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Construction of an approximate solution for an Ising magnet in an external magnetic field

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A method of approximate calculation of the magnetization of an Ising magnet located in an external magnetic field is proposed. This method is based on using an exact or approximate expression for the spontaneous magnetization of an Ising magnet on the same lattice. The method uses the ratio of effective fields for clusters of one and two lattice nodes. Using the proposed method for a magnet located in an external field, the dependence of magnetization on temperature and the magnitude of the external field is calculated. The proposed method is applied in the work to the solution in the mean field approximation, to the solution in the Beta approximation and to the exact solution on a square lattice; for all these solutions, critical indices characterizing the behavior of a magnet in an external field are calculated.

Keywords: the Ising model, phase transitions, the influence of an external field.

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1. Introduction

Magnetic field impact on the behavior of magnetic materials, including those described by the Ising model, has been studied for a long time [1,2]. This impact is of the most interest for such magnetic models for which there is no exact solution [3,4]. In this respect, an approach is proposed herein for construction of an approximation method that can be used to consider external magnetic field impact on the systems described by the Ising model.

An „effective exchange interaction field relation function" is introduced herein [5]. This function is defined as a relation of exchange interaction field values at which the cluster mean spin is equal to the ensemble mean. A relationship between the relation function and spontaneous magnetization as a function of temperature is established in [5]. The relationship makes it possible to calculate the relation function if an approximate or accurate solution for the Ising model is available. In [5], it is assumed that the relation function as a function of spontaneous magnetization in case of non-magnetic dilution is approximately the same as for a pure magnet, and consequences of this approximation are addressed. An assumption on approximate independence of the relation function on an external magnetic field for a pure Ising magnet is discussed in this study, which can be taken as an extension of [5]. It should be noted that the approach described herein may be combined with the approach described in [5]. An assumption on independence of the relation function on an external field for the Bethe lattice can be shown [6,7] to be exact. Therefore, the objective of this study is to investigate the result of this assumption in other cases. More specifically, an expression for the dependence of spontaneous magnetization on temperature as a mean field approximation [8] and exact solution for a square lattice [9] are used. For these cases, a dependence of magnetization on external field is constructed in the given approximation at temperatures above and below the critical temperature and critical indices characterizing behavior in an external field were found.

2. Magnetization and relation function in the Ising model

The Ising model Hamiltonian on a lattice is written as

$$\mathscr{H} = -J\sum_{(i,j)}\sigma_i\sigma_j - H\sum_i \sigma_i, \qquad (1)$$

where σ_i and σ_j are the Ising „spins„ taking on values $+1$ and -1, J is the exchange interaction energy, H is the external field; the first sum is over all pairs of adjacent spins, the second sum is over all sites [9].

If the Ising model is set on a simple lattice with coordination number q, then, as shown in [5], mean magnetization per site M may be calculated as follows:

$$M = \frac{\mathrm{sh}(2w)}{\mathrm{ch}(2w) + t}, \qquad (2)$$

where

$$w = y(M, H)\cdot \mathrm{arcth}\,(M) + KH\big(1 - y(M, H)\big).$$

Here, $K = J/(k_{\mathrm{B}}T)$, k_{B} is the Boltzmann constant, T is the temperature, $t = \exp(-2K)$, and $y(M, H)$ is a function of magnetization M and external filed H. This function defined in [5] is referred to as the relation function. This may be understood as a relation of some „effective fields" in clusters of one and two spins [5]. If an exact or approximate value of spontaneous magnetization as a function of temperature and external field $M = M(t, H)$ or inverse relationship$t = v(M, H)$ are known, then relation function $y(M, H)$ can be found from (2):

$$y(M, H) = \frac{\frac{1}{2}\ln\left(\frac{v(M,H)M+\sqrt{(v(M,H)M)^2+1-M^2}}{1-M}\right) - KH}{\operatorname{arcth}(M) - KH}. \quad (3)$$

Conversely, if function $y(M, H)$ is known from some considerations, then dependence $M = M(t, H)$ corresponding to this function can be find from (2). It should be noted that using the set relation function $y(M)$ at $H = 0$ from (2), not only solution of $M = M(t)$, but also solutions of $M = -M(t)$ and $M = 0$ are obtained with the latter being nonstable at $t < t_c = \exp(-2K_c)$.

