the values of $\gamma$ approach a definite value when the values of $K$ are very close to $K_c$. This limit, the value of $\gamma$ is around $\gamma = 1.75$ obtained from the scaling theory. Figure 2 is plotted for positive values of the parameter $b$. As seen from the figure, the values of $\gamma$ are around $\gamma = 1.1$ when $K$ is very close to $K_c$. Now, we are going to investigate the behavior of the critical exponent $\gamma$ for the values of $K$ greater than $K_c$ in the same manner as it is treated in the $K < K_c$ case. The first thing one can notice is that the terms in $I_1$ are smooth and they all have finite values for all the values of $K$.

This property of $I_1$ easily leads to the following $\gamma$ relation,

$$\gamma = \frac{\ln[f_1(K, 0) + 9(1 - \sinh(2K)^{-4})f_2(K, 0)]}{\ln(K_c - K)},$$

where, for the average magnetization, we used the Onsager’s relation, $\langle \sigma \rangle = [1 - \sinh(2K)^{-4}]^{1/8}$, and the critical exponent $\beta$ of square lattice is equal to $1/8$. The obtained $\gamma$ relation for the case $K > K_c$ is plotted in Fig. 3. From this figure, it is obvious that the values of $\gamma$ around the critical point $K_c$ do not depend on the values of the arbitrary parameter $b$. And the values of $\gamma$ approach 0.91 regardless of the values of the arbitrary parameter $b$.

To elucidate the general feature of the behavior of magnetic susceptibility, the logarithm of the magnetic susceptibility relations obtained for the cases $K < K_c$ and $K > K_c$ in this paper for the square lattice Ising model is plotted in Figs. 4 and 5, respectively.
Fig. 3 The values of $\gamma$ for the case $K > K_c$ in the vicinity of $K_c$ for the three different values of the arbitrary parameter $b$.

Fig. 4 The plot of $\ln(\chi)$ for $K < K_c$ in the vicinity of $K_c$.

Fig. 5 The plot of $\ln(\chi)$ for $K > K_c$ in the vicinity of $K_c$.

At this point, it is important to indicate the cumbersome and lengthy mathematical procedures used in the previous studies. For example, in reference [9], the authors of this paper discussed the properties of the susceptibility of the square Ising model expressing correlation functions in form of $2^j$-fold multiple integral. And they expressed certain closed-form expressions for the subsets of coefficients. In addition, they have generated and analyzed series with more than 300 terms in both high- and low-temperature regimes. Of course, all of these mathematical procedures lead inevitably to cumbersome and lengthy calculations. On the other hand, in this paper, we calculated the susceptibility by taking the derivative of the interrelation for the average magnetization concerning an external magnetic field. By doing so, we have greatly reduced the length of math operations.

4 Conclusion

In this paper, a new approach is introduced to investigate and calculate the susceptibility of the square lattice Ising model. To do so, we start our investigation by applying the exact interrelation for the average magnetization introduced previously. The application of this interrelation in the presence of an external magnetic field produces the relations which relate average magnetization of the lattices to the even spins and the odd spins correlation functions.
We have assumed that the even spins correlation functions behave smoothly and continuously around the critical point. As a result, the derivative of the correlation functions with respect to the external magnetic field gives finite values at the critical point for $H = 0$. We have also assumed that the three spin correlation function obeys the same mathematical form as conjectured in our previous works by just replacing the constant $a$ with a function $a(K, H)$. Exploiting the previously obtained result $a(K, 0)$ at critical point, $a(K, 0)$ is expanded into series around $K = K_c$. Since we aim to calculate the susceptibility of the square lattice for values of $K$ near $K_c$, the function $a(K, 0)$ can be approximated by keeping just two terms in the expansion.

We have observed that the values of the critical exponent $\gamma$ are strongly dependent on the values of the arbitrary parameter for the case $K < K_c$, but the values of $\gamma$ converge to a fixed value if the value of arbitrary parameter takes a value around $-2.65$. Using this consideration, we have determined the values of $\gamma = 1.72$ for $K < K_c$. On the other hand, for the values of $K$ greater than $K_c$, the values of $\gamma$ are slightly dependent on the values of the arbitrary parameter.

In the end, $\gamma$ converges to 0.91. We believe that the approach used in this paper is quite relevant and important. The method can be also applicable to the more complicated untouchable problem such as calculating the susceptibility of the 3D cubic lattice Ising model. These types of problems are going to be the subject of our future research.

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