An assumption on relation function $y(M, H)$ will be made now. More specically, assume that this function does not depend on external field H. As shown in [5] and [6,7], this assumption is exactly fulfilled for the Ising model in an external field on the Bethe lattice. In this case, this relation function is simply equal to constant $\frac{q-1}{q}$. It is certainly not expected that $y(M, H)$ does not depend on H for other lattices and for the Bethe lattice. Moreover, for a square lattice, as will be shown below, this assumption cannot be fulfilled exactly. However, assuming that $y(M, H)$ is independent on H, an approximate solution for magnetization in external field H may be obtained using the solution for spontaneous magnetization at $H = 0$ for the same lattice. For this, proceed as follows. Assume a solution of $M = M(t)$ at $H = 0$ is available (e.g. the Onsager solution for a flat square lattice [9]). Express this solution as $t = v(M)$ and using (3) at $H = 0$, find $y(M)$:

$$y(M) = \frac{\ln(\varphi(v(M), M)) - \ln(1 - M)}{2\operatorname{arcth}(M)}, \quad (4)$$

where

$$\varphi(x, M) = xM + \sqrt{(xM)^2 + 1 - M^2}.$$

Now, substitute $y(M)$ found using (4) for $y(M, H)$ in (2). The obtained expression will be used to find an approximate dependence of magnetization on temperature and external field $M = M(t, H)$. This expression may be analytically represented as inverse relation $H = H(t, M)$:

$$H = \frac{1}{K}\,\frac{\ln\left(\frac{\varphi(v,M)}{\varphi(t,M)}\right)}{\ln\left(\frac{\varphi(v,M)}{1+M}\right)}\operatorname{arcth}(M). \quad (5)$$

Now find magnetic susceptibility at $H = 0$. Differentiating (2) with respect to H at $H = 0$ and assuming that y is independent on H, we obtain

$$\chi(H, T) = \frac{2AK(1 - y)}{1 - 2A\left(\frac{\partial y}{\partial M}\operatorname{arcth} M + \frac{y}{1-M^2}\right)}. \quad (6)$$

where

$$A = \frac{\operatorname{ch}(2w)}{\operatorname{ch}(2w) + t} - M^2.$$

At a temperature higher than the Curie temperature from (6), it follows that

$$\chi = \frac{K(1 - t)}{t - t_c}, \quad (7)$$

where $t_c = \exp(-2K_c)$, $K_c = \frac{J}{k_B T_C}$, T_C is the Curie temperature. Critical index γ is defined from asymptomatic expression $\chi(0, T) \propto (T - T_C)^{-\gamma}$, $T > T_C$ [9]. It can be seen from (7) that $\gamma = 1$, i.e. the Curie–Weiss law is fulfilled [8].

Thus, the proposed procedure allows to construct an approximate solution for the Ising model in an external field using a solution for the same lattice without an external field. The same technique was used in [5] to obtain an approximate solution for the Ising magnet with non-magnet dilution, but without an external field. This means that both situations may be combined, i.e. the method shown herein can be used to construct an approximate solution of a problem of a diluted magnet in an external field.

3. Applying relation function to mean-field theory, Bethe approximation and Onsager solution

Consider the use of the above solution construction method for the Ising model in an external field on some examples. As the first step, apply the method to the mean-field model [9]. External field impact on magnetization can be obviously considered directly in the mean-field method [8]. However, we use the relation function method in the mean-field model to show that the relation function used even in such simplified model given a sufficiently reasonable result, which is not much different from direct consideration of an external field.

As the mean-field approximation [9], spontaneous magnetization for this lattice with $q = 4$ is determined by expression $M =$ th, $(4KM)$, whence

$$v(M) = \left(\frac{1 - M}{1 + M}\right)^{1/4M}. \quad (8)$$

Critical value $t = t_c = \exp(-1/2) \approx 0.6065$. Substituting (8) in (5), find the correlation between magnetization M and external field H (in terms of J). dependences $M(H)$ thus calculated are shown in Figure 1 (curves *1* and *3*). Curve *1* is plotted with $t = 0.5 < t_c$, and curve *3* is plotted with $t = 0.7 < t_c$. For comparison, Figure 1 shows

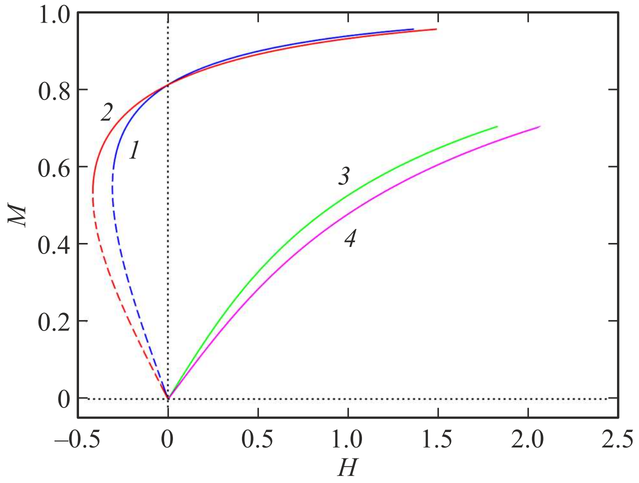

Figure 1. The Ising magnet magnetization as a function of an external field (in terms of $|J|$) to mean field approximation. Curves *1* and *3* are plotted by the relation function calculated for the zero external field, curves *2* and *4* are plotted directly by the mean-field method.

dependences $M(H)$ found as the mean-field approximation by „direct consideration" of the external field, i.e. from $M = \text{th}\,(4KM + KH)$ with the same t (curves *2* and *4*, respectively). It can be seen that the behavior of curves *1* and *2* (as well as *3* and *4*) is qualitatively the same, while quantitative difference between them is low. It should be noted that there are ambiguity sections at $H < 0$ on curves *1* and *2*. Presence of these sections is associated with the fact that the mean-field method [5] and derivation of magnetization through the relation function (Equation (2)) always have solution $M = 0$ which is unstable at $t < t_c$. This means that in the ambiguity region on curves *1* and *2* in Figure 1, lower branches (sections of curves *1* and *2* shown with dashed lines) shall be discarded.

As Bethe approximation [5], spontaneous magnetization on a lattice with coordination number$q$ is equal to

$$M = \frac{1 - hp^q}{1 + hp^q}, \tag{9}$$

where p is the equation root

$$p = \frac{t + hp^{q-1}}{1 + thp^{q-1}},$$

and $h = \exp(-2KH)$.

It is easy to show that at $q = 4$ and $H = 0$

$$v(M) = \frac{\sqrt[4]{1 - M^2}}{\sqrt{1 + M} + \sqrt{1 - M}}. \tag{10}$$

Substituting this expression into (4), we obtain a relation function to this approximation equal to 3/4, i.e. it does not depend on M. Using (9) and (3), with arbitrary H, it can be shown that relation function (3) as the Bethe approximation is always equal to 3/4. This means that our main approximation of relation function independence on H is exact in our case. This certainly means that substitution of (10) into (5) yields the same result as direct calculation of $M(H)$ using (9).

Consider now the Onsager solution for the Ising model on a square lattice without an external field [5]:

$$M^8 = 1 - \frac{1}{\text{sh}^4(2K)}. \tag{11}$$

Hence

$$v(M) = \sqrt[4]{1 - M^2}\,\frac{\sqrt[4]{(1 + M^2)(1 + M^4)}}{1 + \sqrt{1 + \sqrt{1 - M^8}}}. \tag{12}$$

From (11) or (12), critical temperature parameter $t_c = \sqrt{2} - 1 \approx 0.4142$ can be easily derived. Substituting (12) into (5), find the correlation between magnetization M and external field H at various values t.

Figure 2 shows graphs $M(H)$ with $t = 0.35 < t_c$ (curve *1*) and with $t = 0.45 < t_c$ (curve *2*). (As mentioned above, the lower section of curve *1* (dashed line) at $H < 0$ shall be discarded.) From (5) (and (12)), dependences $M(t)$ with constant H may be also derived (Figure 3). All these dependences, which gradually decrease at $H \to 0$, approach the Onsager solution.

At T equal to Curie temperature T_C, dependence of magnetization on external field H is characterized by critical index δ, which is defined from asymptomatic expression $M(H, T_C) \propto H^{1/\delta}$ [9].

To determine δ, substitute $v(M)$ corresponding to exact or approximate solution in the zero field into equation (5) and expand the obtained expression in series in terms of powers of M with $t = t_c$. Substitution of $v(M)$ corresponding to the mean-field approximation and Bethe approximation (expressions (8) and (10), respectively)

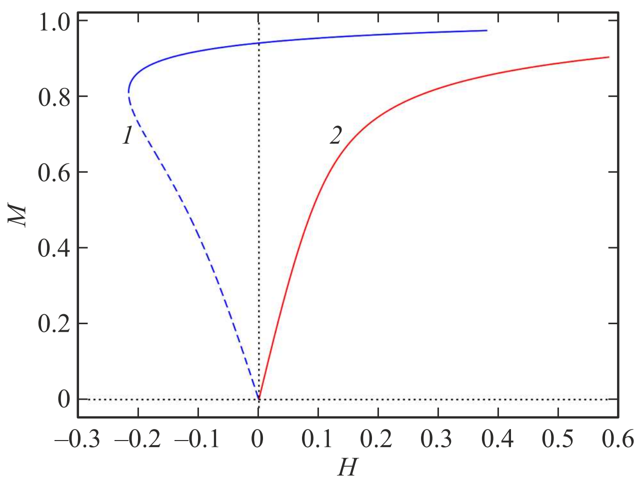

Figure 2. The Ising magnet magnetization as a function of an external field (in terms of $|J|$) constructed by the relation function for an exact solution on a square lattice in the zero external field. Curves *1* and *2* ae plotted or temperatures below and above the critical temperature, respectively.

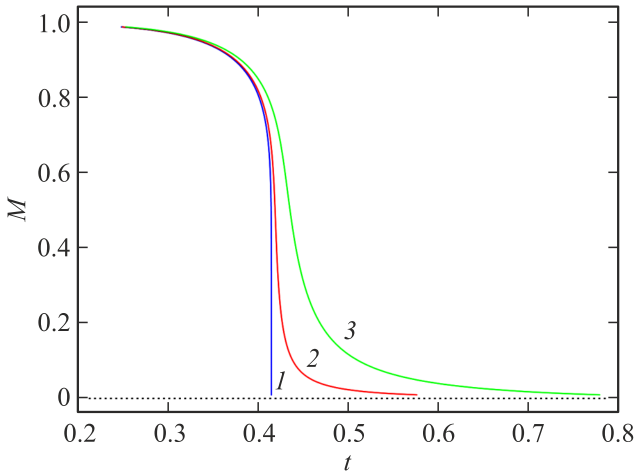

Figure 3. The Ising magnet magnetization as a function of the temperature parameter constructed by the relation function for an exact solution on a square lattice in the zero external field. Curves *1, 2* and *3* are built for fields 0, 0.01 J and 0.05 J, respectively.

yields a traditional value of δ equal to 3. When using expression (12) corresponding to the exact solution for a square lattice, we obtain $\delta = 9$. The above paragraph shows that the Curie–Weiss law (7) is fulfilled in our approach, i. e. $\gamma = 1$. In the zero external field, the dependence of spontaneous magnetization on temperature is characterized by critical index β defined by asymptotic expression $M(0, T) \approx (T_C - T)^\beta$. In the mean-field approximation and Bethe approximation $\beta = 1/2$, and in exact solution (12) $\beta = 1/8$ [5]. It can be seen that in all described cases, β, γ and δ are correlated by $\gamma = \beta(\delta - 1)$ which is derived from the similarity hypothesis [9]. Other relations for critical indices derived from the similarity hypothesis are also fulfilled for those indices that can be calculated directly.

4. Conclusion

The study uses a universal relation function for Ising model $y(M, H, t)$ which correlates the effective fields of single-atom and two-atom clusters. This function generally depends on spontaneous magnetization M, temperature $t = \exp(-2K)$ and external field H. In the zero external field, correlation between M and t obtained from the exact or approximate solution of $t = \upsilon(M)$ defines $y(M)$.

Assuming that for a magnet in an external field the relation function is the same as for a magnet without an external field, the following results are obtained.

1. The adopted assumption results in dependence of magnetic susceptibility on temperature in the zero external field $\chi = \frac{K(1-t)}{t-t_c}$, where $t = \exp(-2K)$, $K_c = \frac{J}{k_B T_C}$, T_C is the Curie temperature, i.e. the Curie–Weiss law is fulfilled.

2. For $\upsilon(M)$ calculated by the mean-field method (8), dependences of magnetization on the external field are plotted (Figure 1). These dependences appear to be rather close to the dependences plotted when the external field is directly considered in mean-field theory (Figure 1).

3. Within the adopted assumption, critical indices γ and δ are found. For the mean-field approximation, the indices have traditional values $\gamma = 1$ and $\delta = 3$, and for $\upsilon(M)$ corresponding to the exact solution (12), $\gamma = 1$ and $\delta = 9$. These results correspond to the similarity hypothesis [9], although, our result or the square lattice does not coincide with the known result [10].

Conflict of interest

The authors declare that they have no conflict of interest.

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